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# Chapter 1

# Introduction

## 1.1 Motivation

The impact of climate change on natural and human systems caused by elevated Greenhouse Gas (GHG) concentrations is increasingly apparent by increases in global average surface temperatures, sea levels, and severe weather events [1]. Energy use and production contribute to two-thirds of total GHG emissions [1]. Furthermore, as the human population increases and previously underdeveloped nations rapidly urbanize, global energy demand will continue to rise. Because energy generation technology selection profoundly impacts climate change, large scale deployment of emissions-free nuclear power plants could significantly reduce GHG production, but faces challenges of cost and safety [1, 2]. The nuclear power industry must overcome these challenges to ensure continued global use and expansion of nuclear energy technology to provide low-carbon electricity worldwide. To enhance the role of nuclear energy in our global energy ecosystem, the Generation IV International Forum was created to lead and plan research and development to support a new and innovative Generation IV of nuclear energy systems [3]. Generation IV nuclear systems' goals are defined in four areas: sustainability, economics, safety and reliability, and proliferation resistance and physical protection [3]. Table 1.1 summarizes the goals in each area.

The Generation IV International Forum's methodology working groups developed an evaluation and selection methodology based on these goals, culminating in selecting six Generation IV systems: Gas-Cooled Fast Reactor System (GFR), Lead-Cooled Fast Reactor (LFR), Molten Salt Reactor (MSR), Sodium-Cooled Fast Reactor (SFR), Supercritical-Water-Cooled Reactor System (SCWR), and Very-High-Temperature Reactor System (VHTR) [3]. This proposed work will consider the MSR and VHTR systems. The MSR system produces fission power in a circulating molten salt fuel mixture. It has a closed fuel cycle tailored to the efficient utilization of plutonium and

Table 1.1: Goals of Generation IV Nuclear Systems [3, 4]

| **Area** | **Goals** |
|---|---|
| Sustainability | - Have a positive impact on the environment through the displacement of polluting energy and transportation sources by nuclear electricity generation and nuclear-produced hydrogen<br>- Promote long-term availability of nuclear fuel<br>- Minimize volume, lifetime, and toxicity of nuclear waste |
| Economics | - Have a life cycle and energy production cost advantage over other energy sources<br>- Reduce economic risk to nuclear projects by developing plants using innovative fabrication and construction techniques |
| Safety and Reliability | - Increase the use of robust designs, and inherent and transparent safety features that can be understood by non-experts<br>- Enhance public confidence in the safety of nuclear energy |
| Proliferation Resistance and Physical Protection | - Provide continued effective proliferation resistance of nuclear energy systems through improved design features and other measures<br>- Increase the robustness of new facilities |

minor actinides. Molten fluoride salts have very low vapor pressure, which reduces stress on the system. MSR systems also have inherent system safety due to fail-safe drainage, passive cooling, and a low inventory of volatile fission products in the fuel. The MSR system is top-ranked in sustainability because of its closed fuel cycle and excellent waste burndown performance. It rates good in safety and proliferation resistance and physical protection, due to its inherent safety features, and rates neutrally in economics because of its large number of subsystems [3]. The VHTR system has a once-through uranium cycle and is primarily aimed at high-temperature heat applications, such as hydrogen production. It is a graphite-moderated, helium-cooled reactor that uses Tristructural Isotropic (TRISO) fuel, which does not degrade at high burnup and temperature. The VHTR system is highly ranked in economics because of its high hydrogen production efficiency, high safety and reliability, and inherent safety features of the fuel and reactor. It rates well in proliferation resistance and physical protection and neutrally in sustainability because of its open fuel cycle [3].

In the proposed work, we explore the Fluoride-Salt-Cooled High-Temperature Reactor (FHR) concept, which is a combination of the best aspects of MSR and VHTR technologies. The FHR uses high-temperature coated-particle fuel (similar to the VHTR) and a low-pressure liquid fluoride-salt coolant (similar to the MSR) [5, 6].

In recent years, Additive Manufacturing (AM) technology, popularly known as ‘3D printing’, has advanced and altered the manufacturing and design of components [7]. The automotive and aircraft industries have successfully fabricated parts with key AM technologies relevant to nuclear reactor core structures [8]. For example, Boeing successfully used AM to reduce weight in the 787 Dreamliner [9] and SES-15 spacecraft [10]. Successful AM applications in the aerospace industry are promising for the nuclear industry since both are highly regulated. Using AM to fabricate nuclear reactor components will drastically reduce cost and timelines, and increase safety and performance by tailoring local material properties and redesigning geometries for optimal load paths [7].

With further advancement of AM technologies, a reactor core could be 3D printed in the near future. Oak Ridge National Laboratory (ORNL) is leading this initiative through the 2019 Transformational Challenge Reactor (TCR) Demonstration Program. The TCR program will leverage recent scientific achievements in advanced manufacturing, nuclear materials, machine learning, and computational modeling and simulation to build a microreactor. The program aims to design, manufacture, and operate a demonstration reactor by 2023 [11]. Applying AM to nuclear reactor design will free complex reactor geometries from previous manufacturing constraints, opening the door for a re-examination of nuclear reactor optimization [12]. Optimization efforts towards classically manufactured nuclear reactors, and now 3D printed nuclear reactors, have focused on parameters such as radius of the core, height of cylinder, enrichment of fuel, etc [12, 13, 14, 15]. Leveraging AM technology enables us to surpass classical manufacturing constraints, such as straight fuel channels or homogenous fuel enrichment, and optimize for arbitrary geometries and parameters such as non-uniform channel shapes, and inhomogeneous fuel distribution throughout the core.

Multi-objective design problems inevitably require a trade-off between desirable attributes [16, 17]. In nuclear reactor design, one example is the trade-off between neutron economy and fuel enrichment. A reactor design must have sufficient neutron economy to ensure criticality but also have a low fuel enrichment to reduce proliferation risk. Conflicting objectives means that there is no *one* perfect solution but a *set* of equally optimal solutions [16]. Multi-objective problems are challenging to optimize; therefore, they cannot be handled by classical optimization methods, such as gradient methods, because only the local optimum will be found [18]. Evolutionary algorithms (EAs) have proven successful methods to optimize multi-objective problems [19], as they can find a solution near the global optimum [18]. They also take advantage of parallel systems for reduced computational cost. The most popular EAs used to solve multi-objective problems are genetic algorithms [16, 19], which imitate natural selection to evolve solutions by (1) maintaining a population of solutions, (2) allowing fitter solutions to reproduce, and (3) letting lesser fit solutions die off, resulting in final solutions that are better than the previous generations [18].

Therefore, in this work, we propose designing an optimization tool that uses the EA optimization technique with nuclear transport and thermal-hydraulics software. This tool will be used to explore nonuniform FHR reactor core parameters, now possible with AM technology, to optimize reactor systems fully.

## 1.2 Objectives

We developed the proposed work's main objectives based on leveraging open-source artificial intelligence tools with validated open-source nuclear transport and thermal-hydraulics software to create an open-source tool which generates optimal reactor designs quickly. Accordingly, the objectives are listed below:

**Model the FHR with established nuclear transport and thermal-hydraulics software**. To demonstrate success in modeling the FHR with nuclear transport and thermal-hydraulics software before using the optimization tool, we will participate in the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA)'s FHR benchmark [20].

**Develop a tool that applies evolutionary algorithms to optimize nuclear reactor design**. This tool will not reinvent the wheel—it will utilize a well-documented and validated open-source EA Python package with established nuclear transport and thermal-hydraulics software. This tool will run parallel on high-performance computing (HPC) machines, be open-source, and follow the rules for ensuring reproducibility, effectiveness, and usability [21, 22, 23].

**Optimize a nuclear reactor design with the optimization tool and a neutronics software**. We will demonstrate successful implementation of the optimization tool with a nuclear transport software by optimizing a simple FHR model for a single objective function.

**Tune hyperparameters with the optimization tool for a neutronics problem**. Hyperparameter selection will impact the effectiveness of the algorithm for our problem. Therefore, we must conduct a hyperparameter search to find ones that work best for our problem.

**Demonstrate nuclear reactor design optimization and hyperparameter search with the optimization tool for a neutronics and thermal-hydraulics problem**. We will demonstrate successful implementation of the optimization tool and hyperparameter tuning with the nuclear transport and thermal-hydraulics tools for a FHR model.

## 1.3 Outline

This document outlines the motivation, preliminary work, and future work proposed towards developing an open-source optimization tool that applies evolutionary algorithms to nuclear transport and thermal-hydraulics software to optimize nuclear reactor design beyond classical parameters to enhance fuel performance and safety further. Chapter 1 describes the motivation and objectives of the proposed work. Chapter 2 will present a literature review that organizes and reports on previous relevant work. Chapter 3 will describe the FHR benchmark specifications and the results obtained thus far. Chapter 4 will detail the computational design of the developed optimization tool. Chapter 5 will demonstrate nuclear reactor optimization with the optimization tool. Chapter 6 will summarize the remaining future work.

# Chapter 2

# Literature Review

This chapter provides a literature review of relevant past research efforts that give context to this proposed work. Recent advancements in AM applications for nuclear reactor core components has removed traditional manufacturing constraints on reactor design, enabling reactor designers to reexamine optimization. In the proposed work, we aim to apply evolutionary algorithm methods to explore non-conventional reactor geometries and fuel distributions, to apply a fresh perspective to nuclear reactor optimization. With growing interest in the nuclear science community and benefits of the FHR, we chose to apply the optimization methods to this reactor type, and also participate in the OECD NEA's FHR benchmarking exercise. Thus, we begin this literature review with an overview of the FHR concept, then go into detail about one specific FHR design: the Advanced High Temperature Reactor (AHTR), previous efforts and technical challenges of modeling the design, and a description of how these efforts led to the OECD NEA's initiation of the AHTR benchmark. Next, we outline AM history and describe the current research towards applying AM to the fabrication of nuclear reactor core components. We also review previous efforts towards nuclear reactor design optimization, describe how AM of nuclear reactor components enables optimization for less constrained reactor geometries, and types of optimization methods that can be leveraged in a large less-constrained design space, such as EAs. Finally, we give a background of EAs, go into detail on a specific EA: the Genetic Algorithm (GA), and how it works to robustly conduct global optimization.

## 2.1 Fluoride-Salt-Cooled High-Temperature Reactor

The FHR is a reactor concept introduced in 2012 that uses high-temperature coated-particle fuel and a low-pressure liquid fluoride-salt coolant [5, 6]. FHR technology combines the best aspects of MSR and VHTR (or High Temperature Gas-Cooled Reactor (HTGR)) technologies. Molten fluoride salts as working fluids for nuclear reactors have been explored since the 1960s and are desirable because of their high-temperature performance and overall chemical stability [24]. Using molten salts for reactor coolant introduces inherent safety compared to water due to the salts' high boiling temperature and high volumetric heat capacity. This eliminates the risk of coolant boiling off, resulting in fuel elements overheating [25]. The leading candidate coolant salt is the fluoride salt $Li_2BeF_4$ (FLiBe), which remains liquid without pressurization up to 1400 °C and has a larger heat capacity than water [25, 5]. FHRs are favorable compared to liquid fuelled reactors, such as MSR systems, because the TRISO particles' solid fuel cladding adds an extra barrier to fission product release [25].

VHTR technology has been studied since the 1970s because it delivers heat at substantially higher temperatures than Light Water Reactors (LWRs), resulting in the following advantages: increased power conversion efficiency, reduced waste heat generation, and co-generation and process heat capabilities [24]. In VHTRs, the helium coolant is held at a high pressure of approximately 100 atm, whereas the FHR's FLiBe coolant is at room pressure, resulting in lower construction costs since a thick concrete reactor vessel is not required. The molten salt coolant has superior cooling and moderating properties compared to helium coolant in VHTRs, resulting in FHRs operating at power densities two to six times higher than VHTRs [24, 5]. Therefore, by combining the FLiBE coolant from MSR technology and TRISO particles from VHTR technology, the FHR benefits from the low operating pressure and large thermal margin provided by using a molten salt coolant and the accident-tolerant qualities of TRISO particle fuel.

Several types of FHR conceptual designs exist worldwide: Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR) at University of California Berkeley (UCB) with circulating pebble-fuel [26, 27], the Solid Fuel Thorium Molten Salt Reactor (SF-TMSR) at the Shanghai Institute of Applied Physics (SINAP) in China with static pebble-fuel [28], the large central-station AHTR at ORNL [29, 30] and the Small Modular AHTR (SmAHTR) at ORNL [31] with static plate-fuel.

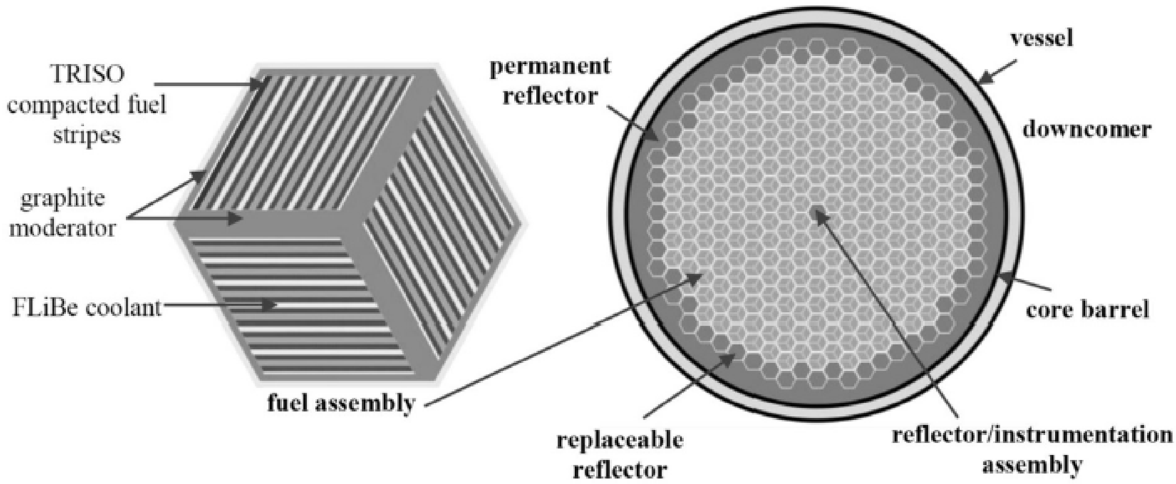


Figure 2.1: Advanced High Temperature Reactor fuel assembly (left) and core configuration (right) [32].

### 2.1.1 Advanced High Temperature Reactor Design

This proposed work focuses on the FHR design with hexagonal fuel assemblies consisting of TRISO fuel particles embedded in planks, i.e., the AHTR design developed by ORNL. The AHTR has 3400 MWt thermal power and 1400 MW electric power with inlet/outlet temperatures of 650/700°C [30]. Figure 2.1 shows the prismatic AHTR's fuel assembly and core configuration. Each hexagonal fuel element features plate-type fuel consisting of eighteen planks arranged in three diamond-shaped sectors, with a central Y-shaped structure and external channel (wrapper). Each fuel plank contains an isostatically pressed carbon with fuel stripes on each plank's outer side. The fuel stripes are prismatic regions composed of a graphite matrix filled with a cubic lattice of TRISO particles. The core consists of 252 assemblies radially surrounded by reflectors [32]. Chapter **??** details the specifications of the AHTR geometry modeled in this proposed work.

### 2.1.2 Previous AHTR modeling efforts and challenges

Modeling and simulation of the AHTR design have been an ongoing effort since its conception in 2003 [33]. The AHTR core design differs significantly from the present LWR-based nuclear power plants. These differences lead to modeling challenges and the need to verify and validate modeling and simulation methods [32]. Verification and validation of neutronics and thermal-hydraulics tools' capability to successfully model the AHTR design are crucial steps in support of licensure

Table 2.1: Phenomena Identification and Ranking Table identified Advanced High Temperature Reactor physical phenomena requiring further research [34].

| **Category** | **Phenomena** |
|---|---|
| Fundamental cross section data | - Moderation in FliBe<br>- Thermalization in FliBe<br>- Absorption in FliBe<br>- Thermalization in carbon<br>- Absorption in carbon |
| Material Composition | - Fuel particle distribution |
| Computational Methodology | - Solution Convergence<br>- Granularity of depletion regions<br>- Multiple heterogeneity treatment for generating multigroup cross sections<br>- Selection of multigroup structure<br>- Boundary conditions for multigroup cross section generation |
| General Depletion | Spectral history |

of the AHTR design towards the eventual goal of deployment [34, 35]. Several neutronic studies conducted along the way to the current AHTR design have shed light on the technical challenges facing the design [32, 36, 31].

Georgia Institute of Technology (Georgia Tech) led an Integrated Research Project to understand challenges in AHTR materials and modeling its neutronics and thermal-hydraulics [37]. During the research project, a panel of subject matter experts generated a Phenomena Identification and Ranking Table (PIRT). The PIRT identifies areas that need additional research to better understand important phenomena for adequate future modeling [34]. Table 2.1 lists the phenomena identified as requiring further research.

The AHTR has a complex core design due to the multiple heterogeneity present in the fuel introduced by TRISO particles' presence embedded in planks [32, 34]. We must obtain detailed reference power distributions to assess lower-fidelity models' accuracy, thus, requiring accurate models of the AHTR's complex geometry with individual TRISO particle fidelity. However, it is challenging, particularly for deterministic codes that use multigroup cross sections and traditional homogenization methods [32], which are insufficient to capture the correct physics in AHTRs due to the multiple heterogeneity [32]. In the AHTR, single and multiple slab homogenization decreased computation time by an order of 10; however, they introduce a nontrivial error of ~3% [32, 38]. To determine the feasibility and safety of the AHTR design, we must calculate core physics parameters to an acceptable uncertainty. For Monte Carlo codes, increasing neutron histories reduces statistical uncertainty but comes at an increased computational cost, requiring the use of supercomputers to run the simulations.

Another technical challenge the AHTR design faces is the uncertainty of the graphite and carbonaceous moderator material properties: densities, temperatures, and thermal scattering data. Problematically, the thermal scattering data ($S(\alpha, \beta)$ matrices) for the bound nuclei in the Fluoride-Lithium-Beryllium (FLiBe) salt are lacking [32]. Mei et al. [39] and Zhu et al. [40] examined the thermal scattering behavior of solid and liquid FLiBe. They concluded that the bound and free atom cross section of FLiBe are identical above 0.1eV and diverges below 0.01eV, which means that the use or absence of thermal scattering data will impact the accuracy of the results [32].

### 2.1.3 AHTR Benchmark

To address and further understand the technical challenges described in the previous section, in 2019, the OECD-NEA initiated a benchmark to assess the modeling and simulation capabilities for the AHTRs with TRISO fuel embedded in fuel planks of hexagonal fuel elements [20]. The benchmark plans to have three phases, starting from a single fuel element simulation without burnup, gradually extending to full core depletion and feedback. The benchmark's overarching objective is to identify the applicability, accuracy, and practicality of the latest methods and codes to assess the current state of the art of FHR simulation and modeling [41]. The benchmark also enables the cross-verification of codes and methodologies for the challenging AHTR geometry, which is especially useful since applicable reactor physics experiments for code validation are scarce [42, 41]. Chapter **??** will provide a detailed description of the benchmark phases and results obtained so far.

## 2.2 Additive Manufacturing

Additive Manufacturing (AM) is the formalized term for what used to be called 'rapid prototyping' and what is popularly called '3D printing' [43]. The basic principle of AM is that a model is initially generated using a three-dimensional Computer-Aided Design (3D CAD) system and then fabricated directly without the need for process planning. In AM, the parts are made by adding materials in layers; each layer is a thin cross section of the 3D CAD designed part, as opposed to subtractive manufacturing methods such as traditional machining [44]. All commercialized AM machines to date use a layer-based approach, and the major ways that they differ are in materials, layer creation method, and how the layers are bonded to each other [43]. These major differences will determine the following factors: accuracy of the final part, material and mechanical properties, the time required to manufacture the part, the need for post-processing, the size of AM machine, and the overall cost of the machine and the process [43]. Initially, AM was used to manufacture prototypes. However, with improvements in material properties, accuracy, and overall quality of AM output, the applications for AM expanded to the point at which some industries build parts for direct assembly purposes [45]. Furthermore, using AM in conjunction with other technologies, such as high-power lasers, has enabled AM to manufacture parts made from various metals [43].

### 2.2.1 Application of Additive Manufacturing to Nuclear Reactor Core Components

AM has progressed rapidly in the last 30 years, from rapid design prototyping with polymers in the automotive industry to scale production of metal components. Examples include Boeing using AM to reduce the 979 Dreamliner's weight [9] and General Electric using AM to produce fuel injection nozzles [46]. The most common metal AM technologies, selective laser melting (SLM), electron beam melting (EBM), laser directed energy deposition (L-DED), and binder jetting, are not currently used to manufacture nuclear power plant parts. Wide-spread adoption of these methods in the nuclear industry could drastically reduce fabrication costs and timelines, combine multiple systems and assembled components into single parts, increase safety and performance by tailoring local material properties, and enable geometry redesign for optimal load paths [7]. Many Generation IV advanced reactor concepts have complex geometries, such as hex-ducts for sodium-cooled fast reactors, that are costly and difficult to fabricate using standard processing techniques. Traditional manufacturing routes also restrict many viable geometries for reactor designers to explore [47]. In summary, the main benefits of using AM for reactor core components is that we are no longer geometrically constrained by conventional fuel manufacturing and can further optimize and improve fuel geometries to enhance fuel performance at lower costs [48].

Experimental work in the nuclear materials' field demonstrates the application of AM to nuclear fuel and structural core material fabrication. Rosales et al. [49] conducted a feasibility study of direct routes to fabricate dense uranium silicide ($U_3Si_2$) fuel pellets using the Idaho National Laboratory (INL) invented Additive Manufacturing as an Alternative Fabrication Technique (AMAFT). $U_3Si_2$ is an accident-tolerant nuclear fuel candidate due to its high uranium density and improved thermal properties. Its current metallurgical fabrication process is expensive and long; the goal of AMAFT is to fabricate $U_3Si_2$ at a lower cost in a timely and commercially-reliable manner [49]. Sridharan et al. [47] demonstrated the application of the laser-blown-powder AM process to fabricate ferritic/martensitic (FM) steel, a type of steel commonly used for cladding and structural components in nuclear reactors. Koyanagi et al. [50] presented the latest AM technology for manufacturing nuclear-grade silicon carbide (SiC) materials; they demonstrated that combinations of AM techniques and traditional SiC densification methods enabled new designs of SiC components with complex shapes. SiC has excellent strength at elevated temperatures, chemical inertness, relatively low neutron absorption, and stability under neutron irradiation up to high doses [51, 52, 50]. These qualities make SiC suitable for many applications in nuclear systems such as fuel cladding, constituents of fuel particles [52] and pellets [53], and core structural components in fission reactors [51]. Trammel et al [54] conducted a preliminary investigation to assess the possibilities of fabricating a fuel element with embedded TRISO fuel using AM techniques, such as binderjet printing and chemical vapor infiltration (CVI). They successfully demonstrated a fabrication method using the following steps (depicted in Figure 2.2):

1. A SiC fuel element structure is first printed with binderjet technology.

2. The designated fueled region of the element is loaded with surrogate TRISO particles and additional SiC powder to fill interstitial spaces between particles.

3. The loaded fuel element is densified in a CVI process to achieve microencapsulation of TRISO particles in a SiC matrix.

Many of the materials and fabrication methods discussed are applicable for FHR-part manufacturing. Therefore, this reiterates the possibility of leveraging AM to 3D print a FHR-type

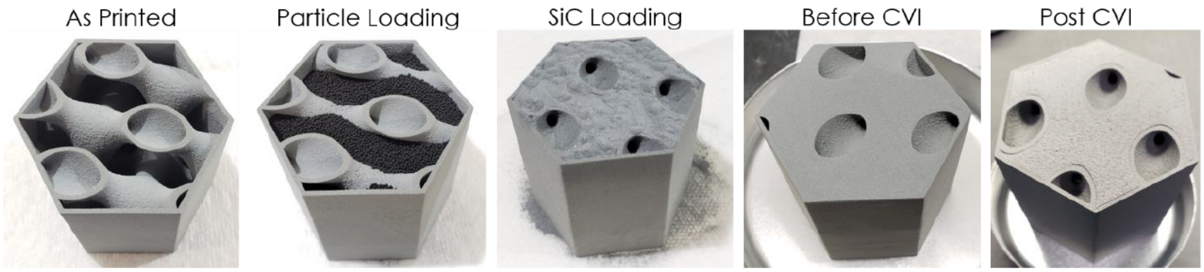


Figure 2.2: Stages of AM fabrication conducted at Oak Ridge National Laboratory to produce a fuel element with non-homogenously shaped coolant channels and TRISO particles embedded in a SiC matrix [54].

reactor with non-conventional geometry.

## 2.3 Nuclear Reactor Design Optimization

The practice of nuclear reactor optimization has been around since the conception of nuclear reactors. Optimization has been applied to many nuclear engineering sub-fields such as reactor design, reactor reloading patterns, and the nuclear fuel cycle. In the proposed work, we will focus on the reexamination of nuclear reactor core design optimization for arbitrary reactor geometries and fuel distributions. Previous efforts towards nuclear reactor core design optimization were limited by traditional manufacturing constraints and utilized deterministic and stochastic optimization techniques, coupled with surrogate models.

Deterministic optimization methods usually start from a guess solution. Then, the algorithm suggests a search direction by applying local information to a pre-specified transition rule. The best solution becomes the new solution, and the above procedure continues several times [55]. Drawbacks of deterministic methods include: algorithms tend to get stuck at a suboptimal solution, and an algorithm efficient in solving one type of problem may not solve a different problem efficiently [55]. Stochastic optimization methods, such as EAs amd simulated annealing, minimize or maximize an objective function when randomness is present; they tend to find globally optimal solutions more reliably than deterministic methods.

A nuclear reactor's complexity results in reactor design optimization being a multi-objective design problem requiring a tradeoff between desirable attributes [16, 17]. When multiple conflicting objectives are important, there is no single optimum solution that simultaneously optimizes all objectives. Instead, the multi-objective optimization problem's outcome is a set of optimal solutions with varying degree objective values [55]. For a multi-objective problem like reactor design optimization, an ideal multi-objective optimization method should find widely spread solutions in the obtained non-dominated front [55].

Recent efforts towards nuclear reactor optimization have relied heavily on the aforementioned stochastic methods, with the occasional addition of stochastic-deterministic hybrid methods. Sacco et al. [13, 56] used stochastic simulated annealing and deterministic-stochastic hybrid optimization techniques to optimize reactor dimensions, enrichment, materials, etc., in order to minimize the average peak factor in a three-enrichment-zone reactor. Odeh et al. [57] used the simulated annealing stochastic algorithm coupled with neutronics and thermal-hydraulics codes, Purdue Advanced Reactor Core Simulator (PARCS) and RELAP5 [58], to develop an optimum Purdue Novel Modular Reactor (NMR-50) core design to achieve a 10-year cycle length with minimal fissile loading. Kropaczek et al. [59] demonstrated the constraint annealing method: a highly scalable method based on the method of parallel simulated annealing with mixing of states [60] for the solution of large-scale, multiconstrained problems in LWR fuel cycle optimization. Peireira et al. [61, 15] used a coarse-grained parallel GA and a niching GA to optimize the same problem as Sacco et al. [13]. Kamalpour et al. [62] utilized the imperialist competitive algorithm, a type of EA, to optimize an fully ceramic microencapsulated (FCM) fuelled Pressurized Water Reactor (PWR) to extend the reactor core cycle length.

Nuclear reactor optimization problems require computationally extensive neutronics and thermal-hydraulics software to compute the objective function and constraints. Multiple papers utilized stochastic optimization methods with surrogate models to replace computationally expensive, high-fidelity neutronics or thermal hydraulics simulations to reduce computational cost. Kumar et al. [14] combined genetic algorithm optimization with a surrogate model to optimize for high breeding of $^{233}$U and $^{239}$Pu in desired power peaking limits and keff by varying these parameters: fuel pin radius, fissile material isotopic enrichment, coolant mass flow rate, and core inlet coolant temperature. Betzler et al. [63] developed a systematic approach to build a surrogate model to serve in place of high-fidelity computational analyses. They leveraged the surrogate model with a simulated annealing optimization algorithm to generate optimized designs at a lower computational cost to understand design decisions' impact on desired metrics for High Flux Isotope Reactor (HFIR) low-enriched uranium (LEU) core designs.

The Sensitivity Analysis (SA) method uses a point-by-point approach: one solution gets updated to a new solution in one iteration, which does not exploit parallel systems' advantages. Finding an optimal solution with SA methods takes very long if high-fidelity computationally expensive codes are used to compute the objective function and constraints. Therefore, using the SA method is only practical if a surrogate evaluation model is used as described in Betzler et al. [63] and Kumar et al. [14].

Contrary to a single solution per iteration in deterministic and stochastic SA methods, EAs use a population of solutions in each iteration [55]. EA methods mimic nature's evolutionary principles to drive its search towards an optimal solution. With the affordability and availability of parallel computing systems, the EA optimization method stands out as a method that easily and conveniently exploits parallel systems. Further, EAs have proved amenable to HPC solutions and scalable to tens of thousands of processors [60]. Therefore, in this proposed work, we will utilize the evolutionary algorithm optimization method.

### 2.3.1 Impact of Additive Manufacturing on Nuclear Reactor Design Optimization

Previous efforts towards nuclear reactor optimization, as discussed in the above section, focused on optimizing classical reactor parameters such as radius of fuel pellet and clad, enrichment of fuel, pin pitch, etc. With the advancements of AM for reactor core components, reactor designers are no longer geometrically constrained by conventional fuel manufacturing and can optimize beyond classical parameters to enhance fuel performance and safety further. Reactor design objectives remain consistent with past objectives, such as minimizing fuel amount and minimizing the maximum fuel temperature for a given power level. However, we can now approach the nuclear design problems with truly arbitrary geometries, no longer limited by traditional geometric shapes that are easy to manufacture with traditional processes: slabs as fuel planks, cylinders as fuel rods, spheres as fuel pebbles, axis-aligned coolant channels, etc [12]. This has opened the door for a re-examination of reactor core optimization in a complete new way, determining the optimal arbitrary geometry for a given objective function [12] with a much smaller set of constraints.

With a substantial increase and change in an arbitrary geometry's design space, it becomes time consuming for a human reactor designer to thoroughly explore and find optimal geometries in the expanded design space. Instead, we can leverage Artificial Intelligence (AI) optimization methods (such as EA) to promptly explore the large design space to find global optimal designs. AI would not replace the human reactor designer but shifts the human designer's focus away from conjecturing suitable geometries to defining design criteria to find optimal designs [12]. Thus, when the human designer changes the reactor criteria, the AI model will quickly adapt and produce new global optimal designs to fit the new criteria.

## 2.4 Evolutionary Algorithms

AI research is the study of 'intelligent agents': any device that perceives its environment and takes actions that maximize its chance of successfully achieving its goals [64]. Therefore, EAs are considered a subset of AI as they create a population of individual solutions, inspired by biological evolution, and induce goals by using a 'fitness function' to mutate and preferentially replicate high-scoring individuals to reach an optimal solution. EAs often perform well at approximating solutions to many problem types because they do not make any assumptions about the underlying fitness landscape. The most popular EAs used to solve multi-objective problems are GAs [16, 19].

### 2.4.1 Genetic Algorithms

GAs imitate natural genetics and selection to evolve solutions by maintaining a population of solutions, allowing fitter solutions to reproduce and letting lesser fit solutions die off, resulting in final solutions that are better than the previous generations [18]. From here, we will refer to a solution as an individual within the population. GAs efficiently exploit historical information to speculate new search points, improving each subsequent population's performance [65]. GAs are theoretically and empirically proven to provide robust search in complex spaces and are computationally simple yet powerful in their search for improvement [65]. GAs are advantageous compared to deterministic and stochastic simulated annealing optimization methods, because (1) it searches

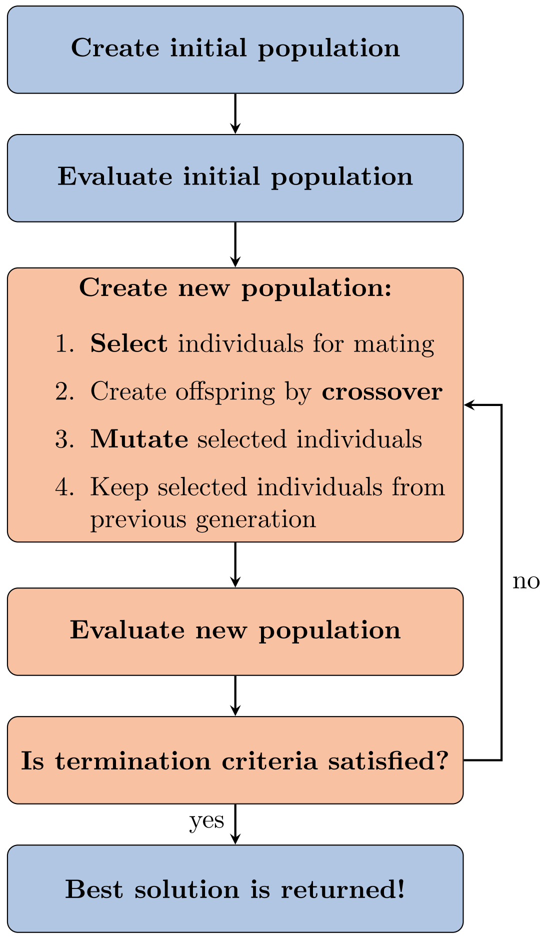


Figure 2.3: Process of finding optimal solutions for a problem with a genetic algorithm [18].

from a population of points; (2) uses objective function information, not derivatives or other auxiliary knowledge of the problem; and (3) uses probabilistic transition rules, not deterministic rules. Figure 2.3 depicts the iterative process of using a GA to solve a problem. The GA generates new populations iteratively until it meets the termination criteria.

GAs use mechanisms inspired by biological evolution such as selection, crossover, and mutation. The three operators are simple and straightforward. The selection operator selects good individuals. The crossover operator recombines good individuals to form a better individual. The mutation operator alters individuals to create better individuals [55]. Next, we provide more description and common methods for each operator.

### Selection Operator

The selection operator's primary objective is to duplicate good individuals and eliminate bad individuals while keeping the population constant [55]. It achieves this by identifying above-average individuals in a population, eliminating bad individuals from the population, and replacing them with copies of good individuals. Selection operator methods utilized in the proposed work include tournament selection, best selection, and NSGA-II selection. In tournament selection, tournaments are played between a user-defined number of individuals, and the best individual is kept in the population. This repeatedly occurs until all the population's spots are filled. In best selection, a user-defined number of best individuals are selected, and copies are made to keep the population size constant. In NSGA-II selection, parent and offspring populations are combined, and the best individuals (with respect to fitness and spread) are selected [66]. Again, copies of the best individuals are made to keep the population size constant.

The selection operator cannot create any new individuals in the population and only makes more copies of good individuals at the expense of not-so-good individuals. Instead, crossover and mutation operators perform the creation of new solutions.

### Crossover Operator

The crossover operator is also known as the mating operator. In most crossover operators, two individuals are picked from the population at random, and some portion of the individuals' attributes are exchanged with one another to create two new individuals [55]. Crossover operator methods utilized in the proposed work include single-point crossover, uniform crossover, and blend crossover. In the single-point crossover, two individuals are selected from the population, and a site along the individual's definition is randomly chosen. Attributes on this cross site's right side are exchanged between the two individuals, creating two new offspring individuals. In a uniform crossover, the user defines an independent probability for each individual's attribute to be exchanged; usually, $p = 0.5$ is used. In blend crossover, two offspring (O) individuals are created based on a linear combination of two-parent (P) individuals using the following equations:

$$O_1 = P_1 - \alpha(P_1 - P_2) \tag{2.1}$$

$$O_2 = P_2 + \alpha(P_1 - P_2) \tag{2.2}$$

where

$\alpha$ = Extent of the interval in which the new values can be drawn
for each attribute on both side of the parents attributes (user-defined)

To preserve some good individuals selected during the selection operator stage, not all individuals are used in a crossover; this is implemented by having the user define a crossover probability ($p_c$). Therefore, the crossover operator is only applied to $100p_c\%$ of the population; the rest are copied to the new population [55].

The crossover operator is mainly responsible for the search aspect of the GAs, whereas the mutation operator is needed to keep diversity in the population [55].

#### Mutation Operator

The mutation operator alters one or more attributes of an individual within a population. Mutation occurs in the GA based on a user-defined mutation probability ($p_m$) that is set low to prevent a primitive random search. Mutation operator methods utilized in the proposed work include polynomial bounded mutation, in which each attribute in each individual is mutated based on a polynomial distribution. The user also defines each attribute's upper and lower bounds and the crowding-degree of the mutation, $\eta$ (a large $\eta$ will produce a mutant resembling its parent, while a small $\eta$ will produce the opposite).

### 2.4.2 Balancing Genetic Algorithm Hyperparameters

In the proposed work, hyperparameters refer to parameters whose value controls the GA's process, such as each genetic operator's associated parameters and population size. A well-performing GA

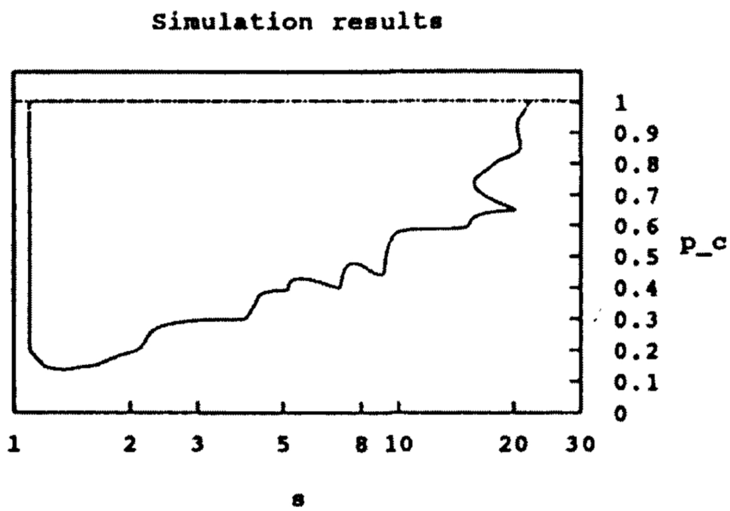


Figure 2.4: Control map region of selection pressure (s) and crossover probability ($p_c$) values in which the genetic algorithm will find the desired optimum for the one-max problem [67, 55].

needs to balance the extent of exploration and exploitation; this is done by finding a balance between the conservation of valuable individuals obtained until the current generation while exploring new individuals. If previously obtained individuals are exploited too much, the population loses its diversity, and premature convergence to a suboptimal solution is expected. Alternatively, if too much stress is given on exploration, the information obtained thus far has not been appropriately utilized, and the GA's search procedure behaves like a random search process [55]. A quantitative balance between these two issues, exploitation and exploration, is challenging to achieve. Deb et al. [55] and Goldberg et al. [67] quantified the relationship between exploitation and exploration. They found that for the one-max test problem, in which the objective is to maximize the number of 1s in a string, a GA with any arbitrary hyperparameter setting does not work well even on a simple problem. Only GAs with a selection pressure (s) and crossover probability ($p_c$) falling inside the control map (Figure 2.4) will find the desired optimum. Another consideration is the population size. A function with considerable variability in objective function values demands a large population size to find a global optimum [55].

Therefore, finding an optimized solution with GAs requires the user to conduct a hyperparameter search. Ng et al. [68] suggest that a coarse to fine sampling scheme is the best way to perform a systematic hyperparameter search. For a two-dimensional example of a coarse to fine sampling scheme, the user first does a coarse sample of the entire square. A fine search is then conducted on the best-performing region of the coarse search.

## 2.5 Summary

This chapter provided a literature review of relevant past research efforts that give context to this proposed work. In summary, additive manufacturing of nuclear reactor components is a quickly developing field thanks to the aerospace and auto industries, which led to breakthroughs in AM fabrication of metal components. The promise of cheaper and faster manufacturing of reactor components with AM frees complex reactor geometries from previous manufacturing constraints and allows reactor designers to reexamine reactor design optimization. Stochastic optimization methods such as evolutionary algorithms have proven to work well for finding global optimums in multi-objective design problems such as nuclear reactor optimization and can be leveraged to explore the vast exploration design space enabled by AM.

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