Application of Metaheuristic Algorithms in the Optimization of Multi-group Cross Section Libraries for Lattice Transport Codes

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1. Introduction

Low-Enriched Uranium Plus (LEU+) is an attractive candidate for improving the fuel economics of Small Modular Reactor (SMR). [1] For LEU+ core design, the existing nuclear core design code system must analyze this system accurately. Previous study has shown that the existing design code analyzes low-enrichment systems with relatively good accuracy, but the error gradually increases at the high-enrichment systems as the enrichment rises. [2] This indicates a necessity for a multi-group neutron cross section library optimized for LEU+ core design.

Recently, Kyung Hee University (KHU) has conducted studies to optimize a multi-group (MG) neutron cross section library for a user-defined target system, based on the KAERI (Korea Atomic Energy Research) library generation system [3-6]. This procedure is called by "library correction," and it can be performed by selecting a reference model that can represent the user-defined target system and conducting iterative corrections for user-defined nuclides and reaction types.

In this study, we will introduce error minimization strategies for MG cross section library correction system based on metaheuristic algorithms. Genetic algorithm (GA) [7] and Simulated Annealing (SA) algorithm [8] are considered, and each algorithm can optimize cross sections or reaction rates.

To verify the library optimization performance of the proposed algorithms, soluble boron free (SBF) SMR benchmarks are conducted. This benchmark consists of single pin cell, 2D fuel assembly, and 2D core problems. To confirm the bias or error trends against ^{235}U enrichment, the SBF SMR benchmark problems with enrichments ranging from 2 w/o to 10 w/o were considered. This benchmark matrix evaluates whether the suggested algorithms can optimize the cross section library across a wide range of problems. The reference Monte Carlo (MC) code used in this study is McCARD [9], and the MG core design code is DeCART2D. [10]

2. DeCART2D Library Correction System

Figure 1 illustrates a flowchart of the MG neutron cross section library correction process. De represents the results from design code, DeCART2D, and MC indicates the results from reference MC code, McCARD. x denotes the type of nuclear reaction, g refers to the energy group, and T denotes the temperature point of nuclide.

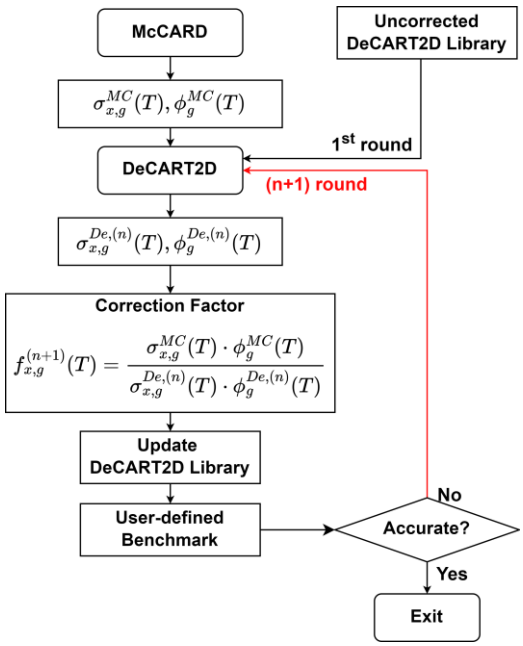

Fig. 1. Flowchart of DeCART2D library correction process

The processes including correction factor generation and updating the cross section library is defined as one round. Typically, the library correction process involves multi-round correction procedures. In the library correction process, the user can determine the following correction options.

a. Reference model for generating correction factor
b. Target nuclides for each round
c. Cross section type ($\boldsymbol{\sigma_x}$) for each nuclide

The reference model usually can be chosen to represent the target benchmark system (e.g., Fuel assembly model that presents the core average reactivity). Once the nuclides to be corrected for each round are determined, the user selects the cross sections to be corrected for each nuclide in each round. Absorption, fission and scattering cross sections are considered.

3. Metaheuristic Algorithms

3.1 Genetic Algorithm (GA)

In this study, GA transforms the correction options into a genetic format and evolves each genome according to genetic operators; selection, crossover, and mutation. It samples round-wise, nuclide-wise user-defined correction options within the given correction round.

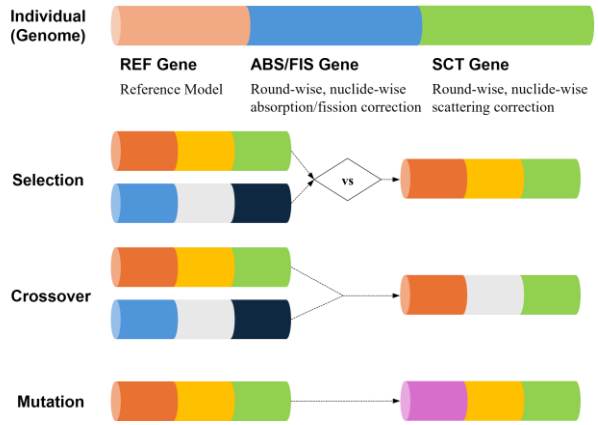

Fig. 2. Description of genome format and genetic operator of GA optimization

Figure 2 illustrates the genome format and genetic operators used for GA optimization in this study. Each individual (genome) consists of data for the reference model, user-defined nuclide groups, and round-wise correction options.

In this study, the selection operator adds the highest fitness individual from the current generation to the next generation. The crossover operator generates new individuals by mixing the genes of the top and bottom individuals for the 70% of the entire population. The remaining individuals are all generated using the mutation operator.

$$Fitness = \frac{1}{RMS_t} \times 10^5, \quad RMS_t = \frac{\sum_i^j w_i R_i}{\sum_i^j w_i} \qquad (1)$$

Fitness of each individual is calculated by (1). w_i is the user-defined weight for the ith unit benchmark, R_i is the RMS error for the ith unit benchmark. RMS_t is a weighted average of all RMS errors of unit benchmarks. Figure 3 shows the flowchart of library optimization using GA.

3.2 Simulated Annealing (SA) Algorithm

In this study, SA perturbs the design parameters of the correction reference model. This includes adjustment of the enrichment of fuel pin, pin pitch, and other design parameters.

$$Score = \frac{1}{RMS_t} \times 10^5 \qquad (2)$$

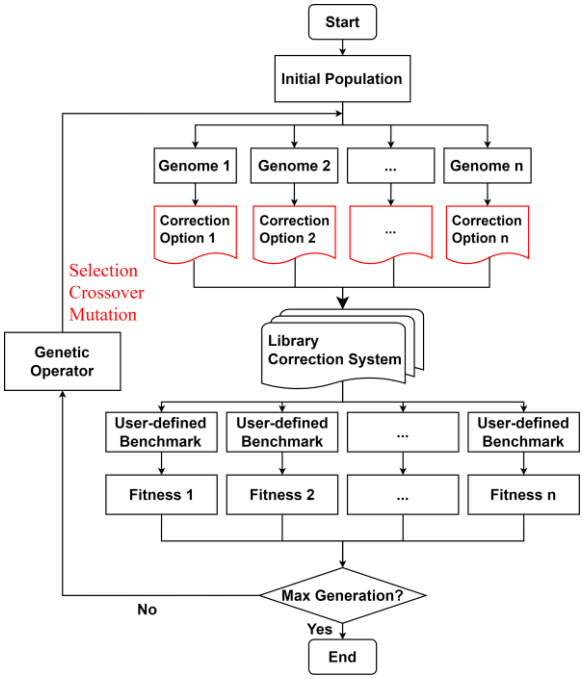

Fig. 3. Flowchart of GA optimization

SA Score evaluation shown in (2) is structurally same with the GA fitness. If the score is better than previous trial, the temperature is decreased by the cooling rate and SA prepares the perturbation for next trial.

$$P_{accept} = \exp\left[-\frac{\Delta E}{T}\right] \qquad (3)$$

If the score is acceptably bad, the probabilistic acceptance logic shown in (3) is applied. This logic is for escaping local solution. Figure 4 shows the flowchart of library optimization using SA algorithm.

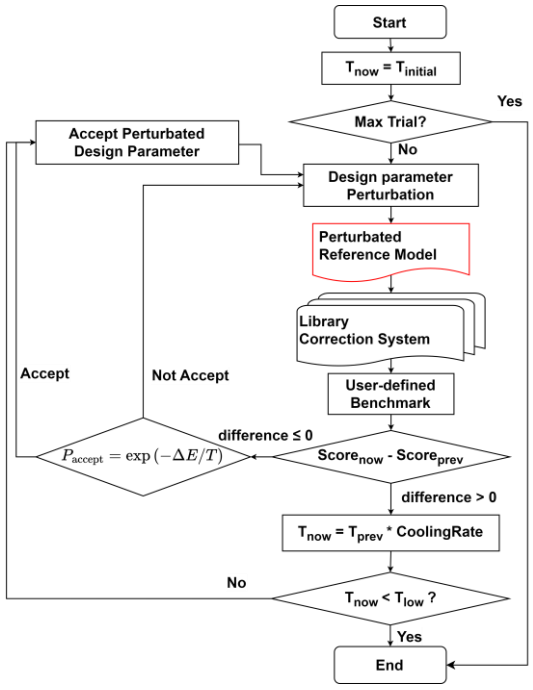

Fig. 4. Flowchart of SA optimization

4. Optimization of Multi-group Cross Section Libraries by Metaheuristic Algorithms

4.1 SBF SMR Benchmark

To evaluate the library optimization performance of the proposed algorithms, SBF SMR benchmark system is organized. The considered SBF SMR uses enriched gadolinium as a burnable absorber and stainless steel (SS304) as a reflector. Figure 5 and 6 shows the modeling of the SMR fuel assembly and core. The benchmark problem includes single pin cell, 2D assembly, and 2D core problems with enrichments of 2, 4, 6, 8, and 10 w/o. This evaluates whether the proposed algorithms can globally optimize various problem geometries and enrichment conditions, including LEU and LEU+ system. The McCARD reference solution is calculated based on ENDF/B-VII.1 library. Table I shows the description of the SMR benchmark problem conditions.

Table I. Description of SMR benchmark problem

Problem	Description
Single pin (5 problems)	5 enrichments (2, 4, 6, 8, 10 w/o)
2D assembly (25 problems)	5 enrichments (2, 4, 6, 8, 10 w/o) 5 assemblies (A01, A02, A03, A04, A05)
2D core (5 problems)	5 enrichments (2, 4, 6, 8, 10 w/o)

* Standard deviation of McCARD solution ≈ ±0.00007
** Temperature condition: Fuel 900K, Clad 600K, Moderator 600K

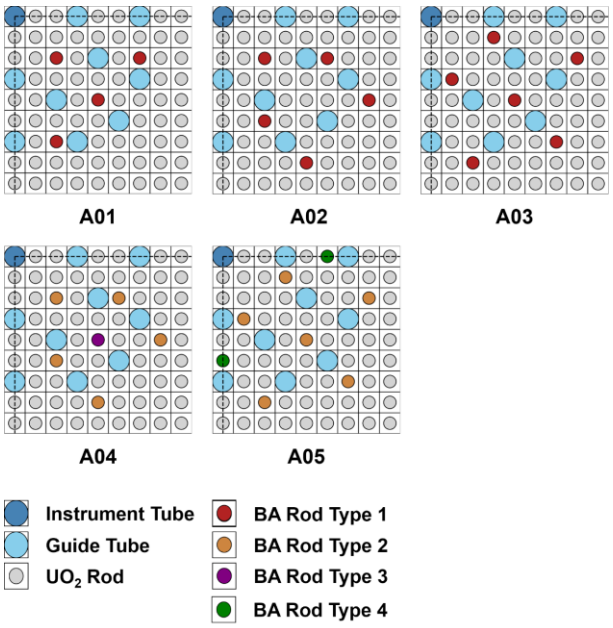

Fig. 5. Fuel assembly modeling for SBF SMR benchmark

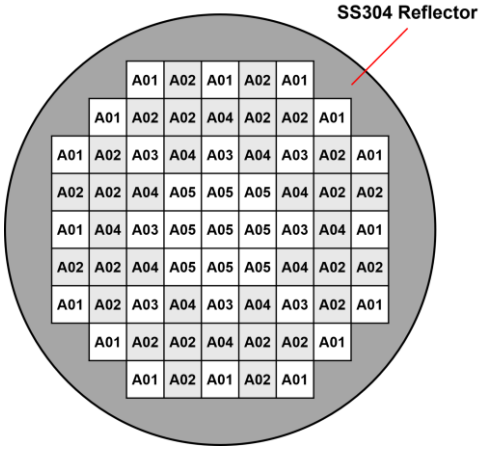

Fig. 6. Core modeling for SBF SMR benchmark

The generated MG cross section library is based on the ENDF/B-VII.1 library and has 47 group for neutron, and 18 group structure for gamma data. Total 4 rounds of correction were considered, and the main nuclides of the reactor (U, Gd, H) are corrected for absorption, fission and scattering cross section.

4.2 GA optimization

For GA optimization, 30 generations of iterations were conducted. Each generation consists of 5 genomes, with each genome containing the correction options for 4 rounds with 3 nuclide groups. The nuclide groups are as follows:

a. ^{235}U, ^{238}U
b. ^{154}Gd, ^{155}Gd, ^{156}Gd, ^{157}Gd, ^{158}Gd, ^{160}Gd
c. ^{1}H

Table II. GA genome data for initial generation

No	Gene		
	REF	ABS/FIS	SCT
1	A01	1111 1111 1111	0000 0000 1111
2	A02	1111 1111 1111	0000 0000 1111
3	A03	1111 1111 1111	0000 0000 1111
4	A04	1111 1111 1111	0000 0000 1111
5	A05	1111 1111 1111	0000 0000 1111

* REF, ABS/FIS, and SCT indicate reference model candidate, correction option for absorption/fission cross section, and correction option for scattering cross section.

In this study, the reference model candidates for GA optimization are the A01, A02, A03, A04, and A05 fuel assemblies from the SMR benchmark using 4.0 w/o UO2 fuel. Table II presents the initial genetic seed for GA optimization.

Gene value ‘1’ indicates that a correction has been performed in a single round, while ‘0’ means that the correction has not been performed. The digit of the gene cluster(e.g., 4 digits of “1111”) means the total number of rounds, and the genes consist of gene clusters arranged in the order of nuclide groups. The genes in Table II

mean 4 rounds of absorption and fission cross section correction for three nuclide groups (a, b, c), while the scattering cross section is corrected only for the third nuclide group (c. ^{1}H) over the same four rounds.

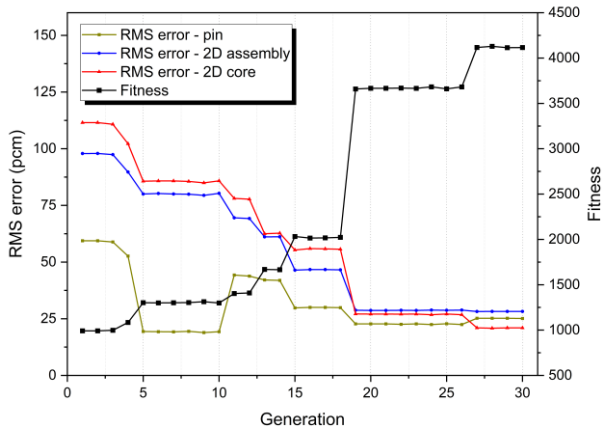

Fig. 7. RMS error changes for pin, 2D assembly, and 2D core problems over 30 GA generations

Figure 7 shows the result of GA optimization over generations. The highest fitness score for the initial generation of GA optimization is 991 points. The fitness improved to 4,116 points in 30 generations. While the initial maximum RMS error is over 100 pcm, RMS errors for all system geometries are converged to within 25 pcm in the final generation. The GA optimized the MG library to solve benchmark problems accurately.

Table III presents the genome data of the highest fitness individuals for representative generations. The genetic operators (selection, crossover and mutation) are working well, and the optimal reference model and round-wise correction options were adjusted.

Table III. GA genome data changes in representative generations

GEN	Gene			Fitness
	REF	ABS/SCT	SCT	
1	A03	1111 1111 1111	0000 0000 1111	991
10	A01	1011 0110 1101	0001 0000 1101	1299
15	A05	1011 1101 1000	0000 0011 1001	2031
20	A05	1110 0001 0100	1100 1111 0000	3666
30	A05	1110 1001 0100	1100 1111 0000	4116

* GEN indicates generation.

4.3 SA optimization

For SA optimization, 70 trials of iterations were conducted. Each trial performs four rounds of corrections for same correction nuclides used in the GA optimization. The reference model is the A03 assembly. SA perturbs the UO2 enrichment and pin pitch of the reference model.

Figure 8 shows the results of the SA optimization over 70 trials. The initial score for the SA optimization was 902 points and the score improved to 2,126 points in 70 trials. During this process, the fuel enrichment was adjusted from an initial value of 4.00 w/o to 3.84582 w/o, and the pin pitch was an initial value of 1.26239 cm to 1.29097 cm. The SA scores gradually improved over trials.

Using 31 processors of Ryzen 9 7950X CPU, the GA took 100 hours for the fitness of 4,116, while the SA costed 140 hours for the score of 2,126 at the same computational environment. In terms of calculation results relative to time spent, the GA approach provides much more accurate and faster optimization result than SA.

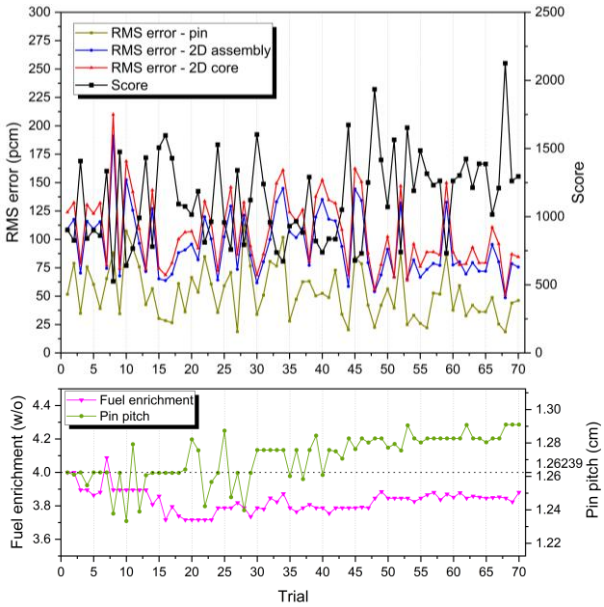

Fig. 8. Changes in RMS error for pin, 2D assembly, and 2D core problems over 70 SA trials (top) and changes in design parameter of correction reference model (bottom)

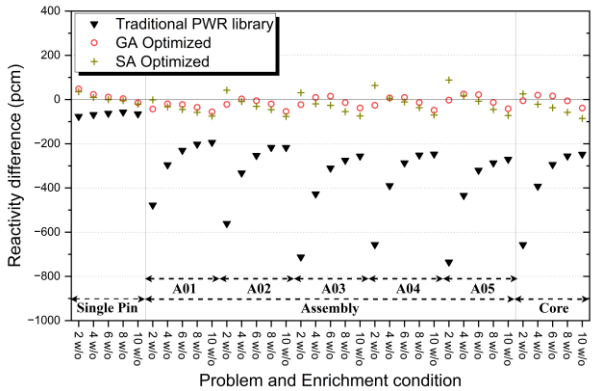

Fig. 9. Reactivity difference for SBF SMR benchmark: GA optimized, SA optimized and traditional PWR library

Figure 9 shows the differences in reactivity for the libraries optimized by each algorithm in the SMR benchmark. For comparison, traditional PWR library optimized for LEU system is plotted.

With respect to various geometries and enrichment conditions, GA optimized library was calculated with a total RMS error of 27 pcm for 30 generations. In comparison, the SA method achieved an overall RMS

error of 46 pcm with 70 trials. Both algorithms provide results that are significantly more accurate than the traditional PWR library, which was calculated with an RMS error of 361 pcm.

5. Conclusion

In this study, new strategies for the MG cross section library optimization based on metaheuristic algorithms are introduced. The proposed GA and SA algorithms both demonstrate the capability to generate a globally optimal cross section library under various conditions (e.g., System geometry and ^{235}U enrichment). Because the proposed SA show less computing time efficiency than the GA algorithm, it is necessary to improve the SA algorithm in the near future. Moreover, the optimized library corrections based on this metaheuristic algorithm will be applied to various SMR and Gen-VI reactor designs.

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