Commun. Comput. Phys.
doi: 10.4208/cicp.090909.180210a

Vol. 8, No. 4, pp. 866-876
October 2010

Analysis of Effectiveness on Monte Carlo Importance Biased Transport Calculation

Haiyan Xu*, Zhengfeng Huang and Shaohui Cai

Institute of Applied Physics and Computational Mathematics, Beijing 100094, China.

Received 9 September 2009; Accepted (in revised version) 18 February 2010

Communicated by Xueqiao Xu

Available online 17 May 2010

Abstract. To obtain fine distributing calculation about the time, space and energy of neutron flux for a kind of non-stationary particle transport problem, the scheme of global Monte Carlo variance reduction is developed. In order to provide the foundation for this scheme, it is necessary to analyze its effectiveness before putting it to use. This paper fulfills this through analyzing the effectiveness of its core which is Monte Carlo transport importance biased calculation. By decomposing the arithmetic and calculating the representative objectives, the effectiveness of the Monte Carlo transport importance biased calculation is demonstrated.

AMS subject classifications: 11K45, 62D05, 82C70, 82D75

PACS: 02.70.Ss, 02.70.Tt, 02.70.Uu

Key words: Monte Carlo, importance biased transport, direct bias, indirect bias.

1 Introduction

It is important to obtain the fine distributing of the neutron flux about the time, space and energy for a kind of non-stationary neutron transport problem whose scale of time, space and energy is far less than that of the average transport problem. For such problems, it is quite difficult to reach the precise result with Monte Carlo (MC) non-biased transport calculation, and then how to get the global solution precisely with MC is put forward. However, most of existing MC variance reduction skills are designed for calculating the local quantity of the steady system, which are not adapted to be applied in this problem except the implicit capture. Therefore the method of MC variance reduction for global solution requires to be studied and developed.

*Corresponding author. *Email addresses:* xu_haiyan@iapcm.ac.cn (H. Xu), huang_canada@126.com (Z. Huang), shaohuicai@126.com (S. Cai)

The study on global solution traces back to the 1990s. Prigarin [1], Voytishek [2] and Heinrich [3, 4] obtained some theoretical results. Spanier et al. [5–7], Cooper and Larsen [8], and Shangguan [9] developed several MC methods which have been applied successfully to some simple models.

Zero variance theory points out a direction of designing the MC simulating scheme, which is capable of reducing the variance of the objective if the approximate importance function is to be found. Based on this idea, different kinds of MC variance reduction techniques were presented by many scholars, such as Booth [10–13], Liu and Gardner [14], Tang [15, 16], Turner and Larsen [17], and Wagner and Haghighat [18], but their research fields were only limited in the local solution of the steady system.

For global MC variance reduction, a scheme [19] is proposed based on zero variance theory through breaking up the whole into parts and coupling MC method with discrete ordinates method. Its core is MC transport importance biased calculation guided by the approximate importance function obtained from the deterministic calculation. This guidance behaves mainly at two aspects: to guide the source function sampling by direct biasing and to guide the transform function sampling by indirect biasing. How about the effectiveness of directly biasing the source function and indirectly biasing the transform function? It is necessary to study and analyze its respective effectiveness to better understand the MC transport importance biased calculation.

The remainder of this paper is organized as follows. The scheme of MC transport importance biased calculation and its decomposed strategy are outlined first. Then the choice of representative objectives is discussed. In Section 4, the numerical results are presented and analyzed statistically. Section 5 summarizes the results of this paper with a conclusion.

2 Biased calculation scheme and its decomposed strategy

The integral Boltzmann transport equation for particle emission density in the phase-space $\vec{P}=(\vec{r},E,\vec{\Omega},t)$ is given by

$$Q(\vec{P})=S(\vec{P})+\int Q(\vec{P}')K(\vec{P}'\to\vec{P})d\vec{P}', \tag{2.1}$$

where $K(\vec{P}'\to\vec{P})$ is the transform function, $K(\vec{P}'\to\vec{P})d\vec{P}$ is the expected number of particles emerging in $d\vec{P}$ about $\vec{P}$ from an event in $\vec{P}'$, and $S(\vec{P})$ is the source function or the source density. This is also the starting equation of MC simulation, in which there are two terms contributing to the particle emission density: one is from the source term, and the other from the transform term.

The scheme of MC transport importance biased calculation is developed based on the zero variance theory. Let $\varphi^+(\vec{P})$ be the importance function with respect to the required objective about the emission density. Multiply Eq. (2.1) by $\varphi^+(\vec{P})/\int S(\vec{P})\varphi^+(\vec{P})d\vec{P}$ and define

$$\hat{Q}(\vec{P})=\frac{Q(\vec{P})\varphi^+(\vec{P})}{\int S(\vec{P})\varphi^+(\vec{P})d\vec{P}}, \qquad \hat{S}(\vec{P})=\frac{S(\vec{P})\varphi^+(\vec{P})}{\int S(\vec{P})\varphi^+(\vec{P})d\vec{P}},$$

$$\begin{aligned}\hat{K}(\vec{P}'\to\vec{P})&=K(\vec{P}'\to\vec{P})\frac{\varphi^+(\vec{P})}{\varphi^+(\vec{P}')}\\&=T\left(\vec{r}',t'\to\vec{r},t\middle|E',\vec{\Omega}'\right)C\left(E',\vec{\Omega}'\to E,\vec{\Omega}\middle|\vec{r},t\right)\frac{\varphi^+(\vec{r},E,\vec{\Omega},t)}{\varphi^+(\vec{r}',E',\vec{\Omega}',t')},\end{aligned}$$

where T is the transfer kernel and C is the collision kernel, and then yield the following transformed equation:

$$\hat{Q}(\vec{P})=\hat{S}(\vec{P})+\int\hat{Q}(\vec{P}')\hat{K}(\vec{P}'\to\vec{P})d\vec{P}'. \tag{2.2}$$

Theoretically a zero variance can be attained starting from Eq. (2.2), but it cannot be realized in practice because the precise importance function cannot be obtained. However, reduced variance can be achieved when using the importance function to bias every sampling (source and transport).

Generally speaking, the source function is the analytic function which has a particular expression and so the biased source function is sampled directly, which is called the scheme of direct biasing. It is very difficult to bias directly the transform function, because the collision term involves so many kinds of reactions of different kinds of nuclides at different energy that its expression is quite complicated especially in the case of the continuous-energy neutron interaction data being adopted. So the scheme of indirect biasing is used to manage the transform function biasing, which first manages transfer and collision just like non-biasing mode does and then performs splitting or Russian roulette according to the size of the importance of the two adjacent emission point.

Splitting and Russian roulette are realized through the weight window which varies with space, energy, time, and direction, which originally come from [18] and have been developed further by adding the two independent variables — time and direction in this paper.

For convenience of description, the following terms are defined as follows:

- `Full-biased Transport`
  `= Source Function Biased Directly + Transform Function Biased Indirectly;`
- `Semi-biased Transport`
  `= Source Function Biased Directly + Transform Function Non-biased;`
- `Non-biased Transport`
  `= Source Function Non-biased + Transform Function Non-biased.`

"Biased Transport" is the biasing skills used during the MC particle calculation, which comprises the two transport modes: a "full-biased transport" and a "semi-biased transport" listed above. This paper analyzes the results from different transport modes and demonstrates the effectiveness of biasing the source function directly and biasing the transform function indirectly.

3 Choice of representative objectives

For performance testing, a one-dimensional sphere test problem was developed. This problem comprises two material zones constructed with twenty spatial cells. The objectives are to calculate fine distributing of the neutron flux about the time, space and energy, that is to calculate the neutron flux integrated in every cell, every energy group and every time range. Usually these objectives have great difference in difficulty in obtaining its associated convergent results. Fixing a certain time range, three representative objectives are selected according to its degree of difficulty in converging after simulating 10^5 histories with non-biased transporting. Table 1 shows the relative errors and efficiency histories of these three objectives and indicates that the objective flux_g1k1 is the most difficult to calculate, and calculating the objective flux_g4k1 is moderately difficult, and the objective flux_g4k19 is the easiest to calculate.

Table 1: Partial results of representative objectives with non-biased transport.

Objective	Relative Error	Efficiency Histories[a]
Flux_g1k1[b]	0.0[c]	0
Flux_g4k1	0.2830	15
Flux_g4k19	0.0162	5988

[a] Refers to the histories contributing to the objective in process of MC transporting.

[b] Refers to the neutron flux integrated in the 1^{th} energy group and the 1^{th} cell.

[c] 1σ uncertainties.

4 Numerical results

Three transport modes — ″full-biased transport′, ″semi-biased transport″ and ″non-biased transport″ are used to calculate three representative objectives through simulating 10^5 histories. To assess the statistics of the mean (the average value of the scores for all the histories calculated in the problem), several statistical quantities are calculated, including the efficiency histories, the ratio of the largest score of each history to the mean (reflect directly the fluctuation of the scores), the relative error, VOV (relative variance of variance) [18], FOM (figure of merit) [20, 21], and the intrinsic error (intrinsic spread of the nonzero scores) and the efficiency error (nonzero history-scoring efficiency error) [21] which make up the relative error. The results are shown in Tables 2-4 and Figs. 1-3. For brevity, in Figs. 1-3, ″error″ refers to the relative error, ″erint″ refers to the intrinsic error, ″ereff″ refers to the efficiency error, and ″flux_gmkn_*″ refers to the value of the quantity ″*″ obtained in the process of calculating the objective flux_gmkn.

Table 2: Main results of objective flux_g1k1.

	Full-biased Transport	Semi-biased Transport	Non-biased Transport
Efficiency Histories	12217	11091	0
Mean (Relative Error)	3.496E+11[a] (0.1447)	5.945E+11 (0.3095)	0.0 (0.0)
Intrinsic Error	0.1444	0.3094	0.0
Efficiency Error	0.0085	0.0090	0.0
FOM	692	119	0
VOV	0.4071	0.4182	0.0
Largest Score/Mean	11383	22683	0.0

[a] Read as 3.496×10^{11}.

The mean from the MC simulation varies with the number of histories and thus the statistic analysis of the MC results comprises two parts: one is the statistics analysis to be done after all the histories are finished, the other is the statistics analysis varying with the number of histories. In general, during simulating the first half of all the histories, it should be normal that the mean, the relative error, the intrinsic error, the efficiency error, FOM and VOV all fluctuate in different degree since MC result does not converge yet; but after that, the converged and reliable result is thought to be obtained, if the mean and FOM stabilize gradually, and at the same time the relative error, the intrinsic error, the efficiency error and VOV decrease with rise of the histories, and in addition the values of the relative error, the intrinsic error, the efficiency error and VOV are all less than 0.1. High FOM, low relative error, low intrinsic error, low efficiency error, and low VOV ordinarily predicate high efficiency and good stability.

Table 2 shows eight statistical quantities of the objective flux_g1k1 from full-biased transport, semi-biased transport and non-biased transport respectively after finishing 10^5 histories, and reveals that semi-biased transport which only use the source biasing skill has a high efficiency compared with non-biased transport and further using the transform biasing skill can increase the computational efficiency more.

Fig. 1 shows the behavior of six statistical quantities of the objective flux_g1k1 from three transport modes with the number of histories. There are no any scores with non-biased transport. With biased transport, not only it has the scores but also the statistics of the mean stabilizes comparatively. Although a reliable mean is not got yet, this indicates that it should be got by adding the histories. Compared with that from semi-biased transport, the relative errors, the intrinsic errors, FOMs, and VOVs from full-biased transport are improved except that the efficiency errors are almost identical.

Table 3 lists eight statistical quantities of the objective flux_g4k1 from three transport modes after finishing 10^5 histories. Its relative error from biased transport recedes by about ten times and 10^7 histories need to be calculated with non-biased transport to reach the same performance. These results further demonstrates the effectiveness of biasing the source function and biasing the transform function.

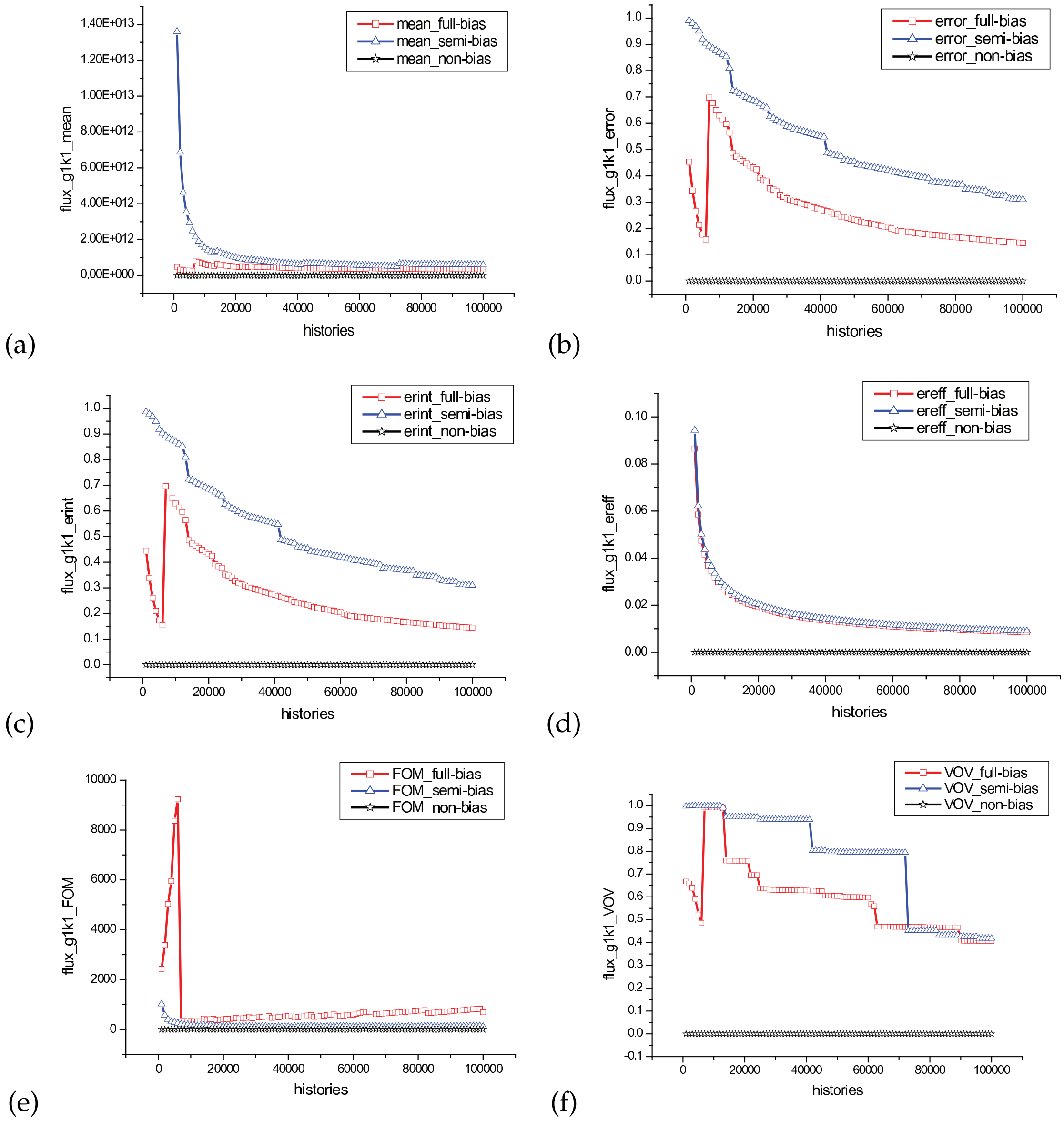

Figure 1: Results for flux_g1k1, (a) mean, (b) relative error, (c) intrinsic error, (d) efficiency error (e) FOM, (f) VOV, versus number of histories.

Fig. 2 presents six statistical quantities of the objective flux_g4k1 vary with the number of histories. With non-biased transport the mean of 10^5 histories does not converge yet, but with biased transport the mean stabilizes quickly and the behavior of its relative error, intrinsic error, efficiency error further shows the reliability of the mean. Biasing indirectly the transform function brings about a rise of FOM and also a little rise of VOV,

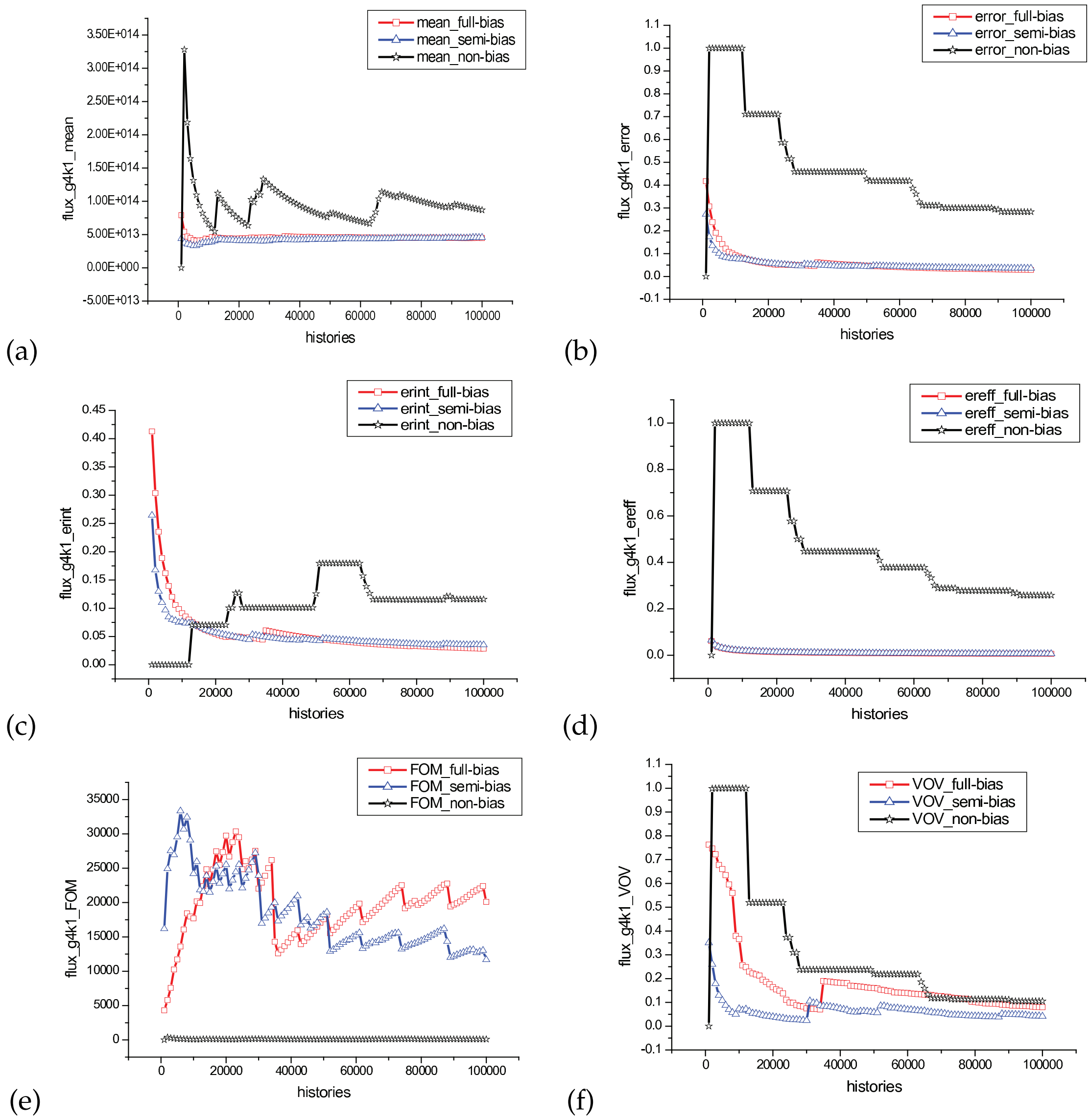

Figure 2: Same as Fig. 1, except for flux_g4k1.

but the influence on VOV is not much and VOV is still in the standard of the reliability evaluation.

Table 4 shows main results of the objective flux_g4k19 from three transport modes. Semi-biased transport increases more than ten times efficiency compared with non-biased transport, and this demonstrates the effectiveness of source biasing. In addition, biasing indirectly the transform function can improve FOM and VOV. Both VOV and the ratio of the largest score of each history to the mean from biased transport are larger than

Table 3: Main results of objective flux_g4k1.

	Full-biased Transport	Semi-biased Transport	Non-biased Transport
Efficiency Histories	22095	20433	15
Mean (Relative Error)	4.481E+13 (0.0289)	4.559E+13 (0.0357)	8.688E+13 (0.2830)
Intrinsic Error	0.0283	0.0352	0.1159
Efficiency Error	0.0059	0.0062	0.2582
FOM	20100	11682	100
VOV	0.0798	0.0413	0.1049
Largest Score/Mean	1437	1283	11573

Table 4: Main results of objective flux_g4k19.

	Full-biased Transport	Semi-biased Transport	Non-biased Transport
Efficiency Histories	72284	72337	5988
Mean (Relative Error)	3.837E+16 (0.0075)	3.847E+16 (0.0075)	4.319E+16 (0.0162)
Intrinsic Error	0.0073	0.0073	0.0102
Efficiency Error	0.0020	0.0020	0.0125
FOM	506388	411651	30669
VOV	0.0338	0.0435	0.0007
Largest Score/Mean	269	275	90

that from non-biased transport, and this indicates for some objectives using biasing skills can produce larger fluctuation of the scores due to correcting the statistical weight of the particles, thus biasing skills should be used more carefully.

For the objective flux_g4k19, its main statistical quantities varying with the histories is plotted in Fig. 3. The mean from non-biased transport fluctuates at beginning and quickly stabilizes after simulating $\sim 2\times 10^4$ histories, which is thought to be comparatively reliable according to the behavior of the mean, the relative error, the intrinsic error, the efficiency error and VOV. It is observed that FOM is lower than that from the biased transport. Compared with non-biased transport, the means from biased transport converge faster and almost stabilize only after simulating 10^4 histories, and at the same time its relative errors, intrinsic errors and efficiency errors have already met with reliable requirements, although VOVs do not until 3×10^4 or 5×10^4 histories are complete respectively with full-biased transport or with semi-biased transport. FOMs from biased transport are always higher than those from the non-biased transport, which demonstrates that the efficiency of biased transport is higher than that of non-biased transport. The means from biased and non-biased transport are different by a factor of 11%∼12%, which goes beyond its error range, and more investigations should be carried out to explain this in the future. For biased transport, whether biasing indirectly the transform function or not almost has no effects on the means, the relative errors, the intrinsic errors

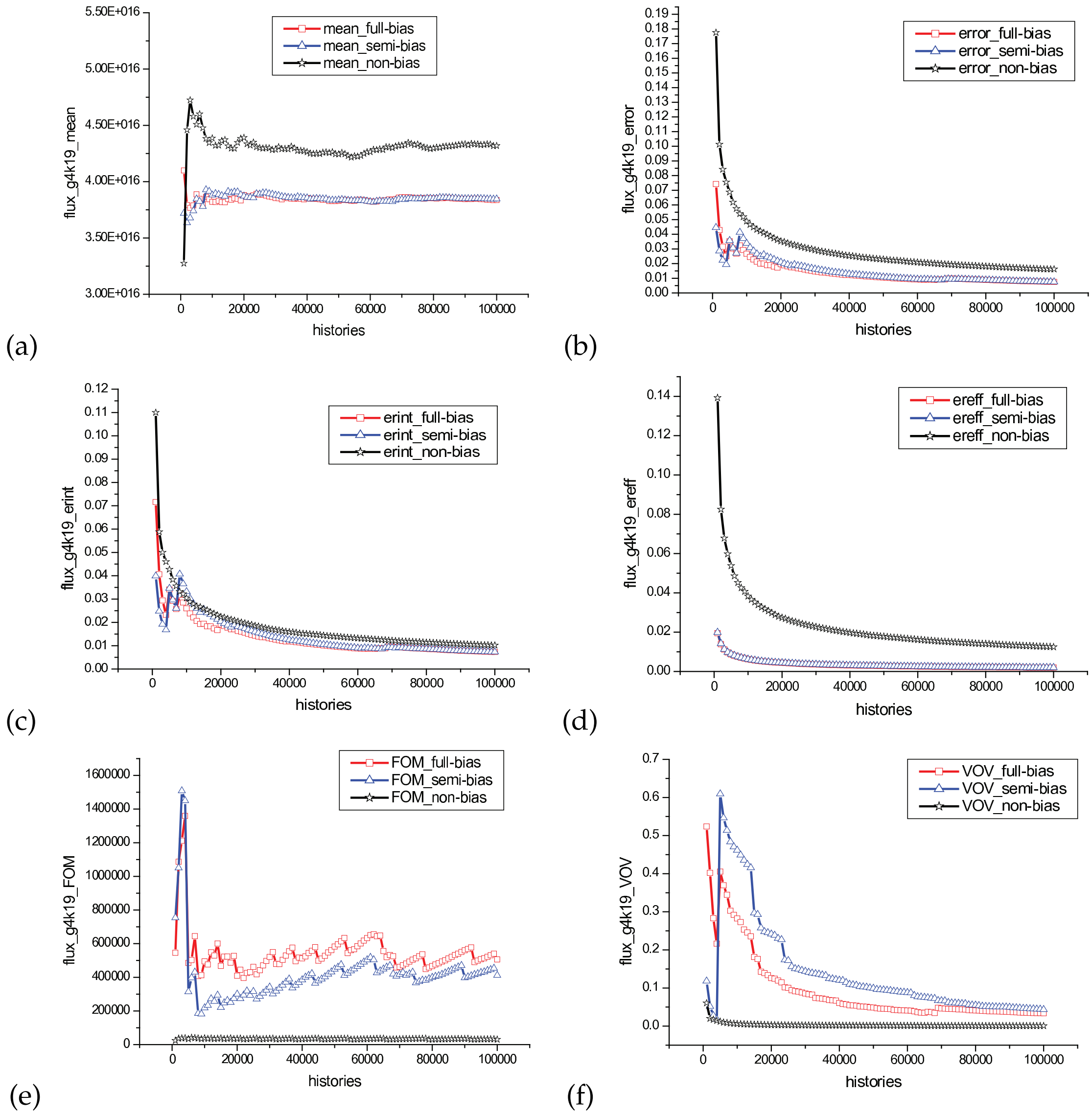

Figure 3: Same as Fig. 1, except for flux_g4k19.

and the efficiency errors. However, biasing indirectly the transform function can raise FOMs and reduce VOVs, which reveals that biasing indirectly the transform function is capable of improving the efficiency and stability.

To sum up, for three representative objectives, the semi-biased transport shows improvement by comparing with the non-biased transport. Based on this, the full-biased transport that further biases indirectly the transform function obtains lower errors and higher efficiency than the other two transport modes.

5 Conclusions

This paper decomposes the scheme of MC transport importance biased calculation into two schemes of full-biased transport and semi-biased transport. The representative objectives are chosen and calculated respectively with different transport modes, and the effectiveness of biasing the source function directly and biasing the transform function indirectly is analyzed and studied.

The simulation results show that semi-biased transport has improved a lot compared with non-biased transport: the ratios of the efficiency histories to all the histories increase, and the relative errors are reduced and FOMs are improved. Based on semi-biased transport, further biasing indirectly the transform function is able to obtain the better efficiency and stability. If the fast and simple method of biasing directly the transform function is found, the effectiveness of MC transport importance biased calculation will reach the optimization. This work provides the foundation for studying the method of global MC variance reduction on particle transport problem.

Acknowledgments

H. Xu would like to thank Prof. Yulin Zhou for his support and encouragements. This work was supported by the Science and Technology Development Foundation of China Academy of Engineering Physics (Grant No. 20060649).

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