Application of Correlated Sampling Algorithm to Depletion Equation

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1. Introduction

It's well known that the depletion equation can be solved by matrix exponential method such as series approximation method or Krylov subspace method. On the other hand, a way of solving it in Monte Carlo method is introduced by Shim [1][2]. In his work, the mathematical formulation of kinetic Monte Carlo (KMC) is derived and the exactness of KMC solution is proved by solving a simple kinetic problem that has analytic solution. Essentially the same work is made in this paper except that the target problem is more realistic depletion equation compared to Shim's work. Besides making depletion code that employs KMC method, the Monte Carlo perturbation algorithm is also introduced based on correlated sampling (CS) algorithm while Shim did the same work by using differential operator sampling (DOS) method. The sensitivity of the input cross section data to the final result is investigated through CS algorithm and compared with the results of the deterministic code.

In the subsequent chapter, the mathematical formulation for KMC will be given. Actually the formulation is exactly the same with the Shim's work but it is unavoidable to repeat here since the explanation of CS algorithm requires it. In chapter 3, the numerical results obtained by KMC are provided in the first place to see whether it matches well the deterministic solution. And then, the results gained from CS algorithm will be presented.

2. Mathematical Formulation of KMC

2.1 Probability Density Function for a Solution Vector

In deterministic method, the depletion equation for nuclide density vector $\vec{X}(t)$ at a position or burn region is represented by a system of first order differential equations:

$$\frac{d\vec{X}(t)}{dt} = \mathbf{A}\vec{X}(t)$$

where $\mathbf{A}$ represent depletion matrix including cross sections and decay constants. The formal solution of this depletion equation is obtained in terms of the exponential of the depletion matrix,

$$\vec{X}(t) = e^{\mathbf{A}t}\vec{X}(0)$$

where $\vec{X}(0)$ is the initial nuclide density vector. The series approximation or Krylov subspace method are commonly adopted for computing matrix exponential in deterministic method. The fundamental difference in KMC approach to the depletion equation comes from the fact that KMC considers the solution vector as a random variable. Let $P(\vec{X},t)$ represents the probability density function for the vector $\vec{X}$ at time t. According to Fichthron and Weinberg [3], if we assume that the depletion process is governed by Poisson process, the probability density function of the solution vector $\vec{X}$ must satisfy the following balance equation:

$$\frac{\partial P(\vec{X},t)}{\partial t} + k(\vec{X})P(\vec{X},t) = S(\vec{X},t) \tag{1}$$

where

$k(\vec{X})$: Total transition rate for the state $\vec{X}$,

$$S(\vec{X},t) = \int_{\Gamma_{\vec{X}'}} d\vec{X}'\, k(\vec{X}' \to \vec{X}) P(\vec{X}',t)$$

$\Gamma_{\vec{X}'}$: Sample space for $\vec{X}'$

By applying integrating factor, Eq. (1) can be written by

$$\Psi(\vec{X},t) = \hat{Q}(\vec{X},t) + \int_0^t \int_{\Gamma_{\vec{X}'}} K(\vec{X}',t' \to \vec{X},t)\Psi(\vec{X}',t')\, d\vec{X}'dt' \tag{2}$$

where

$$\Psi(\vec{X},t) = k(\vec{X})P(\vec{X},t)$$

$$K(\vec{X}',t' \to \vec{X},t) = T(t' \to t \mid \vec{X})C(\vec{X}' \to \vec{X})$$

$$T(t' \to t \mid \vec{X}) = k(\vec{X})e^{-k(X)(t-t')}$$

$$C(\vec{X}' \to \vec{X}) = \frac{k(\vec{X}' \to \vec{X})}{k(\vec{X})}$$

$$\hat{Q}(\vec{X},t) = T(0 \to t \mid \vec{X})Q(\vec{X})$$

$$Q(\vec{X}) = P(\vec{X},0)$$

$\Psi(\vec{X},t)$ is called the transition probability density function and Eq. (2) is the integral equation for it. It's well known that the solution of Eq. (2) can be expressed by Neumann series solution:

$$\Psi\left(\vec{X},t\right)=\sum_{j=0}^{\infty}\psi_j\left(\vec{X},t\right) \tag{3}$$

where

$$\psi_j\left(\vec{X},t\right)=\int_0^t dt_0\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0 K_j\left(\vec{X}_0,t_0\rightarrow\vec{X},t\right)\hat{Q}\left(\vec{X}_0,t_0\right)$$

$$K_0\left(\vec{X}_0,t_0\rightarrow\vec{X},t\right)=\delta\left(\vec{X}_0-\vec{X}\right)\delta\left(t_0-t\right)$$

$$K_1\left(\vec{X}_0,t_0\rightarrow\vec{X},t\right)=K\left(\vec{X}_0,t_0\rightarrow\vec{X},t\right)$$

...

$$K_j\left(\vec{X}_0,t_0\rightarrow\vec{X},t\right)=\int_{t_{j-2}}^t dt\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\cdots\int_{t_0}^t dt_1\int_{\Gamma_{\vec{X}_1}} d\vec{X}_1 K\left(\vec{X}_{j-1},t_{j-1}\rightarrow\vec{X},t\right)\cdots K\left(\vec{X}_0,t_0\rightarrow\vec{X}_1,t_1\right)$$

Eq. (3) shows that the mathematical form of transition probability consists of products and summations of $K\left(\vec{X}',t'\rightarrow\vec{X},t\right)$ which is made up of two probabilities functions $T\left(t'\rightarrow t\mid\vec{X}\right)$ and $C\left(\vec{X}'\rightarrow\vec{X}\right)$ named respectively time flight kernel and event kernel. Eq. (3) tells us that the transition probability for $\vec{X}$ at time t can be computed by summing up all contributions obtained by sequential samplings of random variable $\vec{X}$ and t through the kernel functions.

2.2 Correlated Sampling Algorithm

During repeating the sampling, the response of the system can be measured aside from the random variables itself. The acting of sampling and measurement of the system response can be expressed by the following equation:

$$\left\langle R(t)\right\rangle=\int_{\Gamma_{\vec{X}}} d\vec{X}\, r\left(\vec{X},t\right)\Psi\left(\vec{X},t\right) \tag{4}$$

where $r\left(\vec{X},t\right)$ stands for the response function of the system. One can obtain Eq. (5) by inserting Eq. (3) into Eq. (4).

$$\begin{aligned}\left\langle R(t)\right\rangle&=\sum_{j=0}^{\infty}\int_{\Gamma_{\vec{X}}} d\vec{X}\, r\left(\vec{X},t\right)\psi_j\left(\vec{X},t\right)dt\\&=\sum_{j=0}^{\infty}\left\langle R_j(t)\right\rangle\end{aligned} \tag{5}$$

where

$$\left\langle R_j(t)\right\rangle=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\, r\left(\vec{X}_j,t\right)\psi\left(\vec{X}_j,t\right) \tag{6}$$

Major concerns in depletion equation are the number densities of nuclides and time. Consider that the response function is given by

$$r\left(\vec{X}_j,t\right)=N_\alpha\left(\vec{X}_j\right)-N_\alpha\left(\vec{X}_{j-1}\right)\equiv\Delta N_{\alpha,j}$$

which means the difference in number density having α nuclide index at j-th transition step. Putting it into Eq. (6) gives the following equation.

$$\begin{aligned}\left\langle\Delta N_{\alpha,j}(t)\right\rangle&=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\int_0^t dt_0\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0\,\Delta N_{\alpha,j}\,K_j\left(\vec{X}_0,t_0\rightarrow\vec{X}_j,t\right)Q\left(\vec{X}_0,t_0\right)\\&=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\int_{t_{j-2}}^t dt_{j-1}\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\cdots\int_0^t dt_0\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0\,\Delta N_{\alpha,j}\\&\quad T\left(t_{j-1}\rightarrow t\mid\vec{X}_j\right)C\left(\vec{X}_{j-1}\rightarrow\vec{X}_j\right)\cdots T\left(0\rightarrow t_0\mid\vec{X}_0\right)Q\left(\vec{X}_0\right)\end{aligned} \tag{7}$$

Let us assume $t\gg t_{j-2}$ and introduce the fact that $\int_{t'}^{\infty} ke^{-k(t-t')}dt=1$. It allows to make Eq. (7) in a simple form which is given in Eq. (8).

$$\begin{aligned}\left\langle\Delta N_{\alpha,j}(t)\right\rangle&=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j T\left(t_{j-1}\rightarrow t\mid\vec{X}_j\right)\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\\&\quad\cdots\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0\,\Delta N_{\alpha,j}C\left(\vec{X}_{j-1}\rightarrow\vec{X}_j\right)\Phi\left(\vec{X}_{j-1}\right)\end{aligned} \tag{8}$$

where

$$\Phi\left(\vec{X}_j\right)=\begin{cases}Q\left(\vec{X}_0\right) & j=0\\ \int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}C\left(\vec{X}_{j-1}\rightarrow\vec{X}_j\right)\Phi\left(\vec{X}_{j-1}\right) & j>0\end{cases}$$

The time can be also considered as the response function. In this case, Eq. (9) can be derived without any approximation from Eq. (6).

$$\left\langle\Delta t_j\right\rangle=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\,\Delta t_j\,T\left(t_{j-1}\rightarrow t_j\mid\vec{X}_j\right)\Phi\left(\vec{X}_j\right) \tag{9}$$

Rewriting Eq. (8) and (9) provides Eq. (10) and Eq. (11).

$$\begin{aligned}\left\langle N_{\alpha,j}(t)\right\rangle&=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\,T\left(t_{j-1}\rightarrow t\mid\vec{X}_j\right)\int_{\Gamma_{\vec{X}_{j-1}}}\\&\cdots\int_{\Gamma_{\vec{X}_0}} d\vec{X}_0\,\Delta N_{\alpha,j}C\left(\vec{X}_{j-1}\rightarrow\vec{X}_j\right)\Phi\left(\vec{X}_{j-1}\right)+\left\langle N_{\alpha,j-1}(t)\right\rangle\end{aligned} \tag{10}$$

$$\left\langle t_j\right\rangle=\int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\,\Delta t_j\,T\left(t_{j-1}\rightarrow t_j\mid\vec{X}_j\right)\Phi\left(\vec{X}_j\right)+\left\langle t_{j-1}\right\rangle \tag{11}$$

According to Rief [4], the correlation of sampling is one of the possible ways to avoid the divergence of relative variance of two different Monte Carlo integrations for the two different systems with a small perturbation. One possible way of correlating the Monte Carlo integration between unperturbed and perturbed system is given by

$$\left\langle N^*_{\alpha,j}(t)\right\rangle = \int_{\Gamma_{\vec{X}_j}} d\vec{X}_j T\left(t_{j-1}\to t \mid \vec{X}_j\right)\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\Delta N_{\alpha,j} \quad (12)$$
$$u\left(\vec{X}_{j-1},\vec{X}_j\right)C\left(\vec{X}_{j-1}\to\vec{X}_j\right)\Phi^*\left(\vec{X}_{j-1}\right)+\left\langle N^*_{\alpha,j-1}(t)\right\rangle$$

$$\left\langle t^*_j\right\rangle = \int_{\Gamma_{\vec{X}_j}} d\vec{X}_j\,\Delta t_j\, w\left(t_{j-1},t_j \mid \vec{X}_j\right)T\left(t_{j-1}\to t_j \mid \vec{X}_j\right)\Phi^*\left(\vec{X}_j\right) \quad (13)$$
$$+\left\langle t^*_{j-1}\right\rangle$$

where the asterisk(*) denotes the perturbed system originated from the reference system and

$$u\left(\vec{X}_{j-1},\vec{X}_j\right)=\frac{C^*\left(\vec{X}_{j-1}\to\vec{X}_j\right)}{C\left(\vec{X}_{j-1}\to\vec{X}_j\right)}$$

$$w\left(t_{j-1},t_j \mid \vec{X}_j\right)=\frac{T^*\left(t_{j-1}\to t_j \mid \vec{X}_j\right)}{T\left(t_{j-1}\to t_j \mid \vec{X}_j\right)}$$

$$\Phi^*\left(\vec{X}_j\right)=\int_{\Gamma_{\vec{X}_{j-1}}} d\vec{X}_{j-1}\,u\left(\vec{X}_{j-1},\vec{X}_j\right)C\left(\vec{X}_{j-2}\to\vec{X}_{j-1}\right)\Phi^*\left(\vec{X}_{j-1}\right)$$

3. Numerical results

Based on KMC algorithm, KMC code is developed to solve the depletion equation. It uses ORIGEN 1 group library to compute the number densities of the system as function of time. To begin with, the validity of KMC algorithm is checked through a test problem to see whether the code works properly.

Table I: Initial condition of the test problem

Nuclide	Mol	Nuclide	Mol	Nuclide	Mol
H-1	4.18E+03	Sn-100	3.47E-01	B-11	1.40E+00
C-12	5.47E-01	Nd-130	5.91E-03	O-16	4.22E+03
F-19	4.19E+00	Si-28	2.18E-01	Si-29	1.10E-02
Si-30	7.32E-03	Cr-50	1.71E-01	Cr-52	3.30E+00
Cr-53	3.74E-01	Cr-54	9.32E-02	Mn-55	3.35E-01
Fe-54	6.51E-01	Fe-56	1.02E+01	Fe-57	2.36E-01
Fe-58	3.14E-02	Co-59	2.63E-02	Ni-58	1.99E+00
Ni-60	7.66E-01	Ni-61	3.33E-02	Ni-62	1.06E-01
Ni-64	2.70E-02	Cu-63	5.06E-01	Cu-65	2.25E-01
Zr-90	3.69E+02	Zr-91	8.05E+01	Zr-92	1.23E+02
Zr-94	1.25E+02	Zr-96	2.01E+01	Nb-93	7.85E+00
Mo-92	1.18E-02	Mo-94	7.35E-03	Mo-95	1.26E-02
Mo-96	1.33E-02	Mo-97	7.59E-03	Mo-98	1.92E-02
Mo-100	7.65E-03	Ag-107	1.84E+01	Ag-109	1.71E+01
Cd-110	2.66E-01	Cd-111	2.73E-01	Cd-112	5.14E-01
Cd-113	2.61E-01	Cd-114	6.13E-01	In-113	2.69E-01
In-115	5.99E+00	U-235	5.11E+01	U-238	1.01E+03

Table I shows the initial condition of the test problem. While burn proceeds, the power level is assumed to be constant as 6.4MWt. To treat the results statistically, all KMC calculations are repeated 30 times with different random number seeds. After that, the KMC results are compared with that of deterministic code named MEDEAC [5], which is developed by KEARI and employing Krylov subspace method. Fig. 1 shows the time evolution of Xe-135 and Sm-149. The dashed lines represent the results of MEDEAC and dots with error bar stand for that of KMC. Fig. 2 illustrates the time evolution of U-235 and Pu-239 calculated by both codes. They show two results are well consistent with each other. Note that the size of error bars in Fig. 1 is much larger than that of Fig. 2. Because the number density of a newly produced nuclide is directly related to the sample size in KMC simulation, small number densities of Xe-135 and Sm-149 results in relatively large statistical error.

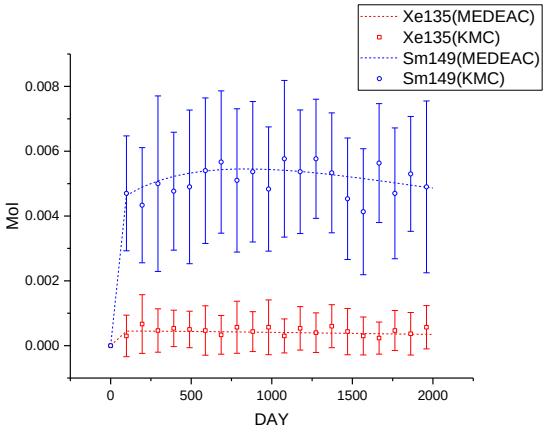

Fig. 1. Comparison of time evolution of number densities of Xe-135 and Sm-149. The dashed lines represent deterministic results, while dots with error bars stand for KMC solutions.

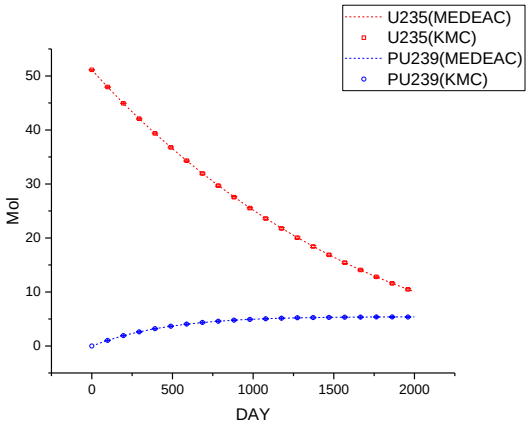

Fig. 2. Comparison of time evolution of number densities of U-235 and PU-239. Error bars of KMC results are relatively small compared to Fig. 1.

To see whether CS algorithm works, the sensitivity of neutron absorption cross section of U-238 with

respect to the number density of Pu-239 are computed. Original value of 1G neutron absorption cross section recorded in ORIGEN library is 8.546e-01 barn. I increased it by 10%~50% and observed how it affects the behavior of Pu-239 number density. The dashed lines in Fig. 3 denote the results obtained by MEDEAC and dots with error bar stand for CS results. It shows that CS algorithm works well in this case. As another example, the sensitivity of neutron absorption cross section of U-235 with respect to number density of Np-237 is calculated and given in Fig. 4. It reveals that reduction of cross section by 10%~50% gives different result in the number density of Np-237 and CS algorithm predicts its sensitivities correctly.

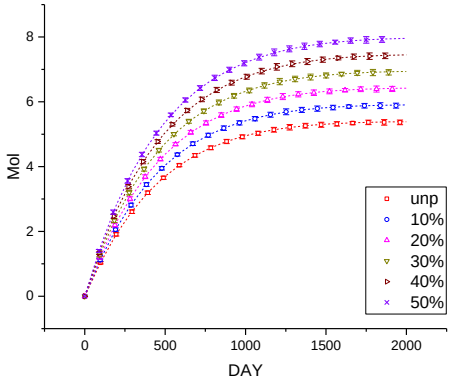

Fig. 3. Sensitivity of U-238 absorption cross section with respect to Pu-239 number density in depletion calculation. The dashed lines represent the deterministic results, while dots with error bars stand for KMC results with CS algorithm.

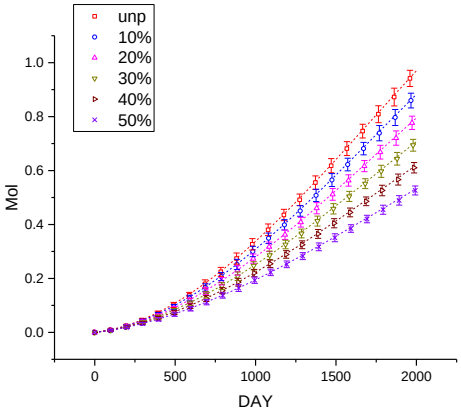

Fig. 4. Sensitivity of U-235 absorption cross section with respect to Np-237 number density in depletion calculation. The dashed lines represent the deterministic results, while dots with error bars stand for KMC results with CS algorithm.

4. Conclusions

Depletion equation solver based on KMC algorithm is developed. It uses 1 group ORIGEN library as an input data. To test whether it works well, the numerical results for the test problem are compared with that of deterministic code, MEDEAC. The results show that they are well consistent. On the other hand, Monte Carlo perturbation algorithm based on CS algorithm is applied to the same KMC code. The mathematical derivation of CS algorithm is a carbon copy of DOS algorithm except for the way of treatment of two perturbation systems. The calculation results show that CS algorithm predicts correctly the sensitivity of input data.

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