DEVELOPMENT OF A MULTIPLE PERTURBATION MONTE CARLO METHODS FOR CRITICALITY PROBLEMS AND IMPLEMENTATION ON PARALLEL PROCESSORS

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ABSTRACT

Monte Carlo correlated sampling technique has been combined with the fission matrix method to calculate reactivity perturbations due to small changes in cross-sections. The actual Monte Carlo simulation is done in a reference system different from both the unperturbed and perturbed systems. This approach allows to correlated the unperturbed system and multiple perturbed systems to the reference system. Hence it is possible to determine multiple reactivities due to multiple cross-section perturbations from a single Monte Carlo simulation. This method has been tested for one energy group isotropic scattering problems. We have also implemented the fission matrix algorithm for eigenvalue calculation and the multiple reactivity calculation algorithm on the IBM-SP2 parallel processor. Speedup performances from the IBM-SP2 parallel computer are presented and a theoretical model is used to predict the speedup curves.

INTRODUCTION

Application of Monte Carlo methods to calculate reactivity perturbations encounters problems as the perturbation gets smaller. For small cross-section perturbations the standard deviation associated with Monte Carlo simulations become comparable to the difference of two multiplication factors. To avoid this difficulty a correlated simulation between the unperturbed (up) and the perturbed (p) systems is required. Correlated sampling technique and the Monte Carlo fission matrix method can be combined to achieve this[1]. In this approach along with the simulation of the unperturbed fission matrix another fission matrix, for the perturbed system, is simulated from the correlated histories reacting with the perturbed system. In an efficient form of correlated sampling the Monte Carlo simulation is carried out in an artificial reference (ref) system which is different from both the unperturbed and perturbed systems[2]. We have utilized this idea for calculation of multiple reactivities due to multiple cross-section perturbations from a single Monte Carlo simulation. We compare Monte Carlo reactivity results with that of a deterministic transport theory code. Since this approach allows to calculate multiple reactivities from a single Monte Carlo simulation, a significant reduction in computational effort is observed.

We have also successfully implemented parallel algorithms for the fission matrix approach of eigenvalue calculation and the correlated sampling approach of reactivity calculation on the IBM-SP2 parallel computer. The parallel algorithms are based on the master-slave approach where the master processor divides the total number of particles, for each fission generation, equally among all the available processors or slaves. These parallel algorithms show good speedup results as are expected from parallel Monte Carlo algorithms. Theoretical models have also been used to predict the speedup curves of IBM-SP2 parallel computer for these algorithms and these predicted curves match closely the observed speedup curves.

MONTE CARLO FISSION MATRIX

Multiplication constant K of a system can be calculated using two Monte Carlo approaches. One is the source iteration approach where K for a fission generation is obtained from a ratio of the cumulative total number of fission neutrons to that of source neutrons. First few generations are discarded to avoid the effect of the first generation source distribution which is usually arbitrarily guessed. An average K for the remaining generations determines the multiplication constant of the system.

Another procedure to evaluate K is to use the Green's function or fission matrix approach. The Monte Carlo fission matrix method defines the multiplication constant as the eigenvalue of the homogeneous transport equation,

$$KQ(\vec{r}) = \int \vec{dr}' Q(\vec{r}') P(\vec{r}' \rightarrow \vec{r}) \quad , \tag{1}$$

where $Q(\vec{r})\vec{dr}$ is the number of fission neutrons produced in the differential volume $\vec{dr}$ about the position $\vec{r}$, K is the multiplication factor, or the dominant eigenvalue of equation (1), and $P(\vec{r}' \rightarrow \vec{r})\vec{dr}$ is the number of next generation fission neutrons produced in $\vec{dr}$ about $\vec{r}$ due to one fission neutron starting at $\vec{r}'$. A spatial grid (V_m; m=1,2,...,N) is imposed on all regions that contain a fission source. Then, integrating over a volume V_m, equation (1) yields:

$$KQ_m = \sum_{l=1}^{N} p_{lm} Q_l \quad , \tag{2}$$

where Q_m is the total number of fission neutrons produced in region m and p_{lm} (elements of matrix P) is the expected number of fission neutrons produced in region m due to one fission neutron starting in region l. The matrix P is estimated during random walk within each fission generation. Once the p_{lm}'s have been evaluated using Monte Carlo method the eigenvalue problem of equation (2) can be solved using standard matrix iterative methods for the dominant eigenvalue. The calculation of the fission matrix constitutes an initial value problem and correlated sampling can be applied directly to it.

CORRELATED SAMPLING

In regular correlated sampling technique the Monte Carlo simulation is done in the unperturbed system [3]. The perturbed histories are forced to follow the unperturbed ones through the same transition points in phase space. Both the unperturbed and the perturbed particles start with a weight of unity. Whenever the unperturbed particle enters a perturbed region the weight of the perturbed particle is multiplied by a biasing factor,

$$B = \frac{F_p}{F_{up}} = \frac{{\Sigma_t}^p exp(-{\Sigma_t}^p l)}{{\Sigma_t}^{up} exp(-{\Sigma_t}^{up} l)} \quad , \tag{3}$$

where l is the distance traveled within the perturbed region and Σ_t is the macroscopic total cross-section. In a special form of correlated sampling the Monte Carlo particle transport is simulated in a reference system which is generally different from both the unperturbed and perturbed systems. Reference systems can be chosen in various ways[4]. One way to choose a reference system is to take the average of the perturbed and the unperturbed systems i.e.,

$$\Sigma_x^{ref} = \frac{1}{2}(\Sigma_x^p + \Sigma_x^{up}) \quad , \tag{4}$$

where x denotes different types of cross-sections. The Monte Carlo particle transport simulation is done only in the reference system with total macroscopic cross-section Σ_t^{ref}. The spatial collision distance s is sampled from ${\Sigma_t}^{ref} exp(-\Sigma_t^{ref} s)$. The biasing factor with which the weight of the unperturbed particle is multiplied is given by,

$$B_{up} = \frac{{\Sigma_t}^{up}}{{\Sigma_t}^{ref}} exp({\Sigma_t}^{ref} - {\Sigma_t}^{up}) s \quad . \tag{5}$$

Similarly the biasing factor for the perturbed particle is,

$$B_p = \frac{{\Sigma_t}^{p}}{{\Sigma_t}^{ref}} exp({\Sigma_t}^{ref} - {\Sigma_t}^{p}) s \quad . \tag{6}$$

To avoid large fluctuations between these two biasing factors, a δ-scatter in the forward direction is added to all three total reaction cross-sections in such a way that the sum of the total reaction cross-section and δ-scatter is same for all three cases. This correlated sampling technique can be used to simultaneously estimate the three fission matrices for the reference, unperturbed and perturbed systems.

MULTIPLE REACTIVITY

Correlated sampling has been applied to the fission matrix method to evaluate multiple reactivities (ΔK_i, i = 1,2,3,...,N) due to multiple small cross-section perturbations (p_i, i = 1,2,3,...,N) of the same unperturbed system. The reference system is chosen such that,

$$\Sigma_x^{ref} = \Sigma_x^{up} + \frac{1}{N}\sum_{i=1}^{N} \Delta\Sigma_x^{p_i} = \frac{1}{N}\sum_{i=1}^{N} \Sigma_x^{p_i} \quad , \tag{7}$$

where $\Delta\Sigma_x^{p_i} = \Sigma_x^{p_i} - \Sigma_x^{up}$ and x denotes a different cross-section type. Choice for a reference system may vary from one problem to another. The Monte Carlo particle tracking is done in the reference system. The spatial collision distance s is sampled from ${\Sigma_t}^{ref} exp(-\Sigma_t^{ref} s)$. The biasing factors for the unperturbed and the multiple perturbed systems are given respectively by,

$$B_{up} = \frac{{\Sigma_t}^{up}}{{\Sigma_t}^{ref}} exp({\Sigma_t}^{ref} - {\Sigma_t}^{up})s \quad , \tag{8}$$

and

$$B_{p_i} = \frac{{\Sigma_t}^{p_i}}{{\Sigma_t}^{ref}} exp({\Sigma_t}^{ref} - {\Sigma_t}^{p_i})s \quad . \tag{9}$$

To avoid large difference between B_{up} and B_{pi}, δ-scatters in the forward direction are added to the total reaction cross-sections of the reference, unperturbed and multiple perturbed systems[5].

During each fission cycle the fission rate is determined, similar to equation (2), as the probability that a particle starting in volume element l generates $p_{l,m}$ particles in element m. For the reference system the matrix elements $p_{l,m}^{ref}$ of the reference fission matrix P^{ref} are scored as,

$$p_{l,m}^{ref} = p_{l,m}^{ref} + W^{ref} \frac{[\nu^{ref} \Sigma_f^{ref}]}{[\Sigma_t^{ref} + \delta^{ref}]} \quad , \tag{10}$$

where ν^{ref} is the number of particles emerging from a fission process in the reference system and Σ_f^{ref} is the macroscopic fission cross-section for the reference system and W^{ref} is the weight of a reference system particle. Simultaneously the fission matrix elements for the unperturbed and multiple perturbed fission matrices, P^{up} and P^{p_i} respectively, are scored as,

$$p_{l,m}^{up} = p_{l,m}^{up} + W^{up} \frac{[\nu^{up} \Sigma_f^{up}]}{[\Sigma_t^{ref} + \delta^{ref}]} \quad , \tag{11}$$

$$p_{l,m}^{p_i} = p_{l,m}^{p_i} + W^{p_i} \frac{[\nu^{p_i} \Sigma_f^{p_i}]}{[\Sigma_t^{ref} + \delta^{ref}]} \quad . \tag{12}$$

The dominant eigenvalues K^{ref}, K^{up} and K^{p_i} of matrices P^{ref}, P^{up} and P^{p_i} respectively, are determined numerically. Then multiple reactivities due to multiple perturbations (p_i, i = 1,2,3,...,N) are calculated as,

$$\Delta K^i = K^{p_i} - K^{up} \quad . \tag{13}$$

We apply survival biasing and Russian roulette techniques to the reference, unperturbed and multiple perturbed systems' particles.

PARALLEL ALGORITHM

Monte Carlo particle transport is an inherently parallel computational method that has been successfully parallelized on different computational platforms[6]. We have implemented parallel version of both the fission matrix algorithm for eigenvalue calculation and the multiple reactivity calculation algorithm on the IBM-SP2 parallel computer. The IBM-SP2 parallel computer is a collection of RISC Systems/6000 processors grouped in a number of frames. At the University of Michigan this computer consists of 32 processors and has an additional high performance switch, called the User Space (US) Communication Subsystem (CSS), other than the Internate Protocol (IP) CSS.

Monte Carlo eigenvalue and reactivity algorithms differ from fixed source algorithms in the sense that both require an iteration procedure to determine the source distribution and the eigenvalue. At the end of each iteration all the processors (master and slaves) need to be synchronized and the slave processors need to exchange information with the master processor. These synchronization and communication requirements increase parallelization overhead compared to fixed source Monte Carlo algorithms. The eigenvalue and reactivity parallel algorithms are based on a master-slave approach. The master processor divides total number of particles, for each fission generation, equally among all the available processors or slaves. Each slave processor simulates random walk for particle histories simultaneously with other slave processors. Each slave processor also stores the sites and the number of next generation fission neutrons produced. These informations are used by each slave processor for the next fission generation. At the end of each fission generation tally results from each slave processor are collected by the master processor and the eigenvalue is computed. This parallel algorithm obeys the principle of reproducibility i.e. any Monte Carlo simulation yields identical results for runs with same number of processors. Independent and reproducible sequences of random numbers are generated and each processor is given its own random number seed. These seeds are generated using the skip ahead approach which allows each processor to generate a sequence of random numbers not overlapping with any other processor's random number sequence.

Speedup, S_N, is defined as the ratio of the time to execute the computational work load on a single processor

to the time on N processors,

$$S_N = \frac{\tau_1}{\tau_N} \quad , \tag{14}$$

where τ_1 is the time to execute the workload on a single processor and τ_N is the time to execute the workload on N processors. The time τ_N is the sum of three terms,

$$\tau_N = \tau_s + \tau_p + \Delta\tau_N \quad : \tag{15}$$

(1) the time τ_s to execute the serial portion of the workload, (2) the time τ_p to execute the parallel portion and, (3) additional time $\Delta\tau_N$ which includes parallelization overhead, communication time, synchronization time etc.

For Monte Carlo simulation the single processor (N=1) execution time can be approximated very well by a simple linear function of the number of histories, N_h, to be simulated.

$$\tau_1 = a + bN_h \quad , \tag{16}$$

where a and b are constants. These constants can be evaluated by observing at least two different workloads (i.e. different N_h) for the N=1 (single processor) case. For the master-slave algorithm serial communication takes place, since the master process can only receive one message at a time. We expect the parallelization overhead and synchronization time to be proportional to (N-1). Hence we express $\Delta\tau_N$ as;

$$\Delta\tau_N = \alpha(N-1) \quad . \tag{17}$$

Now the time for a parallel simulation on N processors can be written as;

$$\tau_N = a + \frac{bN_h}{N} + \alpha(N-1) \quad . \tag{18}$$

In the above equation, after evaluating constants a and b from two serial execution time, all the terms are known except α. τ_N is the actual measured time on N processors of IBM-SP2. Hence α can be determined from equation (18) for each speedup data point. The observed speedup is expressed as;

$$S_N = \frac{\tau_1}{\tau_N} = \frac{\tau_1}{a + b\frac{N_h}{N} + \alpha(N-1)} \quad . \tag{19}$$

The predicted speedup follows the curve given by;

$$S_N(predicted) = \frac{N}{1+\beta N} \quad , \tag{20}$$

where,

$$\beta = \frac{\alpha}{\tau_N} \quad . \tag{21}$$

β represents the fraction of total computation time spent in parallelization overhead, communication, synchronization etc. between two processors[7].

RESULTS AND DISCUSSION

Multiple Reactivity. We have implemented the correlated sampling method for multiple reactivity calculations in x-y geometry and one energy group with isotropic scattering. Multiple ΔKs due to multiple small cross-section perturbations were evaluated using this Monte Carlo test code and the results were compared to that of the TWODANT[8] code with S_{16} Gauss-Legendre quadrature set and the convergence criterion for inner and outer iterations set at 10^{-12}. The dimensions of each square mesh for the TWODANT simulation are .125 mean free path X .125 mean free path. The test problem consists of a square region with dimensions of 16.659 cm X 16.659 cm and inside that square there is another smaller square region of 8.329 cm X 8.329 cm. Cross-section perturbations were performed only in the inner square region. All test cases have vacuum boundary conditions on four sides. Table 1 shows comparisons of ΔK results between the Monte Carlo test code and the TWODANT code for different test problems. We observe that the results are in agreement with a maximum error of $\sim$4%. It appears that it is possible to calculate multiple reactivities due to multiple small perturbations using one Monte Carlo simulation for one energy group transport problems with isotropic scattering. Each additional reactivity calculation requires approximately 10% of extra computational effort. Hence a significant saving in computational time is achieved. It should be noted that this methodology worked for relatively large perturbations (e.g. 10% or more change in ΔK) as well as small perturbations. One possible area of application would be to calculate reactivities due to variations in soluble boron concentrations.

Parallel Speedups. We have measured parallel speedups for both the eigenvalue and the multiple reactivity calculation algorithm. Figures 1 and 2 show observed and predicted speedup results for these two algorithms for different cases (i.e. number of particles/batch (p/b) and number of batch (b)). From the speedup results we see that we obtain almost linear speedup upto 9 (on 10 processors) for these cases and the predicted speedup results match the observed results reasonably well.

TABLE 1. Three ΔK Calculation.

Unperturbed Σ_s=0.9,	cross-sections Σ_a=0.1,	Σ_t=1.0, $\nu\Sigma_f$=0.11	
Perturbed cross-sections	TWODANT ΔK	Three Correlated Monte Carlo ΔK	error (%)
Σ_t=1.0, Σ_s=0.9 Σ_a=0.1, $\nu\Sigma_f$=.108	-.010029	$-.009713 \pm .36E-4$	3.1
Σ_t=1.0, Σ_s=0.9 Σ_a=0.1, $\nu\Sigma_f$=.1109	.004567	$.004422 \pm .16E-4$	3.1
Σ_t=1.0, Σ_s=0.9 Σ_a=0.1, $\nu\Sigma_f$=.121	.05789	$.05606 \pm .19E-3$	3.1
Σ_t=1.01, Σ_s=0.9 Σ_a=.11, $\nu\Sigma_f$=.11	-.04248	$-.04128 \pm .12E-3$	2.8
Σ_t=1.001, Σ_s=0.9 Σ_a=.101, $\nu\Sigma_f$=.11	-.004583	$-.004455 \pm .13E-4$	2.8
Σ_t=1.0001, Σ_s=0.9 Σ_a=.1001, $\nu\Sigma_f$=.11	-.0004619	$-.0004490 \pm .12E-5$	2.7
Σ_t=1.0, Σ_s=.9009 Σ_a=.0991, $\nu\Sigma_f$=.11	.004208	$.004133 \pm .13E-4$	1.8
Σ_t=1.0, Σ_s=.901 Σ_a=.099, $\nu\Sigma_f$=.11	.004680	$.004596 \pm .14E-4$	1.8
Σ_t=1.0, Σ_s=.899 Σ_a=.101, $\nu\Sigma_f$=.11	-.004599	$-.004517 \pm .14E-4$	1.7
Σ_t=1.003, Σ_s=.907 Σ_a=.096, $\nu\Sigma_f$=.10699	.0034704	$.0033154 \pm .56E-5$	4.4
Σ_t=1.002, Σ_s=.86 Σ_a=.142, $\nu\Sigma_f$=0.149	.001951	$.001992 \pm .43E-4$	2.1
Σ_t=1.0001, Σ_s=.897 Σ_a=.1031, $\nu\Sigma_f$=0.114	.0057797	$.0056409 \pm .73E-5$	2.4

Figure 1. Eigenvalue Algorithm Speedups.

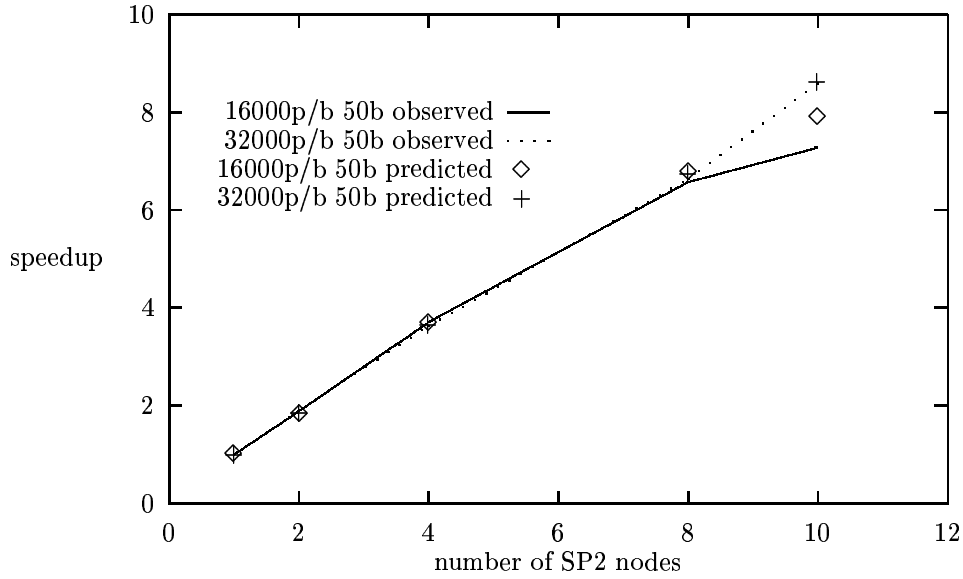

Figure 2. Multiple Reactivity Algorithm Speedups.

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