Chapter 1

Literature Review

This chapter provides a literature review of relevant past research efforts that give context to this proposed work. We begin with an overview of the Fluoride-Salt-Cooled High-Temperature Reactor (FHR) concept, then go into detail about the specific Advanced High Temperature Reactor (AHTR) design, previous efforts towards modeling the design and technical challenges, and a description of how these efforts led to the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA) initiation of the AHTR benchmark. Next, we outline Additive Manufacturing (AM) history and describe the current research towards applying AM to the fabrication of nuclear reactor core components. Next, we review previous efforts towards nuclear reactor design optimization and describe the impact of AM advancements on reactor design optimization. Finally, we give a background of evolutionary algorithms and their applications for optimizing reactor designs constructed with additive manufacturing technology.

1.1 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 [1, 2]. FHR technology combines the best aspects of Molten Salt Reactor (MSR) and Very-High-Temperature Reactor System (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 [3]. Using molten salts for reactor coolant introduces inherent safety compared to water due to the salts' high boiling temperature and high volumetric heat capacity, eliminating the risk of coolant boiling off, resulting in fuel elements overheating [4]. The leading candidate coolant salt is the fluoride salt Li_2BeF_4 (FLiBe), which

remains liquid without pressurization up to 1400 °C and a larger ρC_p than water [4, 1]. FHRs are favorable compared to a liquid fuel reactor, such as MSR systems, because the solid fuel cladding adds an extra barrier to fission product release [4].

VHTR technology has been studied since the 1970s because it delivers heat at substantially high 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 [3]. 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 [3, 1]. Therefore, by combining the FLiBE coolant from MSR technology and Tristructural Isotropic (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 UCB with circulating pebble-fuel [5, 6], the Solid Fuel Thorium Molten Salt Reactor (SF-TMSR) at the Shanghai Institute of Applied Physics (SINAP) in China with static pebble-fuel [7], the large central-station AHTR at Oak Ridge National Laboratory (ORNL) [8, 9] and the Small Modular AHTR (SmAHTR) at ORNL [10] with static plate-fuel.

1.1.1 AHTR design

This proposed work focuses on the FHR design with hexagonal fuel elements consisting of TRISO fuel particles embedded in plates ("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 $650/700°C$ [9]. Figure 1.1 shows the prismatic AHTR's fuel element and core configuration. Each hexagonal fuel element features plate-type fuel consisting of eighteen plates 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

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particles. The core consists of 252 assemblies radially surrounded by reflectors [11]. Chapter **??** details the specifications of the AHTR geometry modeled in this proposed work.
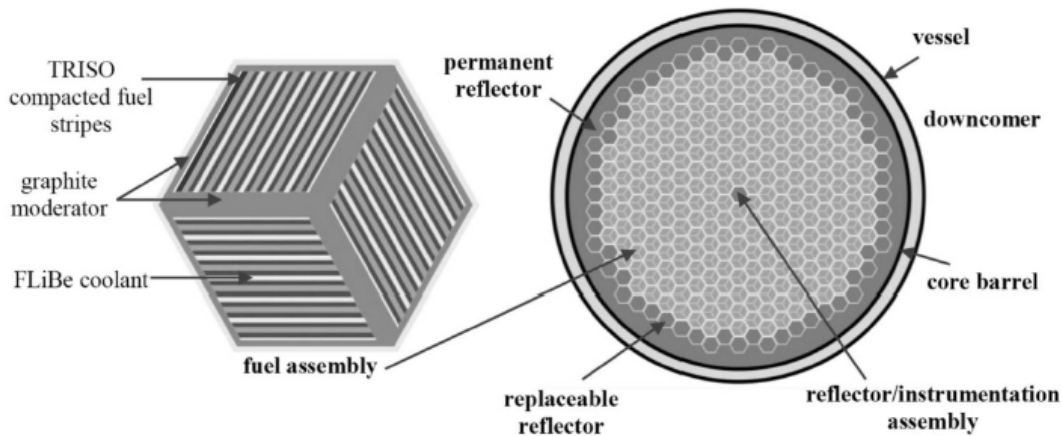

Figure 1.1: FHR core configuration and fuel element [11].

1.1.2 Previous AHTR modeling efforts and challenges

Modeling and simulation of the AHTR design have been an ongoing effort since its conception in 2003 [12]. 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 [11]. Verification and validation of neutronics and thermal-hydraulics tools' capability to successfully model the AHTR design is a crucial step in support of licensure of the AHTR design towards the eventual goal of deployment [13, 14]. Several neutronic studies conducted along the way to the current AHTR design have shed light on the technical challenges facing the design [11, 15, 10].

Georgia Institute of Technology led an Integrated Research Project to understand challenges in FHR materials and modeling the neutronics and thermal-hydraulics in both plate and pebble fuelled FHRs [16]. During the research project, a panel of subject matter experts came together to generate a Phenomena Identification and Ranking Table (PIRT) by identifying phenomena and ranking their importance. The PIRT identifies areas that need additional research to better understand important phenomena for adequate future modeling [13]. Table 1.1 lists the phenomena identified as requiring further research.

The AHTR has a complex core design due to the multiple heterogeneity present in the fuel

Table 1.1: PIRT identified FHR physical phenomena requiring further research [13].

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

introduced by TRISO particles' presence embedded in plates [11, 13]. Accurately modeling the FHR's complex geometry with individual TRISO particle fidelity is necessary to obtain detailed reference power distributions to assess lower-fidelity models' accuracy. However, it is challenging, particularly for deterministic codes that use multigroup cross sections and traditional homogenization methods [11]. These traditional homogenization methods are insufficient to capture the correct physics in FHRs due to the multiple heterogeneity [11]. In the AHTR, single and multiple slab homogenization decreased computation time by 10; however they introduce a nontrivial error of ~3% [11, 17]. 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.

Another technical challenge the AHTR design faces is the uncertainty of the graphite and carbonaceous moderator material properties: densities, temperatures, and thermal scattering data. Also, the thermal scattering data ($S(\alpha, \beta)$ matrices) for the bound nuclei in the Fluoride-Lithium-Beryllium (FLiBe) salt are lacking [11]. Mei et al. [18] and Zhu et al. [19] 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 [11].

1.1.3 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 state of the art modeling and simulation capabilities for FHRs with TRISO fuel embedded in fuel plates ("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 current methods and codes to assess the current state of the art of FHR simulation and modeling [21]. 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 [22, 21]. Chapter ?? will provide a detailed description of the benchmark phases and results obtained so far.

1.2 Additive Manufacturing

AM is the formalized termed for what used to be called rapid prototyping and what is popularly called 3D printing [23]. The basic principle of AM is that a model is initially generated using a three-dimensional Computer-Aided Design (3D CAD) system and is 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 [24]. 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 [23]. 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, size of AM machine, and overall cost of the machine and the process [23]. 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 current point in which some industries build parts for direct assembly purposes [25]. Furthermore, using AM in conjunction with other technologies, such as high-power laser technology, has enabled

AM ~~technology~~ to manufacture parts made from various metals [23].

1.2.1 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 [26] and General Electric using AM to produce fuel injection nozzles [27]. 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 [28]. 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 the viable geometries for reactor designers [29]. 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 and safety ~~with the added benefit of~~ lower cost [30].

Experimental work in the nuclear materials field demonstrates the application of AM to nuclear fuel and structural core material fabrication. Bergeron et al. [30] successfully demonstrated additively manufacturing thorium dioxide using a stereolithography-based 3D printer and photopolymer resin. The high-density thorium dioxide objects were printed and sintered to densities of ~ 90% [30]. Rosales et al. [31] 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 [31]. Sridharan et al. [29] demonstrated

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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. [32] presented AM technology's current status 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 [33, 34, 32]. These qualities make SiC suitable for many applications in nuclear systems such as fuel cladding, constituents of fuel particles [34] and pellets [35], core structural components in fission reactors [33].

1.3 Nuclear Reactor Design Optimization

The practice of nuclear reactor optimization has been around since the conception of nuclear reactors. Optimization has been applied to nuclear reactor design, reactor reloading patterns, and the nuclear fuel cycle. In the proposed work, we will focus on the optimization of nuclear reactor core design. Previous efforts towards nuclear reactor core design optimization include deterministic and stochastic optimization techniques and these optimization methods coupled with surrogate models.

Deterministic optimization methods usually start from a guess solution; then, the algorithm suggests a search direction based on applying local information to a pre-specified transition rule. The best solution becomes the new solution, and the above procedure continues several times [36]. Drawbacks of deterministic methods include: algorithms tend to get stuck to a suboptimal solution, and an algorithm efficient in solving one type of problem may not solve a different problem efficiently [36]. Stochastic optimization methods minimize or maximize an objective function when randomness is present; they tend to find globally optimal solutions more reliably than deterministic methods. Evolutionary algorithms and simulated annealing are examples of stochastic optimization algorithms.

A nuclear reactor's complexity results in reactor design optimization being a multi-objective design problem requiring a tradeoff between desirable attributes [37, 38]. 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 solu-

tions with varying degree objective values [36]. 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 [36].

Recent efforts towards nuclear reactor optimization have relied heavily on stochastic methods such as simulated annealing and evolutionary algorithms, with the occasional addition of stochastic-deterministic hybrid methods. Sacco et al. [39, 40] 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. [41] used the simulated annealing stochastic algorithm coupled with neutronics and thermal-hydraulics codes, Purdue Advanced Reactor Core Simulator (PARCS) and RELAP5, 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. [42] demonstrated the constraint annealing method, a highly scalable method based on the method of parallel simulated annealing with mixing of states [43] for the solution of large-scale, multiconstrained problems in LWR fuel cycle optimization. Peireira et al. [44, 45] used a coarse-grained parallel Genetic Algorithm (GA) and a niching GA to optimize the same problem as [39]. Kamalpour et al. [46] utilized the imperialist competitive algorithm, a type of evolutionary algorithm, 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 optimization methods with surrogate models to replace computationally expensive high fidelity neutronics or thermal hydraulics simulations to reduce the computational cost of utilizing stochastic methods. Kumar et al. [47] combined genetic algorithm optimization with regression splines surrogate model to optimize a reactor model for high breeding of U-233 and Pu-239 in desired power peaking limits, desired keff using the following parameters: radius of a fuel pin cell, isotopic enrichment of the fissile material in the fuel, the mass flow rate of the coolant, and temperature of the coolant at the core inlet. Betzler et al. [48] developed a systematic approach to build a surrogate model to serve in place of high-fidelity computational analyses. They leveraged the sur-

rogate 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 simulation annealing method uses a point-by-point approach. One solution gets updated to a new solution in one iteration, ~~which~~ *but* does not exploit parallel systems' advantages. Finding an optimal solution with simulation annealing methods ~~will take~~ *takes* very long if high-fidelity *not hyphenated earlier* computationally expensive codes are used to compute the objective function and constraints. Therefore, using the simulation annealing method is only practical if a surrogate evaluation model is used as described in [48] and [47]. Evolutionary algorithm *(EA)* methods mimic nature's evolutionary principles to drive its search towards an optimal solution. *use names too*

EAs should be introduced at the beginning of this section / thing, so the reader knows where you're going

Contrary to a single solution per iteration in deterministic and stochastic simulation annealing methods, evolutionary algorithms ~~(EAs)~~ use a population of solutions in each iteration [36]. With the affordability and availability of parallel computing systems, the evolutionary algorithm optimization method stands out as a method that easily and conveniently exploits parallel systems. Further, EAs have proved amenable to high-performance computing (HPC) solutions and scalable to tens of thousands of processors [43]. Therefore, in this proposed work, we will utilize the evolutionary algorithm optimization method.

1.3.1 Impact of additive manufacturing on nuclear reactor design optimization

In section 1.2.1, we discussed how, with the advancements of AM for reactor core components, reactor designers are no longer geometrically constrained by conventional fuel manufacturing and can further optimize and improve fuel geometries to enhance fuel performance and safety. 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 plates, cylinders as fuel rods, spheres as fuel pebbles, axis-aligned coolant channels, etc [49]. ~~Therefore,~~ this has opened the door for a re-examination of optimization ~~in a completely new way,~~ *complete* *methods* determining the optimal arbitrary geometry for a given objective function [49] with a much smaller set of constraints.

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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 [49]. 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.

1.4 Evolutionary Algorithms

EAs mimic natural evolutionary principles to constitute search and optimization procedures [36]. Evolutionary algorithms 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 genetic algorithms (GA) [37, 50].

1.4.1 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 [51]. 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 [52]. GAs are theoretically and empirically proven to provide robust search in complex spaces and are computationally simple yet powerful in their search for improvement [52]. GAs are advantageous compared to deterministic and stochastic simulated annealing optimization methods, because (1) it searches 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 1.2 depicts the iterative process of using a GA to solve a problem. The GA generates new populations iteratively until it meets the termination criteria.

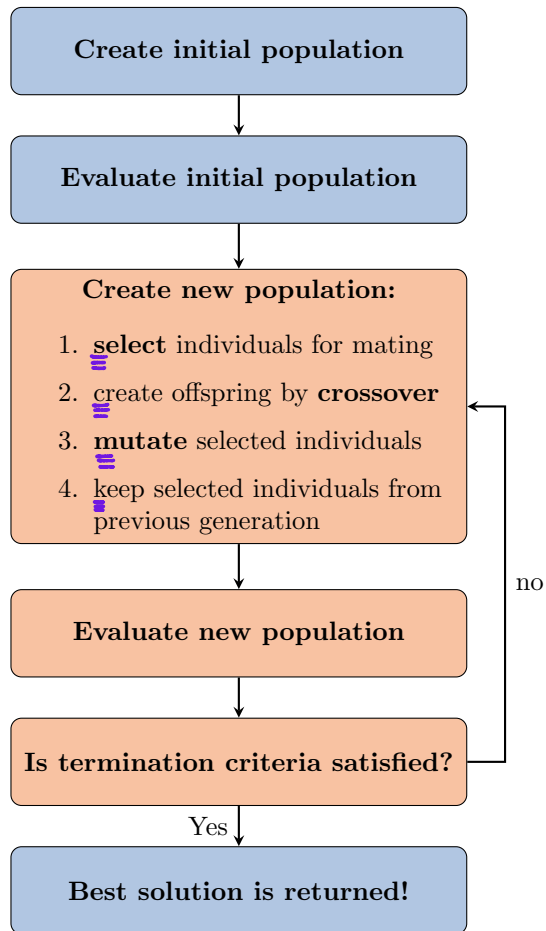GAs uses mechanisms inspired by biological evolution such as selection, crossover, and mu-

Figure 1.2: Process of solving a problem with genetic algorithm [51].

tation. The three operators are simple and straightforward. The selection operator selects good individuals. The crossover operator recombines ~~together~~ good individuals to form a better individual. The mutation operator alters individuals to create a better individual [36]. In the subsequent section, we will provide more description and common methods for each operator.

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Selection Operator

The selection operator's primary objective is to duplicate good individuals and eliminate bad individuals while keeping the population constant [36]. 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 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 [53]. Copies of the best individuals are made to keep population size constant.

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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. The crossover and mutation operators perform the creation of new solutions.

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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 [36]. 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

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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:

$$O_1 = P_1 - \alpha(P_1 - P_2) \tag{1.1}$$

$$O_2 = P_2 + \alpha(P_1 - P_2) \tag{1.2}$$

where

α = 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 [36].

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 [36].

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 polynomial bounded mutation, 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, η (large η will produce a mutant resembling its parent, while a small η will produce the opposite).

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1.4.2 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 good optimization method needs to balance the extent of exploration of information obtained until the current generation through the crossover and mutation operators with the extent of exploitation through the selection operator. If previously obtained individuals are exploited too much, the population loses its diversity, and premature convergence to a sub-optimal solution is expected. Whereas 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 [36]. A quantitative balance between these two issues, exploitation and exploration, is challenging to achieve. Deb et al. [36] and Goldberg et al. [54] 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 1.3), find the desired optimum.

Simulation results
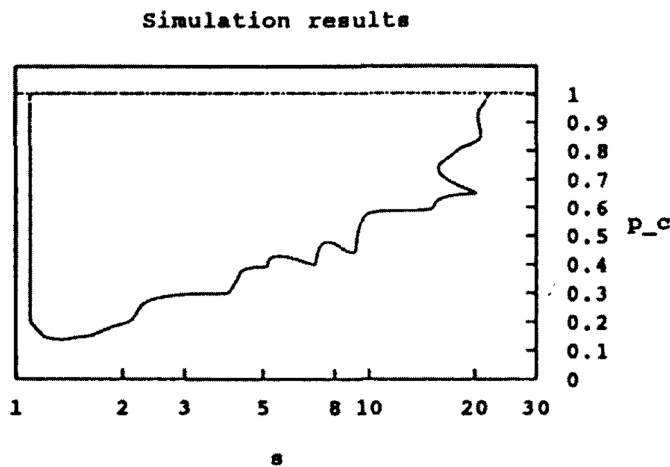

Figure 1.3: Simulation results of the region in which the GA will find the desired optimum for the one-max problem [54, 36].

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 [36]. Therefore,

finding an optimized solution with GAs requires the user to conduct a hyperparameter search. Ng et al. [55] 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.

1.5 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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