

## $\alpha$ -eigenvalue Calculation using the $S_N$ Method with GPU Diffusion Acceleration

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### 1. Introduction

The prompt neutron decay constant  $\alpha$  is a kinetics parameter related to the exponential decay of the number of neutrons in a target system. Using the pulsed neutron source method or the reactor noise analysis method,  $\alpha$  can be measured even in a non-neutron multiplying system. Therefore, we try to utilize  $\alpha$  as a surrogate instead of the critical experiment, to validate neutronics code and to update evaluated nuclear data library by the data assimilation without nuclear fuels. The numerical solution of  $\alpha$  can be obtained by applying a deterministic method to the  $\alpha$ -eigenvalue equation [1]. However, the deterministic method requires many iterations of transport sweeps. Therefore, a diffusion acceleration method is necessary for fast transport calculations. In addition, an effective quadrature set is also required to accurately treat the anisotropic scattering neutron source using a smaller number of discretized neutron flight directions. To address the above problems, we aim to newly develop a fast  $\alpha$ -eigenvalue calculation code based on the  $S_N$  method.

### 2. Methods

#### 2.1 $\alpha$ -eigenvalue Calculation using the $S_N$ Method

The time-dependent neutron transport equation is described as follows:

$$\frac{1}{v} \frac{\partial}{\partial t} \psi + \mathbf{\Omega} \cdot \nabla \psi + \Sigma_t \psi = Q, \quad (1)$$

where  $\psi$  is the angular flux;  $\Sigma_t$  is the total macroscopic cross section;  $Q$  is the scattering source term; and  $v$  is the neutron velocity. Assuming that  $\psi$  decreases exponentially with the prompt neutron decay constant  $\alpha$  in Eq. (1), the time derivative of  $\psi$  can be expressed as

$$\psi \propto \exp(-\alpha t) \Rightarrow \frac{\partial \psi}{\partial t} = -\alpha \psi. \quad (2)$$

Substituting Eq. (2) into Eq. (1), the following  $\alpha$ -eigenvalue equation based on transport theory can be derived.

$$\mathbf{\Omega} \cdot \nabla \psi + \left( \Sigma_t - \frac{\alpha}{v} \right) \psi = Q. \quad (3)$$

By discretizing Eq. (3) in terms of energy and angular variables, Eq. (3) is rewritten by

$$\mathbf{\Omega}_m \cdot \nabla \psi_g(\mathbf{\Omega}_m) + \left( \Sigma_{t,g} - \frac{\alpha}{v_g} \right) \psi_g(\mathbf{\Omega}_m) = Q_g(\mathbf{\Omega}_m). \quad (4)$$

Based on the  $\alpha$ -eigenvalue equation shown in Eq. (4), the  $\alpha$ -eigenvalue calculation is performed using the  $S_N$  method. In this study, the diamond differencing scheme is utilized for spatial discretization.

The anisotropic scattering source  $Q_g$  is expanded by using the real spherical harmonics  $R_l^n(\mathbf{\Omega})$  as follows:

$$Q_g(\mathbf{\Omega}_m) = \sum_{l=0}^{NL} \frac{2l+1}{4\pi} \sum_{n=-l}^l \sum_{g'=1}^{NG} \Sigma_{s,l,g' \rightarrow g} \phi_{l,g}^n R_l^n(\mathbf{\Omega}_m), \quad (5)$$

where  $\phi_{l,g}^n$  and  $\Sigma_{s,l,g' \rightarrow g}$  represent the expansion coefficients for the  $(l, n)$ -th-order neutron flux and the  $l$ -order scattering cross section, respectively. In this study, the transport sweep of the  $S_N$  method is performed using the icosahedral quadrature [2] to achieve the highly accurate integral calculations of spherical harmonics with a small number of discretized directions  $\mathbf{\Omega}_m$ .

#### 2.2 GPU Diffusion Acceleration

GPU (Graphics Processing Unit) is computing devices that perform graphics processing. GPU is capable of parallel computing with thousands of processing cores and has a wide memory bandwidth, allowing them to outperform CPU in specific computations. In this study, taking advantage of the fast computation of GPU, we implemented a fast diffusion acceleration calculation that simultaneously updates the neutron flux distribution and the neutron source distributions by GPU calculation with fine spatial meshes and energy groups. For the GPU diffusion calculation, the linear algebra libraries cuBLAS [3] and MAGMA [4], which are GPU compatible, were used to implement the inner iteration calculation for the neutron flux and the updating calculation for  $\alpha$  per outer iteration. On the other hand, these libraries were not directly used to update the scattering source. Therefore, the processing code was written by CUDA [3], as illustrated in Fig. 1. The processing code was programmed in a manner that memory access is efficient and fast computations can be performed by GPU.

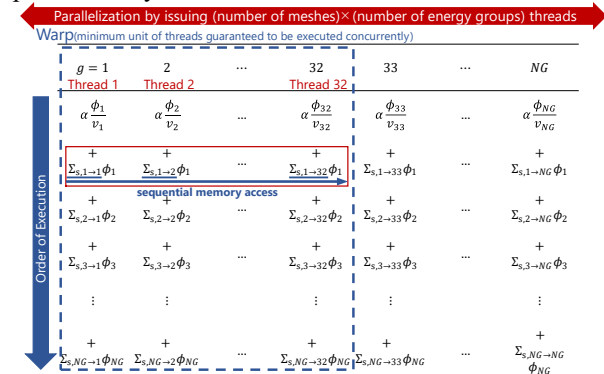


Fig. 1. Diagram of GPU code implementation to update scattering source.

### 2.3 Virtual Scattering Source to Address Numerical Instability

When a material with a small total cross section  $\Sigma_t$  (e.g., aluminum) is included in a target calculation system, the transport sweep calculation becomes unstable because  $(\Sigma_{t,g} - \alpha/v_g) < 0$  in Eq. (4). To address this issue, we used a virtual scattering source (i.e., the delta-tracking method). Considering a virtual scattering neutron source whose energy and flight direction do not change after the scattering, we corrected the numerical instability by adding the virtual scattering cross section  $\Sigma_0$  to the  $l$ -th order self-scattering cross section  $\Sigma_{sl,g' \rightarrow g}$  so that  $(\Sigma_{t,g} + \Sigma_{0,g} - \alpha/v_g) > 0$ . Finally, the corrected  $\alpha$ -eigenvalue equation can be transformed as follows:

$$\begin{aligned} & \mathbf{\Omega}_m \cdot \nabla \psi_g(\mathbf{\Omega}_m) + \left( \Sigma_{t,g} + \Sigma_{0,g} - \frac{\alpha}{v_g} \right) \psi_g(\mathbf{\Omega}_m) \\ &= \sum_{l=0}^{NL} \frac{2l+1}{4\pi} \sum_{n=-l}^l \sum_{g'=1}^{NG} (\Sigma_{sl,g' \rightarrow g} + \Sigma_{0,g}) \phi_{l,g}^n R_l^n(\mathbf{\Omega}_m). \end{aligned} \quad (6)$$

### 3. Results

To validate the developed code and to investigate its effectiveness,  $\alpha$ -eigenvalue calculations were performed for 16 water tank systems measured in previous experiments [5]. JENDL-5 was processed by FRENDDY [6] to obtain multigroup cross-sections for 172 energy groups. The anisotropic scattering was considered up to the P3 component. Using the icosahedral quadrature of IQ72, the total number of flight directions is 72 over the total solid angle. Thanks to the virtual scattering source, we confirmed the stable convergence of  $S_N$  calculations. As a result, we demonstrated that the GPU diffusion acceleration was about 3.7 times faster than the CPU diffusion calculation for the largest water tank system (Figs. 2, and 3). In addition, as shown in Fig. 4, the calculated value of  $\alpha_{\text{calc}}$  was in good agreement with the experimental value of  $\alpha_{\text{exp}}$ , which confirms the validity of our developed  $S_N$  code. Note that  $\alpha_{\text{calc}}$  is slightly overestimated as  $\alpha_{\text{exp}}$  (or neutron leakage) increases. As discussed in our previous study [7], the reason for the difference between  $\alpha_{\text{calc}}$  and  $\alpha_{\text{exp}}$  may be the uncertainty of the TSL data for  $^1\text{H}$  in  $\text{H}_2\text{O}$ , because the TSL data affects  $\alpha_{\text{calc}}$  for the water tank system.

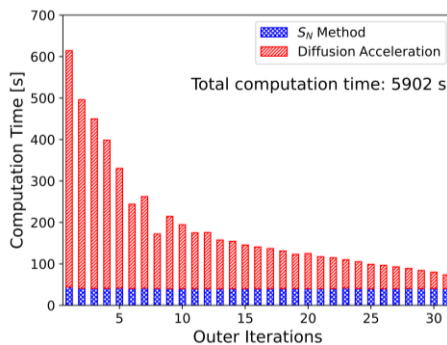


Fig. 2. Computation time for  $S_N$  method with CPU diffusion acceleration calculation

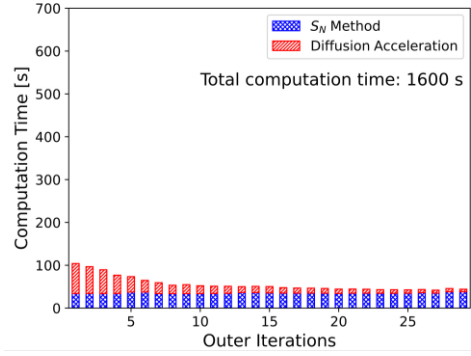


Fig. 3. Computation time for  $S_N$  method with GPU diffusion acceleration calculation

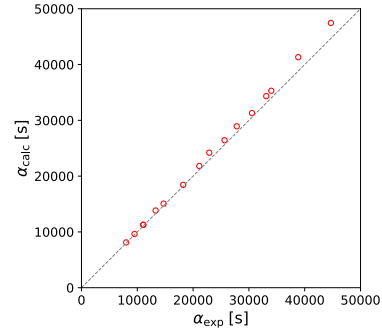


Fig. 4. Comparison of experimental value  $\alpha_{\text{exp}}$  and calculated value  $\alpha_{\text{calc}}$

### 4. Conclusions

In this study, a fast  $\alpha$ -eigenvalue calculation code based on the  $S_N$  method was newly developed using GPU diffusion acceleration, icosahedral quadrature, and delta-tracking method. Future research topic is to apply GPU to the transport sweep iteration of the  $S_N$  method for further GPU acceleration.

### REFERENCES

- [1] T. Endo, A. Noguchi, A. Yamamoto, K. Tada, Perturbation-Theory-Based Sensitivity Analysis of Prompt Neutron Decay Constant for Water-Only System, Transactions of American Nuclear Society, Vol.124, pp.184-187, Jun.14-16, 2021.
- [2] C. Ahrens, G. Beylkin, Rotationally invariant quadratures for the sphere, Proceedings of the Royal Society A, Vol.465, pp.3103-3125, 2009.
- [3] NVIDIA, P. Vingelmann, F.H.P. Fitzek, CUDA, release: 12.2.0, Available from: <https://developer.nvidia.com/cuda-toolkit>, 2023.
- [4] S. Tomov, J. Dongarra, M. Baboulin, Towards dense linear algebra for hybrid GPU accelerated manycore systems, Parallel Computing, Vol.36, pp.232-240, 2010.
- [5] K. Kobayashi, Y. Seki, N. Mizoo, T. Watanabe, T. Watanabe and H. Nishihara, Measurement and Calculation of Neutron Diffusion Parameters in Water, Journal of Nuclear Science and Technology, Vol.3, pp.275-288, 2012.
- [6] A. Yamamoto, K. Tada, G. Chiba and T. Endo, Multi-group neutron cross section generation capability for FRENDDY nuclear data processing code, Journal of Nuclear Science and Technology, Vol.58, pp. 1165-1183, 2021.
- [7] Y. Harada, H. Yamaguchi, T. Endo, A. Yamamoto, Uncertainty Quantification of Prompt Neutron Decay Constant  $\alpha$  due to Thermal Neutron Scattering Law of Water, M&C 2023, Aug.13-17, 2023, Niagara Falls, Canada.