The adjoint problem as physical heuristic for loading pattern optimization

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Abstract

Loading pattern optimization enables longer irradiation cycles while still maintaining the ability to safely operate and shutdown the reactor. The loading pattern optimization problem is characterized by a huge search space and is a multi-objective, nonlinear, NP-hard discrete problem. However, in-core fuel management is an essential part of routine work in a nuclear reactor, hence optimized usage of the fuel inventory enables the economic and efficient utilization of resources. This study is a proof-of-concept for the hypothesis that adjoint-based neutron importance functions can be used for the optimization process of the core loading pattern. New optimization techniques are developed in order to demonstrate the successful utilization of adjoint-based functions as the optimization driving force. Different importance functions are developed and studied. It is demonstrated that the physical insight obtained from the importance function can be used for optimization of loading patterns. Eventually, this new technique should be integrated into a stochastic optimization algorithm, e.g., evolutionary algorithms, in order to accelerate and improve existing optimization algorithms.

Keywords: Adjoint, Loading pattern, Optimization, Neutron importance, Neutron transport

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Highlights

• The neutron importance is used for loading pattern optimization
• Different adjoint-based neutron importance functions are developed and studied
• New neutron importance-based optimization technique is developed and demonstrated
• This idea shows great potential to accelerate and improve existing optimization methods
1. Introduction

The in-core fuel management optimization problem is that of arranging the fuel assemblies (FAs) in the core in a way that best suits the desired objectives, such as maximizing core excess reactivity or maximize energy production, while maintaining the ability to safely operate and shutdown the reactor within the required safety margins [1–8]. This optimization problem is characterized by a huge (computationally prohibitive) search space, and is a multi-objective, nonlinear, NP-hard combinatorial problem. Nonetheless, proper in-core fuel management is an essential part of routine work in a nuclear reactor, and proper use of existing fuel inventory enables economic and efficient use of resources. It is thus important to find clever ways to solve this optimization problem, and to constantly strive to improve existing optimization methods [1, 2, 4, 8].

The objective of this study is to develop new optimization techniques and methodologies for the optimization of loading patterns (LPs) of nuclear FAs in the reactor core, utilizing the adjoint flux as the optimization driving force. The adjoint flux, as the solution to a specific adjoint problem, has a natural physical interpretation as a measure of the importance of a neutron in a point in the parameter space of the core [9]. That is, the adjoint flux is a direct measure of the importance of a locally injected neutron to the response of a detector at that point. So, the importance function assigns each point in the parameter space of the core with an importance value, corresponding to the local influence of a neutron at that point. Integral weighted quantities, e.g., \( \langle \phi^\dagger, \mathcal{A} \phi \rangle \), where \( \mathcal{A} \) is some operator representing a physical process, are also highly indicative.

The hypothesis of this study is that the importance function, and variations upon it, can be utilized to accelerate and improve LPs optimizations. It is demonstrated that importance function supplies valuable knowledge of the LP, which can be used to rearrange it to better suit different purposes. preliminary results show that an existing LP can be improved (with respect to some optimization objective) in an iterative process, using the knowledge of the local importance. This is achieved by integrating the local importance values into a reordering scheme for the creation of the next (better) LP.

For brevity and clarity, and for the proof of concept, this study focuses on a single core parameter, i.e., the effective neutron multiplication factor, \( k_{\text{eff}} \). However, it is shown that the PPF objective can also be optimized using \( k_{\text{eff}} \). For this paper, the best LP is the one yielding the highest or lowest \( k_{\text{eff}} \). One of the objectives is to show that optimized LPs can be obtained through the iterative importance reordering process described above and more thoroughly in the following sections.
2. Scientific Background

2.1. The adjoint operator

The inner product of two real functions $u$ and $w$ of the phase space and time coordinates $(r, E, \hat{\Omega}, t)$ is defined as \[ \langle u, w \rangle = \int_0^T dt \int_0^\infty dE \int_{4\pi} d\hat{\Omega} u(r, E, \hat{\Omega}, t)w(r, E, \hat{\Omega}, t) . \tag{1} \]

The integration domain is the phase space covering the volume of the reactor core and its surface, the solid angles covering a unit sphere, an allowable range of energies, and a time span.

Given a linear operator $L$, two real functions $u$ and $w$, and an inner product (e.g., Eq. 1), the adjoint of this operator, denoted by $L^\dagger$, is defined, and constructed, by the identity:

$$\langle w, Lu \rangle = \langle u, L^\dagger w \rangle + P[u, w] .$$ \tag{2}

That is, $L^\dagger$ is the operator that satisfies Eq. (2), and is constructed by applying all necessary mathematical operations until $u$ stands freely under the inner product and $w$ is acted upon by an operator, denoted $L^\dagger$. $P[u, w]$ is a functional consisted of the residual terms arising from actions on $u$ and $w$ in the process of isolating $u$ from the operator $L$, and usually contains boundary terms originating from integration by parts.

2.2. The adjoint neutron transport equation

The stationary continuous-energy neutron transport equation is written as

$$\hat{\Omega} \cdot \nabla \psi(r, E, \hat{\Omega}) + \Sigma_t(r, E)\psi(r, E, \hat{\Omega}) = \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(r, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega})\psi(r, E', \hat{\Omega}')$$

$$+ S(r, E, \hat{\Omega}) , \tag{3}$$

where $S$ represents the fission source and other external sources ($Q$),

$$S(r, E, \hat{\Omega}) = \frac{\chi(E)}{4\pi} \int_0^\infty dE' \nu(E')\Sigma_f(r, E') \int_{4\pi} d\hat{\Omega}' \psi(r, E', \hat{\Omega}') + \frac{1}{4\pi} Q(r, E, \hat{\Omega}) . \tag{4}$$

The neutron transport equation (Eq. 3) is subjected to boundary conditions defined as

$$\psi(r_b, E, \hat{\Omega}) = \psi^b(r_b, E, \hat{\Omega}), \quad r_b \in \partial V, \quad \hat{\Omega} \cdot \hat{n} < 0, \quad 0 < E < \infty . \tag{5}$$

Expressing Eqs. (3)-(4) in compact operator form gives the notation

$$L \psi = Q , \tag{6}$$
where \( \mathcal{L} \) is defined as the transport operator. In order to construct the adjoint operator \( \mathcal{L}^{\dagger} \) we take the inner product of an auxiliary function \( \psi^{\dagger}(r, E, \hat{\Omega}) \) with \( \mathcal{L} \psi \) and define \( \mathcal{L}^{\dagger} \) as the \textit{adjoint} transport operator that satisfies the identity

\[
\langle \psi^{\dagger}, \mathcal{L} \psi \rangle = \langle \psi, \mathcal{L}^{\dagger} \psi^{\dagger} \rangle + P[\psi, \psi^{\dagger}] .
\]  

(7)

Solving Eq. (7), the adjoint transport operator is

\[
\mathcal{L}^{\dagger} \psi^{\dagger} = -\hat{\Omega} \cdot \nabla \psi^{\dagger}(r, E, \hat{\Omega}) + \Sigma_{s}(r, E)\psi^{\dagger}(r, E, \hat{\Omega})
- \int _{0}^{\infty} dE' \int \frac{d\hat{\Omega}'}{4\pi} \Sigma_{s}(r, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi^{\dagger}(r, E', \hat{\Omega}')
- \nu(E)\Sigma_{f}(r, E) \int _{0}^{\infty} dE' \frac{\chi(E')}{4\pi} \int \frac{d\hat{\Omega}'}{4\pi} \psi^{\dagger}(r, E', \hat{\Omega}') .
\]  

(8)

The corresponding adjoint transport equation is then written as

\[
\mathcal{L}^{\dagger} \psi^{\dagger} = Q^{\dagger} ,
\]  

(9)

with the following boundary conditions (corresponding to void boundary conditions in the forward problem)

\[
\psi^{\dagger}(r_{b}, E, \hat{\Omega}) = 0, \quad r_{b} \in \partial V, \quad \hat{\Omega} \cdot \hat{n} > 0, \quad 0 < E < \infty .
\]  

(10)

2.3. The adjoint 2-group diffusion equations

The neutron diffusion equation is a well-known approximation to the neutron transport equation, which essentially eliminates the angular dependency. It does so by first, integrating over all angles, defining the isotropic flux and isotropic scattering kernel

\[
\phi(r, E) \equiv \int \frac{d\hat{\Omega}'}{4\pi} \psi(r, E, \hat{\Omega}')
\]

\[
\Sigma_{s}(r, E' \rightarrow E)\phi(r, E') \equiv \int \frac{d\hat{\Omega}'}{4\pi} \Sigma_{s}(r, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(r, E', \hat{\Omega}') ,
\]  

(11)

and second, by using Fick’s law, i.e., \( J(r, E) \equiv -D(r, E)\nabla \phi(r, E) \). This yields the steady-state neutron diffusion equation:

\[
-\nabla \cdot [D(r, E)\nabla \phi(r, E)] + \Sigma_{s}(r, E)\phi(r, E) = \int _{0}^{\infty} dE'\Sigma_{s}(r, E' \rightarrow E)\phi(r, E')
+ \chi(E) \int _{0}^{\infty} dE'\nu(E')\Sigma_{f}(r, E')\phi(r, E') + Q(r, E) ,
\]  

(12)
where $D = \frac{1}{3\Sigma_t}$ is Fick’s diffusion coefficient. The multi-group steady-state $k$-eigenvalue neutron diffusion equation is easily derived:

$$-\nabla \cdot [D_g(r) \nabla \phi_g(r)] + \Sigma_{r,g}(r) \phi_g(r) = \sum_{g' \neq g}^{G} \Sigma_{s,g' \rightarrow g}(r) \phi_{g'}(r) + \frac{\Sigma_g(r)}{k_{\text{eff}}} \sum_{g' = 1}^{G} \nu \Sigma_{f,g'}(r) \phi_{g'}(r),$$

(13)

where the subscript $g$ denotes group constant terms that are flux-weight averaged over the energy group $g$, and the removal term is $\Sigma_r \equiv \Sigma_t - \Sigma_{g' \rightarrow g}$.

The core solver used for this work, DYN3D [13, 14], employs here 2-group diffusion equations, homogenized over a spatial mesh. Repeating a similar process to the one in the case of the adjoint transport equation (section 2.2), the adjoint 2-group diffusion equation used by DYN3D is written as:

$$-\nabla \cdot [D_g(r) \nabla \phi_g^*(r)] + \Sigma_{r,g}(r) \phi_g^*(r) = \sum_{g' \neq g}^{G} \Sigma_{s,g' \rightarrow g}(r) \phi_{g'}^*(r) + \frac{\nu \Sigma_{f,g'}(r)}{k_{\text{eff}}} \sum_{g' = 1}^{G} \chi_{g'}(r) \phi_{g'}^*(r),$$

(14)

3. Methodology

3.1. Neutron importance as optimization driving force

The hypothesis is that the neutron importance function, and the insight it provides, can be used to drive an optimization process on a nuclear reactor LP. For example, in order to increase $k_{\text{eff}}$ one needs to increase the neutron flux in high-importance locations in the core. That is because neutrons injected into the system are most influential in high-importance locations. In other words, neutrons injected into high importance locations have a higher probability to induce fission. This is very intuitive reasoning, which simply states that more neutrons are likely to be produced by an LP in which neutrons are born and concentrated where they are more likely to induce fission.

Similar reasoning can be used in order to decrease the PPF in the core below some required threshold. Decreasing the neutron flux in high-importance locations and increasing it in low-importance locations will lead to flattening of the fission power (and to decreasing in $k_{\text{eff}}$).

An iterative importance-driven process is proposed for the optimization of different LPs. An algorithm is constructed which receives an LP and rearranges it according to its importance distribution using different reordering schemes, depending upon the optimization goals for the LP.

First, the forward and adjoint fluxes of the LP are calculated. This produces spatially and energetically discrete functions, i.e., for every assembly, axial layer, and energy group, the forward and the adjoint flux values are obtained. The forward and adjoint neutron fluxes at radial node $i$, axial node $z$ and energy group $g$ are denoted by $\phi_{i,z,g}$ and $\phi_{i,z,g}^*$, respectively. The forward flux is normalized according to the reactor power whereas the adjoint flux is normalized such that its maximal value equals unity.
Second, several importance functions can be defined, e.g.,

\[
\mathcal{I}_{1}^{i,z,g} = \phi_{i,z,g} \tag{15}
\]

\[
\mathcal{I}_{2}^{i,z,g} = \phi_{i,z,g}^{\dagger} \phi_{i,z,g} \tag{16}
\]

\[
\mathcal{I}_{3}^{i,z,g} = \phi_{i,z,g}^{\dagger} \phi_{i,z,g} \phi_{i,z,g} \tag{17}
\]

The quantity \( \mathcal{I}_{i,z,g} \) is denoted as the “local” importance and actually assumes a distribution in space and energy domains. It is useful to define the radial importance \( \mathcal{I}_{1}^{z} \) and the total importance \( \mathcal{I}^{z} \) of the core LP by

\[
\mathcal{I}_{1}^{z} \equiv \sum_{z=1}^{N_{z}} \sum_{g=1}^{G_{z}} \mathcal{I}_{1}^{i,z,g}, \quad \mathcal{I}^{z} \equiv \sum_{i=1}^{N_{i}} \sum_{z=1}^{N_{z}} \sum_{g=1}^{G_{z}} \mathcal{I}_{i,z,g}. \tag{18}
\]

Figure 1 shows a random loading pattern of a typical PWR core (left) with three types of FAs (differing in their \(^{235}\text{U} \) enrichment) and its corresponding calculated radial importance \( \mathcal{I}_{1}^{1} \), \( \mathcal{I}_{2}^{1} \) and \( \mathcal{I}_{3}^{1} \), respectively.

Third, all fuel assemblies (FAs) are then sorted according to their importance values. Once all assemblies are sorted, one of two reordering schemes is applied:

1. Swapping between high enrichment FAs in low importance locations and low enrichment FAs in high importance locations. Namely, reordering the LP in accordance with importance.

2. Swapping high enrichment FAs in high importance locations and low enrichment FAs in low importance locations. Namely, reordering the LP in the opposite with importance.

Once the FAs have been swapped, the algorithm reconstructs the LP in consistency with the resulting arrangement and builds an input deck for the flux solver. The process continues iteratively until a maximal number of iterations is reached, or until the LP is completely ordered by importance, according to one of the two reordering schemes. Once a single swap is performed, the fluxes’ distribution (and hence the importance distribution) are changed, and a new calculation is required for obtaining the accurate fluxes distribution of the new LP. However, the number of FA swaps per iteration is a parameter of the algorithm.
3.2. The core simulator

The core simulator used for the calculations of $k_{\text{eff}}$, the forward and adjoint fluxes and all other properties of the LP is DYN3D [13, 14]. It is a three-dimensional coupled neutron kinetics and thermal-hydraulics core model, developed at Helmholtz Zentrum Dresden-Rossendorf (HZDR), for dynamic and depletion calculations of light water reactor cores with quadratic or hexagonal FA geometry. The multigroup neutron diffusion equation is solved by nodal expansion methods. Cross section libraries generated by different lattice codes for different reactor types can be linked with DYN3D.

3.3. The reactor core

The core considered in this work is a simplified PWR core of a typical advanced (Gen III+) PWR, e.g., APWR [15], with a $17 \times 17$ rectangular lattice containing 257 FAs of three different $^{235}\text{U}$ enrichment levels, i.e., 3.1 w/o, 2.4 w/o, and 1.6 w/o. The axial composition of an FA is assumed to be homogeneous and all FAs are assumed to be fresh. Radial and axial boundary conditions are assumed to be black absorber. The number of FAs of each type is assumed to be constant, so the optimization is performed only on the LP and not on the number of FAs of each type.

4. Results

The two reordering schemes are tested on different initial LPs, with differing amounts of swaps per iteration, sorting the importance, and thus rearranging the LP, according to one of the importance functions. As demonstrated below, the first scheme is found useful for $k_{\text{eff}}$-maximizing LP creation. The second scheme, however, is found to have difficulties in its current basic form. This is due to the hardship in reordering a core so enrichment is in reverse order with respect to importance, since the former affects the latter. Even so, when the number of swaps per iteration is small, it succeeds in lowering the PPF.

4.1. 1st reordering scheme – Maximizing $k_{\text{eff}}$

4.1.1. Effect of importance function

A random initial LP is used for different optimization processes, differing in the importance function used for ordering. The results of the optimization process using the first reordering scheme with importance functions defined in Eq. (15) are shown in Fig. 2. It is evident from Fig. 2 that all three importance function enable the convergence to a maximal $k_{\text{eff}}$ LP. The initial $k_{\text{eff}}$ is 1.2273, whereas the final $k_{\text{eff}}$ is 1.3531, 1.3532, and 1.3533 for $I_1^1$, $I_1^2$, and $I_1^3$, respectively.
Figure 2: Iterative convergence from an initial random LP to maximal $k_{\text{eff}}$ LP with 1 swap per iteration using different importance functions $I_1^i$ (a), $I_2^i$ (b), and $I_3^i$ (c) (total of 140 iterations, shown every $\sim$30, upper - LP, lower - radial importance).

The behavior of the total importance (Eq. 18), as well as that of $k_{\text{eff}}$, as a function of the iterations are shown in Fig. 3 for the three types of importance function. The behavior of the multiplication factor...
Figure 3: The behavior of the total importance (Eq. 18) and $k_{\text{eff}}$ as a function of iterations for the three types of importance function.

$k_{\text{eff}}$ is similar for all three importance functions and is monotonically increasing as the optimization process progresses. The initial significant increase in $k_{\text{eff}}$ occurs during the first 20 iterations and can be attributed to the initial swaps of low enriched FAs located in high-importance locations with high enriched FAs located in low-importance positions. These few initial swaps are the most significant for the increase in $k_{\text{eff}}$ and are mainly composed of swapping 3.1 w/o (red) FAs with 1.6 w/o (green) FAs (see Fig. 1). The second significant increase in $k_{\text{eff}}$ occurs between iterations 80-120 and is attributed mainly to swaps of 2.4 w/o (yellow) FAs with 1.6 w/o (green) FAs.

On the other hand, the behavior of the total importance as a function of iterations is highly complex and non-monotonic. Although the general trend exhibited by the total importance is to follow the increases in $k_{\text{eff}}$ its irregular behavior strongly indicates the non-linearity of the search space and the fact that even a single binary swap of FAs cannot be considered as a small perturbation.

4.1.2. Effect of number of swaps per iteration

As noted above, the number of FA swaps per iteration is a parameter of the algorithm. Once a single swap is performed, the fluxes’ distribution is changed, and a new calculation is required for obtaining the accurate fluxes distribution of the new LP. However, it is possible to perform several swaps before re-calculating the fluxes map of the new LP.

In order to study the effect of the number of swaps per iteration, the same optimization problem is solved with a varying number of swaps per iteration, i.e., 1, 5, 10, 20, and 50. As the number of swaps per iteration is increased, two things are observed. First, the quality of the final LP is decreased, and second, the number of iterations required for convergence is decreased as well. The iterative optimization process with 1-50 swaps per iteration is shown in Fig. 4.
4.2. 2nd reordering scheme – Minimizing PPF

The second reordering scheme aims to order enrichment in the LP in reverse accordance with local importance, i.e., to place high enrichment assemblies in low-importance locations and vice versa. However, taking a high enriched assembly and placing it in a low-importance location raises local importance in that location. Consequentially, this location and the ones in its proximity, with the assemblies in them, possess higher importance than they did in the former LP. Those assemblies are thus likely to become candidates for the next swap, rather than remain in place for the rest of the optimization. Thus, all optimizations using the second reordering scheme experience difficulty to converge to an LP of fuel enrichment in an opposite order to the importance distribution. Examples of this phenomenon can be clearly seen in Fig. 5, whereas the oscillation of the algorithm between 2 repeatable LPs is shown in Fig 6.
5. Conclusions

Preliminary results show that the adjoint flux, with its natural physical interpretation as an importance function, can be successfully utilized as a driving force for the optimization of nuclear core LPs. The physical insight obtained by the importance functions can be used for the improvement of existing optimization algorithms, or for the construction of novel optimization algorithms. Such a basic algorithm, which employs variations on iterative binary shuffling according to local importance, is developed for the purpose of this study as a “proof of concept” tool. Initial results obtained using this algorithm suggest that the local importance is a useful tool that can be utilized for the optimization problem.

The two reordering schemes mentioned above are chosen for their simplicity, for the purpose of constructing and testing the research hypothesis, that adjoint-based importance functions can be utilized in the optimization process of core LPs. The motivation for their specific definition, respectively, is maximizing $k_{\text{eff}}$ and minimizing PPF. The first reordering scheme tends to concentrate fuels according to their enrichment,
i.e., placing the higher-enriched FAs away from core boundaries. This arrangement maximizes fission rate and minimizes leakage, effectively increasing the multiplication factor of the system. The second reordering scheme does the opposite. It creates a pattern of high enriched FAs near core boundaries for maximum leakage or isolating them from each other to avoid high fission rate and flux concentrations. Needless to say that many other reordering schemes can be implemented.

In the case of arranging the LP in accordance with importance it is easy to see why the process is likely to converge. Interchanging the locations of high enriched FAs from low-importance locations with low enriched FAs from high-importance locations creates a positive feedback effect of increasing (decreasing) importance in high (low) importance locations further. Typically, highest importance FAs are found away from core boundaries and in the proximity of (other) high enriched FA concentrations, and lowest importance FAs are found near core boundaries and where FA enrichment is lowest.

Any low enriched FAs within these high enriched clusters are given high importance for their proximity to the high-importance concentrations and are thus natural candidates for a swap with high enriched FAs away from the concentration. So naturally, the iterative process is inching toward a high-$k_{\text{eff}}$ LP of descending-enrichment concentric circles.

The algorithm can perform any number of possible binary FAs swaps per iteration. The number of swaps per iteration is an adjustable algorithm parameter which is tested here and should be further studied. A minimal number of swaps allows the algorithm a more refined process at the expense of an increased number of full core calculations, and vice versa, increasing the number of swaps per iteration minimizes the number of full core calculations at the expense of precision in the convergence process. To wit, swapping one pair of FAs per iteration, thus calculating local importance distribution after every swap, guarantees that each fuel swap is the most influential one in the current LP.

One must bear in mind that once a single swap has been executed, a new LP is generated and the spatial distribution of the adjoint flux is changed. In some cases, the change can be dramatic, indicating that the search space of LPs can be highly nonlinear, discrete, and discontinuous. An illustrative example of this non-intuitive trait of single swaps is shown in Fig. 6.

Two notes should be made regarding this result. First, this result highlights and explains the inherent limitation of perturbation theory based optimization algorithms. Single swaps are generally not small perturbations, as beautifully shown in Figs. 5 and 6. Second, this raises the question of whether two swaps (or more) per iteration will perform better than a single swap per iteration. In this case, there may be a trade-off (or another complex) relation between the number of swaps per iteration and the convergence rate. Increasing the number of swaps per iteration maximizes the utilization of the information available to us at each step (i.e., the adjoint flux). On the other hand, it may well be that the second swap (and any other subsequent swap) is based on irrelevant (or even misleading) information, since the adjoint flux distribution may be significantly altered after any swap.
Finally, the picture that arises from the literature survey (which is beyond the scope of this paper), the adjoint flux and importance have been used as an integral part of perturbation theory calculations for LP optimization schemes. However, the importance function has not been used outside the scope of perturbation theory. The adjoint flux, the total importance, the local importance distribution, the adjoint spectrum, and different variations of those, are factors of the LP which hold in themselves or are connected to, physical interpretation of the core characteristics. In this, they hold physical information about the LP that can be utilized not only in the context of perturbation theory but in constructing optimization schemes for nuclear reactor core LPs.

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