

Topologically Optimal Nuclear Core Designs Using Deterministic Neutronics

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INTRODUCTION

Additive manufacturing (AM) is currently used for high value, high complexity parts across most manufacturing sectors. AM offers order-of-magnitude faster prototyping and development timelines and the ability to manufacture complex geometries that combine multiple components into single parts or create high performance components that cannot be traditionally manufactured.

The Transformational Reactor Program (TCR) at Oak Ridge National Laboratory has developed additive techniques for nuclear reactor manufacturing focused on High Temperature Gas-cooled Reactor (HTGR) technologies. TCR's key achievement is process development of AM fuel blocks using TRISO fuel in a SiC matrix with arbitrary fuel form factors and cooling channels. Notably, the fuel achieves a 60% TRISO packing fraction compared to the previous state of the art of 40% [1]. TCR has characterized AM SS 316L and AM SiC [2] in high temperature and radiation environments and consequently evidenced that AM materials are as viable as traditionally manufactured materials in nuclear environments, moreover exceeding performance of traditional manufacturing. AM's tool chest [3] for reactor design includes effectively arbitrarily graded core compositions, shaped coolant geometries, high packing fraction TRISO-matrix fuels, embedded burnable poisons, and embedded sensors.

Motivation for a new core design paradigm

Manufacturing arbitrarily defined cores appears to be a likely possibility in the near future, but core designs and methods have not yet been developed to exploit these future capabilities. As a result, we do not know what performance gains can be expected. But performance gains may become increasingly important for nuclear core design as civilian nuclear reactors trend towards smaller and safer cores that improve passive safety capabilities and economies of reactor production but suffer from increased neutron leakage and reduced burnup [4]. Space applications for propulsion and power have severe mass costs and may similarly benefit from new core design methodologies.

The immense design space afforded by arbitrary core definition requires computationally efficient design techniques beyond parameter sweep studies. A 1-meter cubic core segmented into millimeter sized voxels yields 10^9 voxels or free parameters, while traditional parametric studies will assess on the order of just 10 parameters. This paper presents scalable topology optimization techniques for designing arbitrarily defined cores.

Previous Work

An important shift in the last decade has been the emergence of parametric design in space reactors including nuclear thermal propulsion and transportable reactors that have allowed increasingly smaller cores using HALEU instead of HEU [5]. Topologically optimized cores will further expand the Pareto fronts for nuclear cores allowing for cores of reduced size, greater energy content, and lower enrichment—important trends for implementing cost-effective infinite coping time reactors.

Core design has traditionally been limited to simple shapes and geometries. Conventional core design knobs might include the pitch, orientation, or thickness of various reactor components. Material knobs might include the fuel or moderator type, fuel enrichment, and clad types. The design space is explored by sweeping the parameter ranges or searching the design space. Each core must be evaluated with neutron transport codes and any other codes necessary for computing the optimization value functions.

Sobes et. al. [6] minimized temperature peaking in a TCR core by changing geometry parameters while maintaining criticality. To reduce the number of neutron transport evaluations, they approximate expensive neutronic and thermal hydraulic calculations at each design iteration with a machine learning surrogate, allowing fast evaluation of designs that deviate slightly from the reference. This is still a parametric search with limited geometric knobs, albeit accelerated by machine learning surrogate models. Their optimization improved average temperature peaking by 3x.

Substantial literature on topology optimization exists for structural components including evolutionary and PDE-constrained optimization approaches [7]. Moreover, the mathematical underpinnings of optimization in function spaces under PDE constraints has been developed as well, summarized in [8]. These methods essentially consist of iterative gradient-guided variation of geometric input to physics analysis.

Topology optimization in nuclear engineering problems based on gradient techniques was first suggested in [9]. High dimensional gradients were calculated using MCNP PERT or KPERT cards. Chabod successfully demonstrated the automated design of a neutron spectrum shaping device which scatters a source of 14.1 MeV neutrons to match the spectrum of a fast reactor within a detection volume. Similarly, he solved a critical mass minimization problem in which varying densities of LEU were mixed with polyethylene in a layered spherical shell geometry in order to obtain the lowest possible critical mass.

The expanded article by Chabod [10] explores a variety of related problems, including the optimization of a reactor in order to minimize the mass of fuel that obtains criticality. It involved 3% enriched uranium with the balance of material

being water. The result obtained consisted of a cylindrical mass of a homogeneous mixture of fuel/water mixture, the fuel fraction primarily remaining around 4% and with higher concentration towards the center of the geometry.

A NEW METHOD

Chabod's result on the reactor fuel mass optimization under a criticality constraint goes against the conventional knowledge in reactor physics that a heterogeneous fuel/moderator layout with low-enriched fuel will maximize reactivity using the smallest amount of fuel. The homogeneous result likely comes as a result of a lack of resolution of the spatial mesh. If the mesh were finer, perhaps the optimization would obtain the expected heterogeneous result. Refining the mesh could give far better heterogeneous results.

However, each iteration was tremendously expensive, requiring eleven hours per iteration using 150 generations of 50,000 fission neutrons on a 16 CPU machine. After testing a similar model without tallies in OpenMC [11], our results suggest that the PERT cards on a fine Cartesian mesh introduce a factor of roughly 1500 overhead compared to simulation without tallying, barring speed differences between each of our CPUs and respective Monte Carlo codes. The expense can perhaps be attributed to the enormous number of memory transactions required of the iterated fission probability method on a fine Cartesian mesh.

Consequently, to explore the enormous design space afforded by voxelized PDE-constrained optimization problems, we developed a workflow based on the characteristics-based neutronics code called MOCKingbird [12]. This comes with a few enormous advantages over Monte Carlo neutronics, with the tradeoff of introducing some modeling error of the transport physics. Firstly, because the design iteration is carried out iteratively, the previously obtained fluxes can be used as a starting guess in the next analysis iteration. In combination with CMFD acceleration, each analysis step over a space of the same dimensionality that Chabod used can be done orders of magnitude faster. Moreover, because the energy discretization is multigroup, implementing an adjoint flux solver is as easy as transposing two matrices. The latter point contrasts continuous energy Monte Carlo enormously. Optimization results from the fast deterministic optimization algorithm can be improved in continuous energy Monte Carlo codes down the line.

The issue of resonance shielding models deserve special attention here. Because the geometry is being varied arbitrarily, resonance shielding models conventionally made for homogenizing shielded cross sections over fuel lumps are not necessarily the best choice: how should one define a lump in this paradigm? At the moment, we simply generate multi-group cross sections on a reference geometry in OpenMC. This assumes a constant state of resonance shielding despite potentially enormous variation in the geometry. While clearly this is incorrect, future research could employ geometry-independent resonance self shielding models. Nonetheless, we are able to experiment with our optimization algorithm regardless of our rather crude assumption.

Thus, we consider the following spatially and angularly

continuous, discrete energy optimization problem in spatial domain $V \subset \mathbb{R}^m$ with $m \in \{1, 2, 3\}$, BCs a mix of reflecting and vacuum. We only optimize k_{eff} but the algorithms here can extend to more interesting objective functions.

$$\begin{aligned} \max_{\alpha(r) \in A} \quad & k_{\text{eff}} \\ \text{s.t.} \quad & \hat{\Omega} \cdot \nabla \varphi + \Sigma_t(\alpha(r))\varphi = \\ & \frac{1}{4\pi} \Sigma_s(\alpha(r))\phi + \frac{1}{4\pi k_{\text{eff}}} \chi \otimes \nu \Sigma_f(\alpha(r))\phi \end{aligned} \quad (1)$$

A is the space of functions taking on the value 0 or 1 throughout the volume V . The cross section symbols take on the meanings described in [12]. The angular flux φ is a g -dimensional column vector, where g is the number of groups; it is a function of the position on the unit sphere $\hat{\Omega}$ and spatial location $r \in \mathbb{R}^m$. The cross sections are $g \times g$ matrices which multiply the scalar flux (even Σ_t is to be interpreted as a diagonal matrix), and $\phi = \int_{4\pi} \varphi|_{\hat{\Omega}} d\hat{\Omega}$, a length g column vector which is a function of r . The cross sections are defined as a function of $\alpha(r)$:

$$\Sigma_x(\alpha) = \Sigma_{x,\text{graphite}}(1 - \alpha) + \Sigma_{x,\text{fuel}}\alpha \quad (2)$$

We base our algorithm off of the classic reactivity perturbation formula from any reactor physics textbook:

$$\Delta\rho \approx \frac{\int_V \phi^* \cdot \left(\frac{1}{k_{\text{eff}}} \delta(\chi \otimes \nu \Sigma_f) - \delta \Sigma_t + \delta \Sigma_s \right) \phi}{\int_V \phi^* \cdot \frac{1}{k_{\text{eff}}} \chi \otimes \Sigma_f \phi} \quad (3)$$

Where $\phi^* = \int_{4\pi} \varphi^*|_{\hat{\Omega}} d\hat{\Omega}$, and φ^* solves the associated adjoint eigenproblem:

$$-\hat{\Omega} \cdot \nabla \varphi^* + \Sigma_t(\alpha(r))\varphi^* = \frac{1}{4\pi} \Sigma_s(\alpha(r))^T \varphi^* + \frac{1}{4\pi k_{\text{eff}}} \nu \Sigma_f(\alpha(r)) \otimes \chi \varphi^* \quad (4)$$

The question then is how to maximize ρ , equivalently k_{eff} . To find the optimal perturbation of fixed size, find the function $I(r) \in A$ (the previously defined function space) which solves this associated optimization problem:

$$\begin{aligned} \max_{I(r) \in A} \quad & \int_V I(r) \Delta\rho_{\text{flipflop}}(r) \\ \text{s.t.} \quad & \int_V I(r) = a \end{aligned} \quad (5)$$

with $\Delta\rho_{\text{flipflop}}(r)$ defined as:

$$\Delta\rho_{\text{flipflop}}(r) = \frac{\phi^* \cdot \delta T(\alpha(r))\phi}{\int_V \phi^* \cdot \frac{1}{k_{\text{eff}}} \chi \otimes \Sigma_f \phi} \quad (6)$$

$a \in \mathbb{R}^+$ is a parameter chosen ahead of time: the volume of space to flip materials within. If a is small, the prediction of the adjoint expression will be accurate. This resembles limiting the step size of an infinite dimensional gradient ascent method. The spatially varying matrix $\delta T(\alpha(r))$ is:

$$\begin{aligned} \delta T(\alpha(r)) = \frac{1}{k_{\text{eff}}} & \left(\chi \otimes \nu \Sigma_f(1 - \alpha(r)) - \chi \otimes \nu \Sigma_f(\alpha(r)) \right) - \\ & \Sigma_t(1 - \alpha(r)) + \Sigma_t(\alpha(r)) + \Sigma_s(1 - \alpha(r)) - \Sigma_s(\alpha(r)) \end{aligned} \quad (7)$$

So, note as a consequence that if we are iterating on the function $\alpha(r)^{(n)}$ with the rule:

$$\alpha(r)^{(n+1)} = (1 - \alpha(r)^{(n)})I(r) + (1 - I(r))\alpha(r)^{(n)} \quad (8)$$

Then

$$\rho^{(n+1)} \approx \rho^{(n)} + \int_V I(r) \Delta \rho_{\text{flipflop}}(r) \quad (9)$$

All of this can be put together to Algorithm 1 to find a locally optimal solution to Eq. 1.

Algorithm 1 Maximizes k_{eff}

```

User inputs  $\alpha(r)$  guess
 $\phi \leftarrow 1$ 
 $\phi^* \leftarrow 1$ 
 $k_{\text{eff}} \leftarrow 1$ 
while  $k_{\text{eff}}$  increasing do
  Update  $k_{\text{eff}}, \phi$  by solving Problem 1 constraint
  Update  $\phi^*$  by solving Eq. 4
  Calculate  $\Delta \rho_{\text{flipflop}}$  from Eq. 6
  Solve Problem 5 for  $I(r)$ 
   $\alpha(r) \leftarrow (1 - \alpha(r))I(r) + (1 - I(r))\alpha(r)$ 
end while

```

RESULTS

We generated 33 group isotropic scattering group constants with transport corrections applied using OpenMC [11] on a natural enrichment UO_2 pin cell embedded in graphite with a density of 1.8 g/cm^3 and 2 ppm natural boron impurity. The group constants have been uploaded to `ridleygav.in/groupconstants.json` for others to use. The $\alpha(r)$ and $I(r)$ functions are discretized into piecewise constant functions on the same mesh as the flat source mesh. We employ 32 azimuthal angles with a standard TY-3 polar quadrature set, and a ray spacing equal to the mesh cell size divided by 2.5.

Reflective Unit Cell

In an infinite square lattice of 5 cm pitch, the optimal pin radius was first found. From there, the area of the pin was divided into three smaller pins of equal area such that total fuel area was conserved. The smaller pins were placed at the coordinates $(-.707, .707)$, $(.707, .707)$, $(-1, 0)$. This geometry was approximated on a 100×100 piecewise constant mesh. Fig. 1 shows how the shape and k_{eff} evolved over iterations. As is commonly known in reactor physics, the lumping of low enriched fuel enhances reactivity, which the algorithm is seen to successfully replicate. Despite assuming the resonance shielding state to be constant by using the same group constants globally, capture in resonance groups still contribute less to the chain reaction.

Graphite Pile

This example with vacuum boundary conditions yields a more interesting result. We use a geometry reminiscent of the MIT graphite pile to kick off the optimization. A 12×12 centered pin lattice is laid down on a 200×200 cm graphite square.

This is approximated with voxels on a 200×200 mesh. Fig. 2 shows how the design and k_{eff} changes over the iterations. The algorithm finds a fixed point around step 400. Because the fast neutron cross section in the fuel is about 4x as large as in the graphite, it decided to place fuel near the outer boundary of the pile in order to reflect leaking fast neutrons back to the core. Moreover, this largely prevents the leakage of thermal neutrons. It also removed the outer layer of pins to create an 11×11 lattice in order to thermalize outgoing fast neutrons. With constraints on fuel volume added in, an even more interesting solution could be obtained since this use of fuel on the boundary is clearly wasteful.

CONCLUSION

We present the first published use of a deterministic neutronics tool in topological optimization to solve the reactor material layout problem that maximizes k_{eff} . While the discretization method we employ has known flaws, it stands as a starting point for further application and improvement of deterministic topological optimization methods in neutronics. Future directions include use of more complicated objective functions, multi-objective optimization methods which sweep the Pareto front, and advanced optimization algorithms. PDE-constrained optimization coupled to other physics such as heat conduction or fluid flow is another direction to advance this field of research.

ACKNOWLEDGMENTS

The first author is supported by a Department of Energy University Nuclear Leadership Program Graduate Fellowship. This research made use of Idaho National Laboratory computing resources which are supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517. We thank Logan Harbour of Texas A&M for his invaluable assistance in MOOSE usage.

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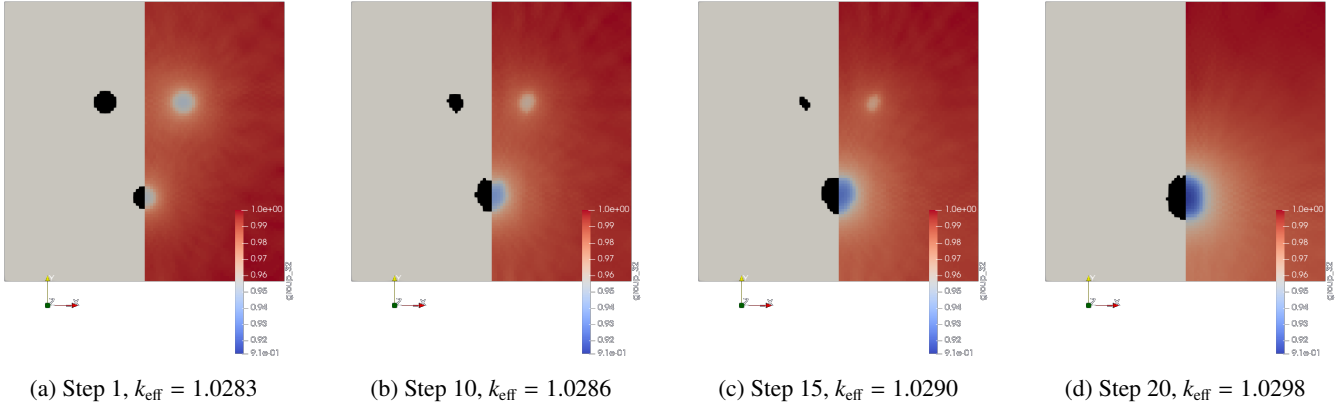


Fig. 1: Evolution of triple-pin unit cell problem $\alpha(r)$ value and thermal (group 32) flux

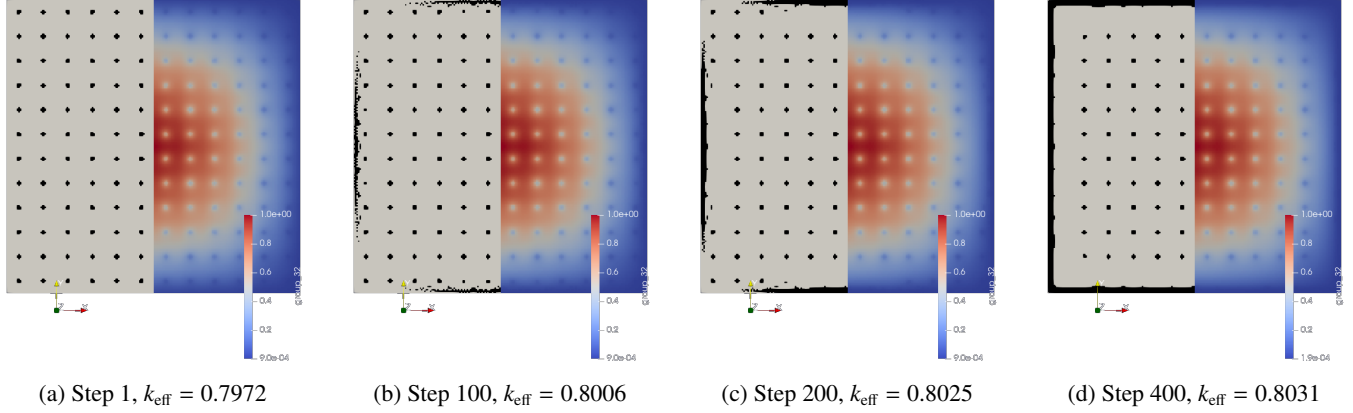


Fig. 2: Evolution of graphite pile problem $\alpha(r)$ values and thermal (group 32) flux

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