# Application of the Generalized Perturbation Theory to the Optimization of Neutron Sources for BNCT

Keita Yamakata [a*], Go Chiba [a]
[a] *Graduate School of Engineering, Hokkaido University*
[*] *Corresponding author: yamakata@eis.hokudai.ac.jp*

## 1. Introduction

In the boron neutron capture therapy (BNCT), the neutron beam must be rich in epithermal neutrons, and gamma-rays and neutrons in the unfavorable energy range, which are not useful for therapy or harmful to the body, must be suppressed as much as possible. Accelerator-based BNCT therapy systems include a beam shaping assembly (BSA) to obtain such a neutron beam that is favorable for the treatment. Several neutron beam quality factors are presented in the international standards document on BNCT [1]. Table 1 shows reference values of these reference neutron beam quality factors.

Table I: Reference values of neutron beam quality factors

| | Epithermal flux | Thermal to epithermal flux ratio | Fast neutron dose per unit epithermal fluence | Gamma dose per unit epithermal fluence |
|---|---|---|---|---|
| | [$cm^{-2}\cdot s^{-1}$] | [-] | [$Gy\cdot cm^2$] | [$Gy\cdot cm^2$] |
| Reference value | $\geq 5\times10^8$ | $\leq 5\times10^{-2}$ | $\leq 7\times10^{-13}$ | $\leq 2\times10^{-13}$ |

When designing a BSA, it is necessary to satisfy the reference values. A significant number of radiation transport calculations must be performed to optimize the material arrangement in a BSA. Monte Carlo codes are usually used for radiation transport calculations [2]. Since the Monte Carlo code results include statistical uncertainties, the number of radiation tracks (or particle histories) must be increased to obtain accurate results, and the calculation time is a major issue when using Monte Carlo codes. In recent years, attempts have been made to utilize calculation codes based on deterministic methods that can obtain numerical solutions in a relatively short time [3]. In this case, also, it is essential to reduce the computation time. In previous studies on BSA design, the roles of BSA components, such as the "moderator" and "gamma-ray filter," have been clarified and BSA has been designed. On the other hand, if a greater degree of freedom in the choice of structure and materials is allowed, it is expected that a preferred material arrangement for BSA can be obtained. The objective of this research is to optimize BSA in a short computation time by allowing a large degree of freedom in the choice of structure and materials applying the generalized perturbation theory commonly used in the field of nuclear reactor physics.

## 2. Theory

In this section some of the techniques used to optimize BSA material arrangement are described.

### *2.1 Hill climbing algorithm*

The hill climbing algorithm is an optimization algorithm used to search for solutions to a given problem. It iteratively evaluates new solutions in the neighborhood of the current solution and moves in the direction of a better solution if exists. Specifically, it generates candidate solutions randomly, evaluates them, and then moves to a better solution. By repeating this process, the quality of the solution is expected to be improved. It can converge to a local optimal solution, and there is no guarantee of reaching the global optimum.

In this research, we perform the optimization of BSA using the hill climbing algorithm by replacing a part of the system with other material. When evaluating a new solution, the objective functions of all candidates are thoroughly compared. In other words, the case of material arrangement at any one of all positions in the system is considered, and the material to be substituted is considered for substitution to any one of all materials. This calculation must be performed quickly.

### *2.2 Generalized perturbation theory*

In the field of nuclear reactor physics, the perturbation theory is used, and it is related to reactor reactivity, which is a critical parameter indicating how much the number of neutrons in a reactor changes. Reactivity is vital for reactor control and safety. The perturbation theory helps to assess the impact of small changes in reactor design or operational conditions on reactor reactivity. The generalized perturbation theory (GPT) is a generalized application of the perturbation theory that allows us to assess the effects of small changes in various parameters other than reactor reactivity [4-5]. It perturbatively determines how integral quantities, in the form of ratios of functionals related to the neutron and adjoint neutron fluxes inside a nuclear reactor, change with variations in reactor parameters. It helps to predict how different perturbations, such as alterations in material properties, variations in environmental conditions, or adjustments to control rod positions, will impact a system's behavior or performance, aiding in understanding the implications for system design and operation.

When the neutron transport equation is defined by equation (1) and the response parameter $R$ is defined by equation (2), we present a method to estimate the variation of $R$ when a perturbation is added to the system using GPT. Note that the definitions of the operators and notations are omitted here since they are classical.

$$A\phi = S \quad (1)$$
$$R = \langle \phi, \Sigma \rangle \quad (2)$$

The neutron transport equation after the perturbation is added is expressed by Equation (3).

$$(A + \Delta A)(\phi + \Delta\phi) = S \quad (3)$$

In GPT, the adjoint equation in equation (4) is defined for equation (1).

$$A^{\dagger}\phi^{\dagger} = \Sigma \quad (4)$$

From equations (1)-(4), we obtain equation (5).

$$\Delta R = -\langle \phi^{\dagger}, \Delta A(\phi + \Delta\phi) \rangle \quad (5)$$

If the added perturbation is sufficiently small, the infinitesimal quantity can be regarded as $\Delta A \Delta\phi = 0$ and equation (5) can be expressed as in equation (6).

$$\Delta R \approx -\langle \phi^{\dagger}, \Delta A \phi \rangle \quad (6)$$

With equation (6), $\Delta R$ for any perturbation $\Delta A$ can be easily calculated from $\phi^{\dagger}$ and $\phi$ in the unperturbed system. As long as the added perturbation $\Delta A$ is sufficiently small, $\Delta R$ can be estimated without solving the neutron transport equation of the perturbed system. This allows for quick estimation of $\Delta R$ for various perturbations in $A$.

By employing GPT, it becomes possible to quickly evaluate the impact on the neutron beam characteristics at the downstream of BSA when partially replacing material in the system by other material. This allows for a quick estimation of the best candidates using the hill climbing algorithm.

## 3. Problem specification and numerical method

In this section specific problems addressed in this research and the numerical method used to address them are described.

### *3.1 Problem specification*

The target system is a one-dimensional infinite slab and system size is fixed at 60 cm. The external neutron source is located at the left end of the system, and the irradiation field is located at the right end of the system. The energy range of epithermal neutron is defined as 0.5 eV to 10 keV. The external neutron source is modeled based on the Be-9(p,n) reaction with an incident proton energy of 8 MeV. There are 13 candidate materials that make up the system, namely LiF, C, Fe, Pb, Ni-60, Al, BeO, B-10, Cd, Poly-B, $CaF_2$, $AlF_3$, and $MgF_2$. Each of these 13 materials has been selected for one of the following purposes: as neutron moderators to slow down fast neutrons and transform them into epithermal neutrons without significant loss of epithermal neutrons, as thermal neutron filters, as fast neutron filters, or as gamma-ray filters. Graphite, Al, BeO, $CaF_2$, $AlF_3$, and $MgF_2$ serve as neutron moderators, while LiF, B-10, Cd, and Poly-B are thermal neutron filters. Fe and Ni-60 act as fast neutron filters, and Pb is a gamma-ray filter.

### *3.2 Numerical method*

All the calculations were carried out with the deterministic reactor physics code system CBZ [3]. The multigroup cross sections were calculated from the multigroup library based on JENDL-4.0. The number of neutron energy groups is set to 45, covering the energy range from 0.01 eV to 10 MeV, with each energy group employing a constant lethargy width ln(10)/5 (5 groups per digit). The number of gamma-ray energy groups is set to 42, covering the energy range from 10 keV to 50 MeV. In the present work, the neutron and gamma-ray diffusion equations were solved. When calculating the neutron and gamma-ray fluxes, the system is divided by 0.1 cm spatial meshs.

The objective function quantifies the adaptability of BSA to the treatment and is calculated from the neutron and gamma-ray flux spectra at the irradiation field, and is defined as equation (7) below in the present work. This equation consists of four terms: an epithermal flux term, a thermal to epithermal flux ratio term, a fast neutron dose per unit epithermal fluence term, and a gamma dose per unit epithermal fluence term. Each of them is proportional to the relative difference of the calculated values from the reference values shown in Table I. The first term is a "gain" term, and the others are "penalty" terms, and the weight parameter $w_{epi}$ is set positive and the other weights $w_{th}$ , $w_f$ and $w_g$ are set negative. Based on these definitions, each term should be positive to satisfy the reference values.

$$R = w_{epi}\frac{(\phi_{epi} - 5e^{8})}{5e^{8}} + w_{th}\frac{(\phi_{th}/\phi_{epi} - 0.05)}{0.05}$$
$$+ w_f\frac{(D_f/\phi_{epi} - 7e^{-13})}{7e^{-13}} + w_g\frac{(D_g/\phi_{epi} - 2e^{-13})}{2e^{-13}} \quad (7)$$

In the hill climbing algorithm, it is difficult to optimize problems with multiple constraint conditions. In this research, weight parameters in the objective function are changed according to the optimization stage. In this way, optimization that satisfies all the constraint conditions is performed. The optimization in this study consists of two optimization stages: the first is to increase the epithermal flux sufficiently while suppressing the other three factors (Stage I), and the second is to satisfy all conditions (Stage II). Table II shows the specific values of the weight parameter for each stage. Stage II is started when the optimization of stage I is fully completed.

Table II: Weight parameters

| Weight parameter | $w_{epi}$ | $w_{th}$ | $w_f$ | $w_g$ |
|---|---|---|---|---|
| Stage I | 1.0 | -1.0 | -1.0 | -1.0 |
| Stage II | 0 | -1.0 | -1.0 | -1.0 |

## 4. Numerical results

Optimization was performed with a graphite slab as the initial system. The change in the material arrangement of BSA due to this optimization is shown in Fig. 1, and Stage I is up to step 61, and Stage II is from step 62 to step 78. The change in the neutron and gamma-ray flux spectra in the irradiation field is shown in Figs. 2 and 3, respectively. Table III shows the reference neutron beam quality factor during the optimization phase. Note that epithermal flux is a value that should be evaluated as a relative value, not as an absolute value, since it is proportional to the intensity of the external neutron source defined as the problem condition. Numerical values expressed in bold letters mean that the reference value is satisfied. As for the optimization result, fast neutron filter materials like Fe and Ni-60 are positioned near the neutron source, while neutron moderators such as AlF3, Al, MgF2, and BeO are positioned in the central area. Near the irradiation field, Ni-60, serving as a fast neutron filter material, and Pb, functioning as a gamma-ray filter material, are positioned.

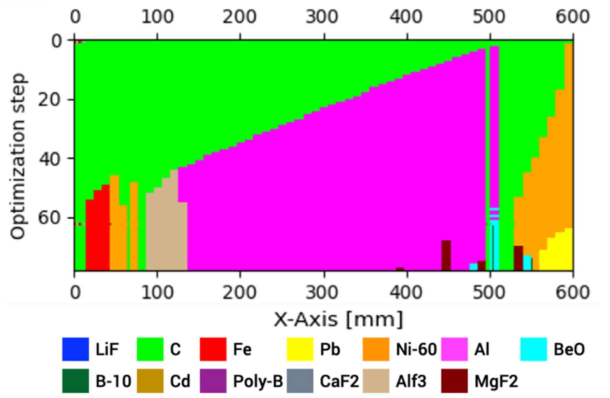


Fig. 1. Change of BSA material arrangement during optimization

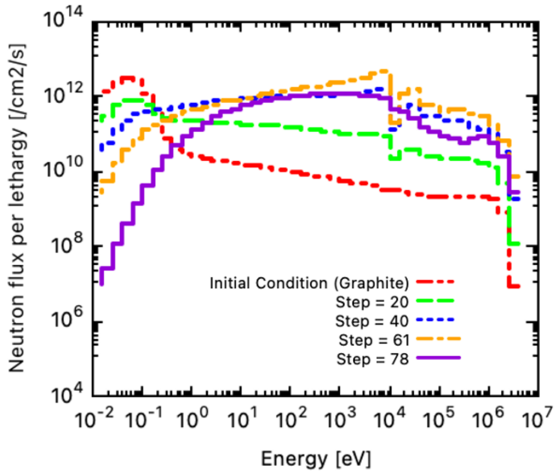


Fig. 2. Change of neutron flux spectrum in irradiation field during optimization

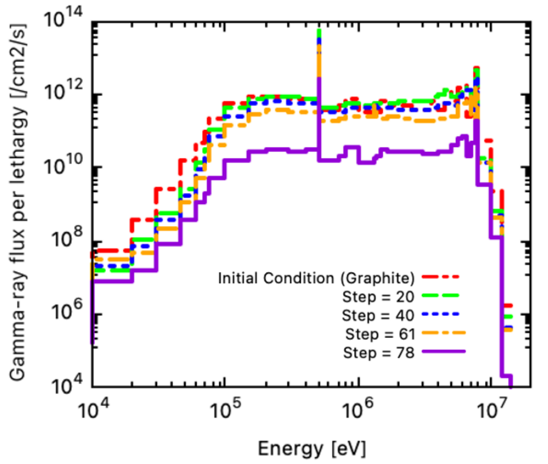


Fig. 3. Change of gamma-ray flux spectrum in irradiation field during optimization

| | Epithermal flux | Thermal to epithermal flux ratio | Fast neutron dose per unit epithermal fluence | Gamma dose per unit epithermal fluence |
|---|---|---|---|---|
| | [$cm^{-2}\cdot s^{-1}$] | [-] | [$Gy\cdot cm^2$] | [$Gy\cdot cm^2$] |
| Reference value | ($\geq 5\times10^{8}$) | $\leq 5\times10^{-2}$ | $\leq 7\times10^{-13}$ | $\leq 2\times10^{-13}$ |
| STEP = 0 | **$1.37\times10^{11}$** | $4.27\times10^{1}$ | $8.29\times10^{-13}$ | $1.75\times10^{-10}$ |
| STEP = 20 | **$1.62\times10^{12}$** | $1.14\times10^{0}$ | **$6.41\times10^{-13}$** | $1.62\times10^{-11}$ |
| STEP = 40 | **$1.01\times10^{13}$** | $9.73\times10^{-2}$ | $9.65\times10^{-13}$ | $1.73\times10^{-12}$ |
| STEP = 61 | **$1.69\times10^{13}$** | **$1.88\times10^{-2}$** | $1.20\times10^{-12}$ | $5.59\times10^{-13}$ |
| STEP = 78 | **$7.76\times10^{12}$** | **$2.53\times10^{-3}$** | **$6.50\times10^{-13}$** | **$1.36\times10^{-13}$** |

Table III: Neutron beam quality factors during optimization

## 5. Conclusions

In the calculation for a one-dimensional slab, the combination of GPT and the hill climbing algorithm enabled optimization that satisfied all the reference values of the neutron beam quality factor in a short time. This method allows optimization with a greater degree of freedom in the choice of structure and material. Therefore, it is expected that more favorable material arrangement can be obtained for BSA. The hill climbing algorithm has the potential to converge to the nearest local optimal solution from its initial conditions, and it can be said that the current research does not achieve global optimization. In the future, we plan to introduce GPT for global optimization.

## REFERENCES

[1] INTERNATIONAL ATOMIC ENERGY AGENCY, Advances in Boron Neutron Capture Therapy, Non-serial Publications , IAEA, Vienna (2023)

[2] R. Inoue, F. Hiraga, Y. Kiyanagi, Optimum design of a moderator system based on dose calculation for an accelerator driven Boron Neutron Capture Therapy, Applied Radiation and Isotopes, 88, 225228 (2014).

[3] G. Chiba, H. Handa, M. Ishikawa, Improvement and benchmarking of the deterministic transport calculation code CBZ to design beam shaping assembly for BNCT, Applied Radiation and Isotopes, 190, 110465 (2022).

[4] G. C. Pomraning, Variational Principle for Eigen-value Equations, J. Math. Phys., 8, 149 (1967).

[5] A. Gandini, A Generalized Perturbation Method for Bi-linear Functionals of the Real and Adjoint Fluxes, J. Nucl. Energy, 21, 755 (1967).

Answer sheet (2023.9.8 Fri)

Keita Yamakata

Q1. The titile of this paper is "Application of the Generalized Perturbation Theory to the Opimization of Neutron Source For BNCT". However, the author omit the description of GPT. And the descriptions about 'why GPT' and 'How GPT is applied in this study' is not enough.

A1. I have added content to Section 2.2 of the main text.

Q2. As one of reader, recommend separating a long sentence to two or more. The reader who is not familiar with this field can be confuesed easily.

A2. Longer sentences were split.

Q3. The auther used the Hill climbing algorithm for optimization. The Hill climbing algorithm is technique which belong to the family of local serach. As mentioned in the paper, there is no quarantee of reaching the global optimum. Could the author descibe why the Hill climbing algorithm is selected compared with other optimization methods.

A3. As previously stated in Section 2.2 of the main text, using GPT enables us to conduct the exploration of neighboring solutions in optimization problems much faster than explicitly seeking them. The primary objective of this research is to establish new optimization methods that were previously impossible due to computational cost constraints. However, when using GPT for the exploration of neighboring solutions, it becomes impossible to handle significant perturbations due to the inclusion of errors related to first-order perturbations. Consequently, careful management of the perturbation range is necessary. Therefore, in this study, we prioritize the ease of managing the perturbation range, and for this reason, we employ the most basic gradient-based method, which is the hill climbing algorithm. The hill climbing algorithm has the potential to converge to the nearest local optimal solution from its initial conditions, and it can be said that the current research does not achieve global optimization. In the future, we plan to introduce GPT for global optimization.

Q4. Is the 'evaluation function' well-known concept or auther defined concept? If it is well-known concept, please add some reference for who are not familiar with this field.

A4. I have replaced the term 'evaluation function' with a more appropriate expression, 'objective function'. In this study, we have defined the objective function as Equation (7) to serve as the optimization criterion.

Q5. Could you explain how weight parameters is handled in the optimization stage?

A5. I have added content to Section 3.2 of the main text.

Q6. In the introduction, auther mentioned uses of MC method and deterministic method for BNCT related analyses. Which method did author used for this paper work (1D infinit slab)? Please add code and library information (such as inhoused transport code with ENDF7.1)

A6. I have added content to Section 3.2 of the main text.

Q7. (For Fig 1) Could you add some description about optimization results based on characteristic of 13 material candidates

A7.
(About 13 material candidates)
 I have added content to Section 3.1 of the main text.
(About optimization results)
 I have added content to Section 4 of the main text.

(minor)

1. Explain why you used the hill climbing algorithm, despite its limitation. → Q3
2. Explain the GPT based optimization algorithm. → Q1
3. How were 13 candidate materials selected? → Q7
4. How the evaluate function and weight parameters were determined? → Q4,Q5
5. Modify figures to include the results of the last step(STEP=141 in Table II)
→The figures for step in old Table II were incorrect and have been corrected to the correct table (new Table III).