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Metaheuristic Optimization Method for Neutron Spectra Shaping

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INTRODUCTION

Numerous research fields are interested in an accurate and efficient methodology to tailor available neutron spectra to their specific application needs. For example, neutron sources that meet the requirements for producing synthetic debris and fission products (FPs) for post-detonation nuclear forensics, detector calibrations, study of radiation damage to different materials, cross section measurements, materials science, design of targets for the production of medical isotopes, or medical applications such as Boron Neutron Capture Therapy (BNCT) often do not exist. Each of these applications has widely varying neutron spectrum and intensity requirements, making progress in one area difficult to apply to other areas using the current set of tools and literature basis. The lack of a coherent, coordinated approach to a difficult problem at least partially explains why state-of-the-art spectral modification techniques have not advanced significantly since the first use of hydrogen thermalization and cadmium filters in 1935 [1].

We have developed an optimization tool for automated neutron beam spectral tailoring based on a set of pre-determined constraints. Two software packages were developed to perform the optimization and design of energy tuning assemblies (ETAs) [2]: *Gnowee* is a general-purpose metaheuristic optimization algorithm, and *Coues* couples *Gnowee* to a radiation transport solver to automatically generate an ETA design given a set of constrains and an objective spectrum. Both packages are available on *GitHub*[1][2]

As an initial application, we used these tools to design an ETA for modification of the National Ignition Facility (NIF) [3] neutron spectrum to mimic sources of interest to the technical nuclear forensics (TNF) program [4]. NIF uses laser inertial confinement to drive a deuterium-tritium (DT) fusion reaction to produce a very high flux of 14.06 MeV neutrons with very few lower energy neutrons.

Gnowee and *Coeus* were not developed as ends unto themselves but instead as a set of tools to enable ETA design. These software packages have ongoing development for generalization to allow for optimization of a larger set of engineering design problems and for use outside of NIF target chamber applications. This paper highlights the key features and attributes of *Gnowee* and *Coues*, example applications of both algorithms to the design of ETAs, and the future planned upgrades to *Coues* to allow for the optimization of a larger set of design challenges.

OPTIMIZATION SOFTWARE: *GNOWEE/COEUS*

The two codes which perform neutron spectra tailoring, *Gnowee* and *Coeus*, were developed as a set of tools to enable ETA design.

Gnowee uses metaheuristic search patterns [5] to sample the design space in an efficient manner to lead to fast, nearly global convergence. The nature of the algorithm makes the search routine problem independent, allowing the optimization algorithm to be applied to a wide range of problems. The search algorithm is coupled to a hybrid Denovo-MCNP [6,7] radiation transport engine enabled by ADVANTG [8]. This approach allows for more computational time to be allotted to high "fitness" solutions while keeping the computational requirements tractable for the hundreds or thousands of radiation transport calculations that can occur in an optimization.

Coeus is developed as the interface between *Gnowee*, the metaheuristic optimization algorithm, the radiation transport codes required to evaluate the ETA objective function and constraints, and the job scheduling system used to submit jobs on High Performance Computing (HPC).

Gnowee: Metaheuristic Optimization Algorithm

Gnowee is a modular, Python-based, open-source hybrid metaheuristic optimization algorithm, designed for rapid convergence to nearly globally optimum solutions for complex, constrained engineering problems with mixed-integer and combinatorial design vectors and high-cost, noisy, discontinuous, black box objective functions..

To illustrate the design challenge, the ETA optimization problem for the creation of synthetic debris for post-detonation nuclear forensics on NIF is illustrated. Here, the objective was to create a tailored neutron spectrum consisting of D-T fusion and prompt fission components. To achieve this, the objective function was formulated as a flux-weighted relative least square minimization given by Eq. 1. The objective function is not fixed and can be changed to fit the optimization objectives.

$$f_1(\overrightarrow{x_P}) = \sum_{g=1}^{G} \left(\frac{\phi_g^O - \phi_g^D(\overrightarrow{x_P})}{\phi_g^O} \right)^2 * \frac{\phi_g^O}{\phi^O} \qquad (1)$$

where ϕ^O is the objective spectrum and $\phi^D(\vec{x}_P)$ is the spectra corresponding to a candidate design. $\vec{x}_P$ is a design

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[1] https://github.com/SlaybaughLab/Gnowee
[2] https://github.com/SlaybaughLab/Coeus

vector of the variables corresponding to a candidate design, which contains continuous variables (cell dimensions), discrete variables (materials, densities, and numbers of cells), and combinatorial variables (the ordering of the cells in the geometry). The assessed suitability of a given candidate design is subject to the following constrains on weight (Eq. 2), and efficiency (Eq. 3):

$$g_1(\vec{x}) = \sum_{n=1}^{N} \rho_n V_n - W \leq 0 \tag{2}$$

$$g_2(\vec{x}) = N_f^{min} - \phi^C(\vec{x}) V \Sigma_f^{HEU} \leq 0 \tag{3}$$

In Eq. 2, ρ_n and V_n are the mass and volume of the nth component, respectively, and W is the maximum system weight allowed. In Eq. 3, $\phi^C(\vec{x})$ is the candidate design's neutron spectrum produced across the highly enriched uranium (HEU) foil, V and Σ_f^{HEU} are the volume and macroscopic cross-section of the HEU foil, respectively, and N_f^{min} is the minimum number of fissions required.

Optimization problems are often categorized based on the design vector, $\vec{x}_p$ - the type, number and behavior of the objective function, and the constraints. Thus, ETA design is a single objective, non-linear, constrained, mixed-integer and combinatorial multi-modal optimization problem. This complexity is compounded by the requirement of "black-box" radiation transport codes to evaluate the objective function for each design.

Due to the nature of the problem being solved, metaheuristic techniques have been adopted instead of gradient-based deterministic approaches because: (1) defining an appropriate search gradient is difficult or impossible for many problems, (2) increases in the generality of the algorithm across applications can be obtained, and (3) nearly global convergence in highly multi-modal landscapes can be achieved.

For the development of *Gnowee*, emphasis was placed on nearly global convergence as practical considerations such as manufacturing tolerances and cost often limit the utility of true global optima. To accomplish these goals, *Gnowee*'s hybrid metaheuristic framework is based on a set of diverse, robust heuristics that appropriately balance diversification and intensification strategies across a wide range of optimization problems. To develop this framework, Lones's and Sorensen's [9, 10] approach to classification of heuristic search operators was utilized to alter the behavior of many common search heuristics from top metaheuristic algorithms such as particle swarm optimization, differential evolution, genetic algorithm, and cuckoo search. The *Gnowee* algorithm was then benchmarked against a diverse set of 18 optimization benchmarks using six different metaheuristic algorithms. These benchmarks[3] showed that *Gnowee* demonstrated significant improvement in both the quality of the solution obtained and the number of function evaluations required (i.e. radiation transport calculations) to achieve the optimized solution [2].

Coeus: ETA Design Software

Coeus provides an efficient capability to design and optimize ETAs for spectral shaping. *Coeus* takes advantage of the "embarrassingly parallel" nature of both *Gnowee* and MCNP to achieve efficient parallel computation through both Open MPI and slave node tasking using the SLURM job scheduler.

The primary purpose of *Coeus* is to manage the interaction with *Gnowee*, creation of MCNP inputs, submitting of jobs, reading of MCNP outputs, and updating the population and results. *Coeus* also has to manage the creation of the ADVANTG inputs, submission of jobs, and reading of the ADVANTG outputs, but these are essentially just extensions of the MCNP processes due to the tight integration between MCNP and ADVANTG.

Coeus initializes surface and geometry objects to create a cylindrical/conical 2-D ETA geometry initially used for the NIF target chamber applications. The variables associated with each surface are sampled by *Gnowee*. All of the surface and cell object updating and MCNP geometry logic is handled within each operator as needed for the variables under consideration for that particular operator. The MCNP parameters, surface, and cell objects are then passed to a function that generates an MCNP input for the new candidate design. However, nothing about *Coeus* or *Gnowee* requires the tight integration of the search operators and geometry update, and this can be handled in a much more generic, modular fashion.

After each MCNP calculation, the specified MCNP tallies are read and used to calculate the objective function and constraints. A significant improvement in efficiency is obtained by tying the statistical convergence of a design to the assessed fitness. If a current design is outside the constraints imposed on the system or is a poor candidate, less particles are simulated to avoid wasting computational resources. As the fitness improves, the number of simulated particles is increased to reduce statistical uncertainty and ensure chosen designs are not statistical anomalies.

GNOWEE/COEUS APPLICATIONS AND RESULTS

Coeus was developed originally for shaping the NIF source spectrum for forensic applications, and this case represents the most complete results obtained to date. For illustration purposes, the following sections detail what has been done as well as a BNCT example study to demonstrate the capabilities of the software.

ETA Design Optimization for TNF

Since the cessation of nuclear weapons testing, synthetic debris has been made in a limited fashion using sample-doping techniques. ETAs designed by *Coeus* are a robust alternative approach. The ETA developed in this work generates realistic synthetic fission and activation

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[3] https://github.com/SlaybaughLab/Gnowee/tree/master/Benchmarks/results

products through irradiation of samples with a combined thermonuclear and prompt fission neutron spectrum (TN+PFNS) [11]. Currently, there are no active sources which are capable of producing this spectrum to compare the ETA results to. When used with fissile foils, this irradiation will produce a synthetic FP distribution that is realistic across all mass chains.

Coeus was run to generate a TNF relevant ETA design given the starting NIF source spectrum, the objective TN+PFNS (see Figure 1), and the constraints shown in Equations 2-3. The optimization run computed 4500 designs over the course of 76 hours (wall time). The resulting optimized ETA design and comparison of the objective and achieved neutron spectra are shown in Fig.1. As shown in the comparison of the objective and ETA neutron spectrum, the ETA accomplished a significant shift from a 14 MeV mono-energetic source and matched the overall objective neutron spectrum remarkably well. The areas of disagreement, < 10 keV and 6-12 MeV, represent a low fraction (~2-3 %) of the overall spectrum. The differences below 10 keV were driven by the weight constraints on the system, and the 6-12 MeV region differences were driven by known modeling errors associated with using bare critical assemblies to derive a representative TN+PFNS.

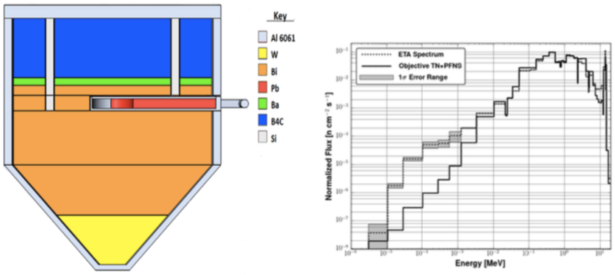

Figure 1. Design of the nearly optimum ETA production of synthetic fission and activation products and the shaped flux in the sample cavity.

TABLE I presents the comparison of the FPs produced by the ETA to those produced by the objective spectrum using Nagy fits of experimental data and the GEneral description of Fission observables (GEF) [12,13]. Across all FPs of interest, the ETA yield is consistent with the objective spectrum FP yields within error. One consistent systematic deviation is in the valley FPs, which are ~5-10% higher for the ETA. This is due to the 10-20 MeV flux in the ETA spectrum being ~14% higher than the TN+PFNS objective, which was a limitation based on the mass requirements to field on NIF.

These modeled results show promise for improving TNF outcomes and the ability to generate realistic synthetic FPs and debris. Just as importantly, they represent a step forward in being able to design *customizable* neutron energy spectra for a variety of applications.

TABLE I. Nagy and GEF-based FPs cumulative yield (fcum(A,Z)) estimates of select FPs from a 93.15% ^{235}U HEU foil exposed to the TN+PFNS objective spectrum and the TN+PFNS achieved by the ETA.

	Nagy		GEF	
FP	Objective	ETA	Objective	ETA
$^{95}_{40}$Zr	6.17±0.09	6.15±0.09	6.47±0.09	6.47±0.09
$^{95}_{40}$Zr	5.75±0.09	5.74±0.09	6.47±0.09	6.46±0.09
$^{111}_{47}$Ag	0.25±0.01	0.26±0.01	0.21±0.01	0.22±0.01
$^{115}_{48}$Cd	0.25±0.01	0.26±0.01	0.24±0.01	0.26±0.01
$^{133}_{53}$I	6.41±0.13	6.38±0.13	6.04±0.13	6.01±0.13
$^{140}_{56}$Ba	5.71±0.07	5.68±0.07	5.41±0.07	5.41±0.07
$^{147}_{56}$Nd	2.12±0.03	2.11±0.03	2.00±0.03	1.99±0.03
$^{151}_{61}$Pm	0.47±0.02	0.47±0.02	0.46±0.02	0.46±0.02
$^{153}_{62}$Sm	0.18±0.01	0.18±0.01	0.17±0.01	0.17±0.01

Alternate Use Cases: BNCT

Many studies were done in the past to determine which neutron energy is the most suitable for treatment of shallow and deep-seated brain tumors in the context of BNCT, and how to produce those optimal neutron beams regardless of the initial neutron source energy. It was found [12, 13] that for deep-seated tumors, the neutron energy range at the skin level needs to be between 1 to 20 keV, with a maximum therapeutic gain for neutrons around 8 keV, while for shallow tumors the most effective are neutrons between 1 and 10 keV. The goal of these studies was to maximize the dose to tumor for a given normal tissue dose (12.5 Gy-equivalent). At the same time, both the high-energy neutron "tail" and neutrons in the thermal energy range needed to be eliminated. The optimal Beam Shaping Assemblies (BSA) were developed by using MCNP simulations for each neutron source and by painstakingly trying many combinations of various materials, their arrangements and thicknesses. The optimal BSA designs were obtained for accelerator based neutron sources (p-^{7}Li) [13], and for D-D and D-T neutron sources [12]. For the purpose of this paper, we decided to test *Coeus/Gnowee* capabilities and try to reproduce optimal BSA for the case of the D-T neutron generator.

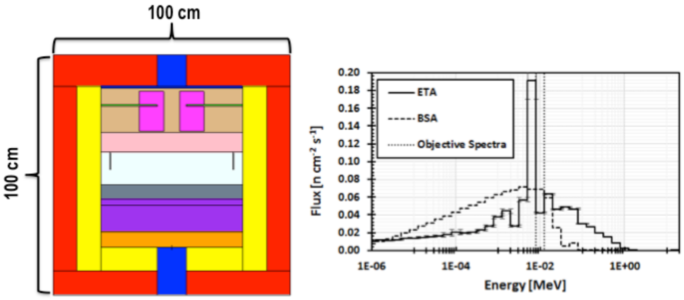

Figure 2. Design of the nearly optimum ETA and the exit shaped flux for the BNCT.

The neutron source for the BNCT study remains the same as for the TNF case, using the 14 MeV NIF neutron source. The objective function drives a focus on 10 keV neutrons differentiating it from the TNF application. The input to *Coeus* was generalized to allow new larger geometries, and modification of the material library. The material library included new compounds, such as lithiaded polyethylene, heavy water, aluminum fluoride, which have been shown to be effective for the BNCT application in the past. New options were also added to *Coeus*: the exclusion of isotopes with missing cross sections, the flexibility of changing fitness parameters, and the adding of weights on the objective spectrums to focus the optimization on reducing neutrons that contribute to the dose to normal tissue dose. For BNCT, the weights used represent the ratio of tumor dose over normal tissue dose.

Figure 2 illustrates that *Coeus* was able to find an ETA design nearly reproducing the optimal neutron spectrum from [13] in a dramatically shorter optimal design search period and smaller dimension (100x100 vs. 140x140 of the reference BSA). However, further improvements in *Coeus* are needed to allow more flexibility to the user to fully develop an ETA design for BNCT, which will provide further calculations for a valid quantitative comparison with the reference design. Specifically, *Coeus* currently is unable to support modeling of a patient phantom, the use of dose distributions as the objective function, and the system constraints on treatment time.

CONCLUSION AND ONGOING WORK

In the current stage of the development, *Gnowee/Coeus* optimizes the design of ETAs with objective functions relevant to comparing two neutron spectra. These modeled results show promise for improving TNF outcomes and the ability to create customizable ETA designs. This represents a dramatic improvement over current spectral shaping options and potentially enables radical improvements in experimental outcomes across a wide range of applications. We have shown that *Gnowee/Coeus* could be easily applied with minor modification to *Coeus,* as the case of BSA optimization for BNCT shows. The further goals are to develop a general-purpose nuclear engineering code that is flexible enough to accommodate different transport engines, HPC architectures, modeled geometries, objective functions, and constraints.

The near term ongoing work is focused on achieving a larger generalization of the software. For that, we needed to develop a more expanded new input system for both MCNP and ADVANTG. The goal is to allow a generic geometry specification for MCNP; to introduce all the ADVANTAG input options as the two methods of spatial discretization; to introduce an automatic ADVANTG switch to change from once-per-generation to once-per-evaluation for very dynamic problems where the weight windows rapidly become non-ideal; and to expand to *Coeus* the ability presented in *Gnowee* to have user-defined constraints and objective functions.

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