
GEOMETRICALLY OPTIMIZED FLUX REACTOR (GOFR)

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SUBMITTED BY:

SULTAN JILANI

IVAN MELNIKOV

ADVISED BY:

DR. DAVID MEDICH

DR. CRAIG WILLS



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Abstract

Nuclear reactors are useful for more than just power - they are the practical neutron sources, but are held back by their large size and prohibitive cost. Neutron sources are essential for academic research, medical isotope generation, and allow for advanced imaging. This project attempts to demonstrate the feasibility of a novel reactor, designed for academic use. The safety features are inspired by Generation-IV reactor designs and thus is designed to be passively safe and proliferation resistant. The Geometrically Optimized Flux Reactor (GOFR) is a small device, approximately 8 cubic meters in volume, and has neutron flux that can exceed much larger reactors. This combination of size, safety, and beam flux makes GOFR ideal for a variety of applications and institutions.

1 Introduction

Neutron sources are needed for a wide variety of applications and expanding access to sources that are smaller and higher intensity allows for increased productivity in all of these these areas.

1.1 Medical Isotope Production

Isotopes are elements with a uncommon number of neutrons. These materials often have properties that can be used in various fields, such as industry and defense, but most notably in medicine. Irradiation of malignant cells and precise diagnostic imaging require short-lived radioactive sources that attach themselves to specific structures and systems within the body. Due to these requirements, radioactive material used for medicine has to be continually generated and in constant demand. Radiopharmaceuticals allow precise delivery of therapeutic radiation, including from within the malignant cells by the clever application of biology and the chemical similarities between isotopes, and for imaging of chemical processes within the body.

1.2 Imaging

Neutron imaging is currently performed in few places and even fewer still do it at frame rates that take full advantage of the method's potential. This imaging technique is faced with difficulties in the production of usable neutrons in terms of quality, scale, and cost. The lack of small, high-flux, and cheap neutron sources creates an artificial bottleneck in the speed at which experiments can be done and advancements made. Despite this limitation, initial results have already provided a glimpse into what this technology has to offer. The advantages include imaging ever smaller surfaces and volumetric details of solids and liquids in real-time, as well as unprecedented resolution of living organics, especially in the field of medical physics.

Volumetric Imaging

X-rays, highly energetic photons emitted by the acceleration of electrons, were discovered in the late 19th century and immediately became the center of attention. Scientists quickly realized the value of being able to see inside the body and turned it into a diagnostic tool, making it possible to diagnose various maladies much earlier and with more certainty. This method of diagnosing issues in the human body has now become a routine part of modern life and it is taken wholly for granted that a doctor can look inside the body without costly and dangerous exploratory surgery. X-rays are additionally used in ensuring that goods are not flawed or damaged without unpacking and without destructively dissecting. Security in sensitive locations and at points of mass travel is also made infinitely easier with the use of X-rays. The molecular structures of various solids are able to be determined by use of diffraction and scattering, for example in the discovery of DNA. Anywhere something needs to be imaged but is under or within something, X-rays can help. However, this is not a perfect technology. X-rays are ionizing, highly energetic, and generally damaging. There have been improvements in the sensitivity of X-ray imaging, leading to a decrease in the energy needed to image but the technique can still be damaging. For this reason, real-time imaging is not considered safe for long periods of time. This damaging quality is especially an issue when working with delicate materials such as living tissue. Another issue, intrinsic to the imaging method, is one of contrast. X-rays are deeply penetrating and are usually only stopped by high-Z materials or are scattered, which makes distinguishing similarly heavy materials difficult, if at all possible. The lessons from this technology were instrumental in the development and discovery of various other advances.

Magnetic resonance imaging is dissimilar from other kinds of imaging in that there is no physical probe that interacts with the sample, however, it still provides insight into objects. MRI works on the principle of nuclear magnetic resonance, which is the tendency of nuclei to re-emit photons of particular, resonant frequencies when under the influence of a strong magnetic field. What this means, is that based upon the frequencies compounds

respond to, one can determine the composition of the sample. Having multiple receivers to catch and triangulate this signal allows for a three dimensional reconstruction of the sample and its cross section. This is generally used for medical imaging and so, for simplicity, hydrogen is targeted. Since the human body is largely water, this approach allows for the tracking of concentrations of water. Due to blood concentrating in areas of activity, such as the brain, or an infected region, MRI can be used to understand how the body behaves. Different parts of the body have differing amounts of water and thus hydrogen, so various internal structures can be imaged. The real-time application of this imaging technique is called fMRI and it has allowed for great strides in the fields of neuroscience and oncology. The brain can be seen thinking by way of blood flow to areas of activation, cancer can be seen growing, and infections festering. With this live view into the body, doctors can understand and view processes that could only be inferred and act with certainty. However, this imaging method is limited in resolution by the strength of magnetic field and that, in turn, is limited by humanity's limited understanding of superconductors. Currently, MRIs are large, helium cooled, claustrophobic and have a decidedly macroscopic resolution, on the scale of square millimeters. They also cannot be used near any appreciable quantities of most metals, as the strong magnetic fields would interact dangerously, possibly shredding the sample beyond salvaging. However, they do not cause ionizing radiation damage like X-rays. MRIs and computed tomographic X-ray scans are sometimes used together to garner a more complete picture of a patient's internals.

Surface Imaging

As mentioned before, X-rays can be scattered off of surfaces to reveal the exact surface of a sample. Due to the difficulty of reconstructing a complete image from irregular scattering, this imaging technique is generally used on crystals, polymers, and other regularly ordered samples. X-rays are damaging and often too energetic for more delicate samples, so electrons are often used instead. Scattering electrons off of high-Z atoms can result in bremsstrahlung radiation, the energy of which, when related to the incident

energy of the electron, is peculiar to Z-value, which indicates the element of the emitting nuclei. To map the surface of the sample, a different approach is used, in which the electron is used in a manner akin to photons in a microscope. Since the wavelength of an electron is significantly smaller than that of a similarly energetic photon, much greater resolution can be achieved.

In a scanning electron microscope (SEM), samples must be conductive or coated in a conductive material to image the surface but the resolution is much higher than any optic system and can image a window on the scale of a few square millimeters. A transmission electron microscope (TEM) functions by passing electrons through samples to image and can achieve sub-Angstrom resolution. However, the sample thickness must be on the scale of only hundreds of nanometers and the TEM may damage the sample. Furthermore, both of these can only operate in a vacuum, severely limiting the samples that can be imaged.

The latest in electron imaging is the scanning tunneling microscope, which uses the quantum tunneling effect to gauge how much current is required to tunnel through the sample. This indicates how many and what energy levels can be occupied by the electron, thus mapping electronic characteristics of the surface. The energy levels can be algorithmically extrapolated to determine elemental and charge properties of the surface. A scanning TEM requires a thin sample as well but can operate outside of a vacuum. Its complexity and sensitivity allow for atomic resolution but also require extensive control of the scanning environment.

Atomic force microscopy (AFM) uses a physical probe to interact with surfaces via a variety of methods, ranging from physical contact to change in resonant frequency of the probe due to electrical forces. AFM achieves sub-nanometer resolution but requires thin samples and can damage them. However, this approach, unlike electron imaging, requires little to no preprocessing.

Neutron Imaging

Neutron imaging, in general, has most of the positive aspects of the aforementioned imaging techniques without most of the drawbacks. Neutrons can be moderated to an energy level corresponding with a de Broglie wavelength of nearly an angstrom, allowing for high resolution diffraction data. This manipulation of the energy level, similarly to electrons, is relatively easy, as long as the moderator is adequately cooled, and can thus be safe enough for medical imaging or energetic enough to be used for therapeutic radiology. Neutron scatter is similar to both X-rays and electrons but does so off of nuclei rather than the electron cloud due to its neutral charge. Because of the direct interactions with the nucleus, this method allows for much greater resolution and allows it to penetrate, and image, high-Z materials. Neutron scattering can image samples that X-rays cannot and to do so with greater detail and less harm to the sample. Injecting contrast agents into a person can help improve the visibility of various structures or help ensure that enough neutron radiation can precisely target malignant cells. Neutron radiation can also be used, with enough flux, to create images in real-time of the sample and if a contrast agent is used, blood flow can be observed by this method as well, and in much greater resolution than an MRI. However, neutron imaging is not an all-encompassing solution. It can make certain materials radioactive, sustained exposure is damaging to equipment, and producing the neutron beam has certain difficulties and idiosyncrasies. Given the demonstrated potential of neutron imaging, this project intends to play a small part in making this technology more available.

Neutron Scattering

Small angle scattering from a surface results in deflections from the incident path of the radiation. This allows for the interrogation of minute details of the material being investigated. This technique is most commonly performed with X-rays and has revealed much about the structure of various molecules, including the double helix of DNA. However, as X-rays interact primarily with the electron cloud of a sample and thus mostly with atoms with more protons and electrons, high-Z materials, the resolution is

limited. Neutrons interact with low-Z materials and the scatter behavior is dependent on nucleus. This allows for an unprecedented level of access to the workings of organic systems. Furthermore, as deuterium is an isotope of hydrogen, it can be substituted into samples to change the neutron scattering behavior of certain parts while the system is chemically unaffected.

Similar to X-rays, neutrons can also be diffracted, revealing the internal structures of dense materials. Neutrons penetrate deeply, as they do not significantly interact with the large electron clouds of atoms. An atom is mostly empty space, and so the neutron passes through many layers of material, diffraction from deep inside.

1.3 Neutron Production

There are three main approaches to neutron production, each with their trade-offs. Most large-scale neutron research is done with spallation sources or nuclear reactors modified for the purpose of neutron emission, rather than power generation. Fusion neutron sources are currently used in commercial applications where a cheap, low power neutron source is needed.

Common Techniques

Fusion In a neutron generator that utilizes fusion, an ionized hydrogen isotope collides with another isotope, releasing neutrons as it fuses into helium. This process is either done with a sealed neutron tube or a fusor. A sealed neutron tube does this with a deuterium gas that is ionized and accelerated towards a tritium infused hydride by means of a differential electric field in a vacuum tube. A fusor, a variant of an inertial electrostatic confinement (IEC) fusion device, accelerates ionized deuterium into the center of the device by means of two concentric rings that create an electric field between them on the order of four kilovolts. Fusion occurs when the ions collide but the ionization method is not strictly defined. All that either of these require is an electric current to be provided. The neutron tube will function until the hydride is depleted but there are ways to replenish the hydride. These produce neutrons but the fluxes are not very high. Fusion on a larger

scale may one day provide the highest neutron flux yet but that is not yet viable. The reality of fusion as a neutron source today is that it is a small scale neutron generator.

Spallation Spallation is a much more widely used method of producing neutrons. The general concept is accelerating a proton in a particle accelerator and hitting a spallation target. This target is a large, heavy metal target, typically lead or mercury. This process degrades the target and it must be replenished. This is not the most efficient way to generate neutrons and is rather large but this neutron source can be turned on and off with great ease. The fluxes are comparable to some reactors and the SINQ facility has achieved continuous beam output from spallation. These are generally large facilities and users can apply for beam time. Despite having good beam characteristics and a wide range of neutron energies, the size and cost of such installations is prohibitive for many scientists and the institutions they belong to.

Reactors Nuclear reactors are the conventional way to produce neutron flux. Critical nuclear reactions generate and capture enough neutrons to ensure the reaction continues until outside intervention. However, not all neutrons that are produced end up colliding with another nucleus. The ones that escape the core are free to radiate outward until they are captured or scattered. The likelihood of a neutron being captured is inversely proportional to the energy of the neutron which means that more energetic neutrons must be moderated in order to maximize fission and thus wattage. Moderation is the process of reducing the energy level of neutrons, usually by absorbing kinetic energy as the neutrons scatter. Current research reactor designs moderate the entirety of the output of the core and redirect most of the flux back into the core by means of reflectors, which are thick crystalline moderators with the express purpose of redirecting neutrons. The neutrons are moderated further as they leave the reactor core, generally in a collimator connected to the beam port. Liquid helium is a popular coolant for the collimator but most research reactor cores are cooled by light water. Most of the recent advancements in research reactor technology are in new safety features built into the core design, switching to low enriched uranium fuel (LEU), and converting power reactors into research reactors. This

conversion process is rather difficult because of the wild disparity in design considerations but this has been achieved in some facilities.

Research Reactors Today

There are four predominant research reactor designs, of which only one has no currently operational examples.

The SLOWPOKE design is the simplest implementation of a research reactor and is correspondingly low energy and, in relation to the other research reactors, low flux. It is a tank-in-pool reactor of Canadian design, comprised of a light water pool and a reactor core. The core uses 19.9% enriched uranium in a uranium dioxide ceramic as a fuel and is encased in a reflector - a beryllium cylinder. Varying the thickness of the reflector at one end allows for maintaining criticality as the fuel is depleted. It operates at only a few kilowatts but can do so unattended for long periods of time. It is inherently safe and cannot undergo a runaway reaction.

The DIDO design is entirely retired and, in one instance, replaced by OPAL. This design is British and was widely used, reliably, for decades. The core was a cylinder made of an alloy of aluminum and 80% enriched uranium submerged in heavy water, which acted as both the moderator and coolant, and surrounded by a graphite reflector. In some instances, reactors of this type were modified to either use low enriched uranium, or to operate at 25 MW. The original design operated at 10 MW.

The OPAL design is a tank-in-pool reactor that uses low enriched uranium ceramic plates and is the only nuclear reactor in Australia. It is of Argentinian design and uses both light and heavy water. The heavy water acts as the neutron reflector and the light water cools the core. It operates at 20 MW and replaced a DIDO design reactor.

The TRIGA reactor design is considered immensely safe due to its innovative use

of zirconium hydride as a moderator. The zirconium hydride is alloyed with the low enriched uranium in the core, allowing for a very dense concentration of hydrogen to act as a reflector and moderator. Hydrogen has the highest scattering coefficient of any other material and outperforms beryllium by a factor of nearly 11. This means the reactivity nearly instantly goes down as the core heats, making it hard to meltdown. It is a tank-in-pool reactor and is often used in universities and other institutions. This reactor can operate at 16 MW and it can be pulsed to up to 22,000 MW.

1.4 Our Approach

This project aims to offer a direction of design when creating a neutron source that can expand the use and research of neutrons, especially for the purpose of neutron imaging. Towards that goal, the neutron source should be small, high flux, and affordable for smaller institutions. The initial plan was to convert a modern Gen IV reactor into a research reactor because of the inherent safety of the core design, higher wattage, and the small size of the core. However, due to the fundamental incompatibilities in design requirements, it was quickly determined that this was not possible for the current project. Other research reactors were studied to see if there was some amalgamation of existing solutions that could be used. It was decided to do a feasibility study of a somewhat novel approach in the hope that some useful knowledge could be gleaned from the experience.

Design

The primary guiding motivation for the design decisions was to maximize the neutron flux of the beam. This meant both operating at a higher wattage, by increasing the amount of fissions per second, and getting neutrons through the beam port. Barring adding more fuel, the way to increase the wattage was to facilitate more neutron capture. To that end, reflectors would be placed around the core, to ensure the neutron path would encounter fissile nuclei, and neutrons would be moderated, to ensure neutrons were readily captured. Ensuring that neutrons made it out of the core and into the beam port seemed like a geometric issue, so the shape of the reflectors was altered to impart

a radial forward bias in the distribution of neutrons using a ellipsoidal reflector, while ensuring enough neutrons return to the core with the use of a retarding surface. To allow for the neutrons reflecting off of the ellipsoidal reflector to make it to the beam port without being absorbed, they need to be fast or miss the fissile material. This design uses both techniques. The neutrons reflected off of the ellipsoidal reflector miss the core due to the neutron transparent space, composed of aluminum, between the core and the reflector. Between the retarding surface and the core, there is an additional moderating material alloyed with the aluminum and zirconium hydride, to ensure that the retarded neutrons were thermalized enough to guarantee fission. Directly behind the core, the ellipsoidal reflector ensures that the neutrons reflect through the core. With tuning of the ratios of these surfaces, a higher neutron flux can be achieved while still maintaining adequate criticality for any size core. From this principle of optimizing the geometry for the highest neutron flux, the name of the design, Geometrically Optimized Flux Reactor (GOFR), was chosen.

Monte Carlo Simulations

In order to test the effectiveness of the novel design, Monte Carlo simulations were used. Said simulations rely on the principle of random sampling, and hence are extremely useful for investigating large population behaviors. Random sampling, or dart throwing, attempts to simulate particle interactions in a probabilistic manner. At the start, a neutron is launched at a random direction, with a random speed consistent with its energy distribution. When this neutron collides with another particle, the interaction is again modeled randomly. A good graphical explanation of a sample particle simulation can be seen in Figure 1.

For example, the collision angle and change of speeds will be different at every simulation run. The underlying assumption here is that eventually, after many samples (on the order of magnitude of 100,000) the results will converge to the actual value. Another way to look at this is a coin toss problem. If one tosses a coin, it's evident that the probability of getting a head is the same as of getting a tail - 50%. However, after 10 tosses, the

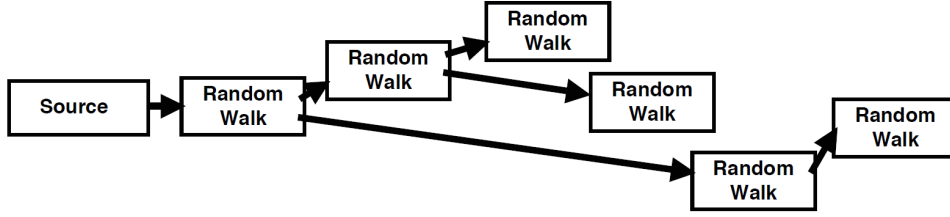


Figure 1: MCNP random walk.

coin may not have landed on its head 5 times and on its tail 5 times. However, as one starts tossing the coin 100 times, or 1,000 times, the results will distribute themselves more evenly - converging towards the 50-50 split of heads and tails. This is the exact same approach used in Monte Carlo simulations. Encompassing these random samples and properties of various materials is MCNP, or Monte Carlo N-Particle Transport Code.

MCNP

The Monte Carlo N-Particle Transport Code was developed by the Los Alamos National Laboratory in the 1950s. Primarily, it is used to simulate nuclear processes, such as fission. Other applications It is ideal for this project since the main reaction used is fission in the novel reactor. There have been several versions of MCNP released over the years, with further improvements to its vast materials library. The library contains information of physical properties like melting and boiling points of materials, as well as more advanced aspects like neutron capturing properties and atomic cross sectional areas. Version 5.1 and X were used for the design and simulation of the Geometrically Optimized Flux Reactor (GOFR). In order to simulate any particle interactions, MCNP solves the Boltzmann transport equation, defined as:

$$\Psi(\vec{r}, \vec{v}) = \int \left(\int \Psi(\vec{r}', \vec{v}') C(\vec{v}' \rightarrow \vec{v}, \vec{r}') d\vec{v}' + Q(\vec{r}', \vec{v}) \right) T(\vec{r}' \rightarrow \vec{r}, \vec{v}) d\vec{r}' \quad (1)$$

The $\Psi(\vec{r}, \vec{v})$ term defines the collision density of particles across the whole simulation space. The C is called the collision kernel, which accounts for particles changing their velocity at a given location. The T term, on the other hand, is the transport kernel and

accounts for the opposite case - a particle changing its location at a given velocity. The Q term is the source of particles. In the case of GOFR, the term is defined as:

$$Q(r, v) = S(\vec{r}, \vec{v}) + \int \Psi(\vec{r}, \vec{v}') F(\vec{v}' \rightarrow \vec{v}, \vec{r}) d\vec{v}' \quad (2)$$

S defines the fact that the source is stationary, and that the primary particles will be emitted from a fixed point in the simulation space. The collision density term accounts for the fact that the core will be undergoing fission, defined as F . What makes MCNP so powerful is the simultaneous use of the collision and transport kernels. Taking both factors into account allows the simulation to look at particles that change velocity and direction at any point in the simulation space. Every interaction that a particle has with another particle is stored in the simulation memory. The states of the particles - energy, velocity, direction - are saved in order to extrapolate results and determine the convergence. The flow diagram in Figure 1, can also be seen in terms of particle histories, seen in Figure 2.

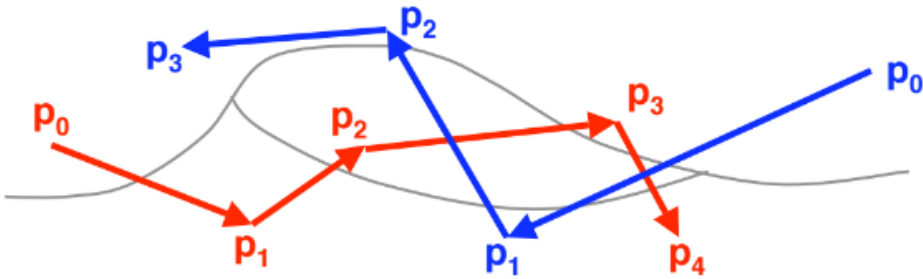


Figure 2: Particle interaction histories.

With the histories, MCNP is able to extrapolate where the particles will end up after future runs and what their energies will be. The final results are defined in the following way:

$$A = \int A(p) \Psi(p) dp \approx \frac{1}{M} \sum_{m=1}^M \left(\sum_{k=1}^{\infty} A(p_{k,m}) \right)$$

The final, average state of the particle is the integral of the product between the collision density and the particle states. The integral can be estimated through a classic

Riemann sum, where M is the number of particle histories and samples. The larger the value of M , the more accurate the final results are.

Through the extensive calculations that MCNP carries out, the decades of development put into it, as well as its ability to take into account all physical properties of materials used, the software package proved ideal for the design and simulation of the Geometrically Optimized Flux Reactor (GOFR).

2 MCNP

2.1 General information

MCNP is built on Fortran, specifically Fortran-90, as it takes time to vet and confirm compatibility with the extensive libraries of MCNP. The basic programming principle is similar to that of punch cards: a program is split into several blocks, where various aspects of a simulation are defined. The first block defines cells, the second one defines surfaces, finally, the last block defines what simulations MCNP is supposed to run. An example MCNP program structure can be seen in Figure 3. The blocks are separated by blank lines, which are required for MCNP to properly read in the file. If the lines are omitted, then the definitions will not be seen correctly. Comments can be added to the input files as well. A full line comment starts with the letter "c", whilst an inline comment starts with a dollar sign (\$). It is important to note that all lines should not exceed 80 characters in length.

Message Block + <i>blank line delimiter</i> {optional} One Line Problem Title Card Cell Cards [<i>Block 1</i>] <i>blank line delimiter</i> Surface Cards [<i>Block 2</i>] <i>blank line delimiter</i> Data Cards [<i>Block 3</i>] <i>blank line terminator</i> {optional}

Figure 3: MCNP program structure.

MCNP programs contain definitions for geometries in a 3D dimensional Cartesian coordinate system. A good way to look at cells, surfaces and their material definitions is the following. In Figure 4, A and B are two surfaces. Each surface has a negative and positive value, which is important for particle interactions. If a value is negative, then the surface is facing inwards relative to the origin. The mathematical depiction can be seen in Figure 5, where the normal vector n_2 is expressed by a negative surface number, whilst the vector n_1 is a positive surface number.

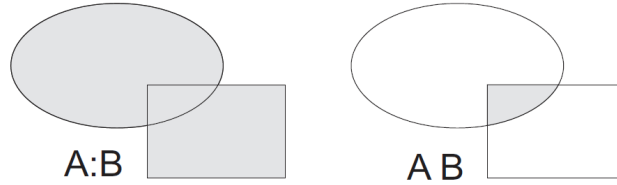


Figure 4: Example MCNP regions.

Surfaces can be combined together to create cells. Defined as either unions or intersections, the resulting cells from surfaces A and B are seen in Figure 4. An important MCNP concept to remember is that when looking at a typical geometrical shape, for example a cube, one must double the number of faces. In a cube, the number of faces is 6, however, because of positive and negative surfaces, the shape should be looked at as having 12 faces¹. Understanding this was a key point in the project. Being able to identify which regions were required and which surfaces to ignore allowed us to carry out simulations more effectively and accurately.

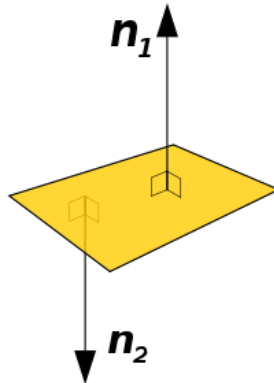


Figure 5: Normal vectors to a plane.

2.2 Example geometry

A good way to understand MCNP syntax and its complexity is a simple example. For this, a graphite cube will be submerged into a spherical container and that container will be filled with water. Throughout the project, it was found that specifying surfaces first was an easier approach, followed by the cell definitions. The input file was structured out

¹Similarly, a sphere will have 2 surfaces - an inner one and an outer one.

of order, however, this allowed for a more step-by-step approach to the simulation setup. In order to create a cube, the procedure is the following:

1. Specify 6 outward facing surfaces.
2. Specify 6 inward facing surfaces.
3. Combine all of the relevant surfaces into a cell. Here, the outside of the cube would be a union of the outward facing surfaces, and the inside will be a union of the inward facing ones.

Although this is only 3 steps, the procedure is fairly complex. In order to specify a single surface, one must figure out the side length, center and boundaries of the square in question. Doing this specification 12 times becomes monotone and challenging, especially when dealing with complex, irregular geometries. MCNP does have a solution, however - macrobodies. With one command, MCNP will know that the shape specified is a cube, sphere or pyramid, to name a few. The command for a rectangular parallelepiped is **RPP**. In order to create a cube centered at the origin with a side length of 10cm, the command is:

```
10 RPP -5 5 -5 5 -5 5
```

In the above example, 10 is the number of the macrobody, which will be important in the cell block - it is an identifier. The first two numbers indicate a starting and ending x-coordinate², followed by the same syntax for y and z coordinates. The next step is to add a container around the cube. This can be a sphere, again, specified by a macrobody, the command for which is **SO**. If the radius is to be 100cm, then:

```
20 SO 100
```

The structure is similar - 20 is the label for the macrobody, SO is the command, 100 is the radius. For this example, we need water and graphite as the materials. These are

²MCNP units are metric, with length defaulting to centimeters.

specified in the final, data block. Material definitions are fairly straightforward. To label a material, one types the letter "M", followed by a number. After that, the material is defined by elemental and atomic abundances. Water, having 2 hydrogen atoms and an oxygen atom, is defined as:

```
M1 1000 2
      8000 1
```

The general format for isotope specification is *ZZZAAA*, where *ZZZ* is the atomic number and *AAA* is the mass number. Specifying *AAA* as 000 tells MCNP to use the elemental form, as is done above. The 1000 and 8000 specify the forms of hydrogen and oxygen, respectively. To specify graphite, the label can be M2, with the atomic and mass numbers being equal to 12 and 60, respectively. To specify 100% composition, we define graphite as³:

```
M2 06012 1
```

Since the surfaces and the materials have been defined, the cells' block can be examined now. The syntax is similar to previous definitions - a cell number, followed by its material, its density, surface number (positive or negative facing) and its importance. The density sign should match the surface number sign - if a surface is defined by a negative cell, then the density⁴ will be negative as well. The importance is a property of the material to interact with particles. In this project's case, setting `imp:N=1` means that this cell will only interact with neutrons. Below is the definition for the graphite cube cell:

```
1 2 -1.7 -10 imp:N=1
```

The above definition completely sets up the cube at the center of the universe. In order to setup the surrounding water, the definition is presented below:

³The 1 at the end of the command specifies fractional composition - 1 being equal to 100%.

⁴Density is specified in terms of MCNP's constants - found either in the manual or primer.

```
2 1 1 (10 -20) imp:N=1
```

The setup is the same as for the previous cell - its label is 2, M1 is used for the material (water), and the cell is defined as the union of the outward facing surfaces of the cube, but the inward facing surfaces of the sphere. The water will interact with the neutrons only. The setup is almost complete, however, the graveyard must be added. This is the boundary of the simulation where the particles simply vanish. To do this, the outward facing surface of the sphere has to be set to 0 importance and material 0, which is vacuum:

```
3 0 20 imp:N=0
```

The setup is complete and the full file can be found in Appendix 1. Assuming the code is saved in the file **example.txt**, there are several ways to run the program. The commands depend on your operating system, but primarily the version of MCNP used:

```
mcnp example.txt
mcnp6.mpi ir inp=example.txt
```

Since the data block does not have any simulation specifications (only the material definitions), MCNP will not output anything meaningful. In the second version of the command above, the flag "ir" was used to specify that the file should be run. In order to inspect the geometry and see if it is valid (assuming you have the graphical MCNP geometry editor), the flag "i" should be used by itself.

2.3 Data block

Criticality tests

The final data block is where the simulation specifications, as well as other aspects like unit conversions are defined. In Layman's terms, this is where one tells MCNP what to do with the provided geometry. Two main types of simulations were run for the project - a criticality tests and an FMESH tally. The criticality test takes a fissionable source

and sees if the geometry will be able to sustain the reaction. The value returned is called the k-coefficient. If the value is greater than 1, then the geometry (mainly the fissionable core that is being tested) is super critical. If it is equal to 1, then the setup is critical. Anything under 1 is non-critical and will die out. A typical criticality test is run using two commands: **kcode** and **ksrc**. The first command specifies the number of particle histories to look at, the k-coefficient value to attempt to obtain, number of cycles and samples. An example command is seen below:

```
kcode 1000 1.0 15 115
```

The above line indicates that 1000 particles will be looked at to attempt to obtain a criticality value of 1, with 115 samples and 15 cycles per sample. The only step left to do is to specify the source of the reactions, in this case the origin:

```
ksrc 0 0 0
```

The k-code will emit particles from the source into a random direction and see if they trigger other fission reactions. This procedure links back to the random walk problem - every interaction a particle has with something else in the defined geometry is randomly generated/processed. After running for the specified number of samples, MCNP will output the criticality that results from the specified geometry. The results returned are in the forms of confidence intervals, however, the average value is the one to look at, which MCNP will also give you. This was the main approach to determining the size and composition of the core. Obtaining a value as close to $k = 1$ was crucial for the GOFR since a runaway reaction would cause safety concerns. On the other hand, a sub-critical core would die out and the beam of neutrons emitted will not last long (or be powerful enough).

FMESH tally

The second type of simulations run on the GOFR was an FMESH tally. A tally in MCNP is a counting mechanism for the number of particles that will pass through a certain region over the course of the whole simulation. The units are MeV/cm², and

for this project the neutrons were counted only, using a special variation of an MCNP tally - the FMESH⁵. In order to count the particles in an FMESH, one must specify its dimensions, as well as the bins, which will count the particles themselves. A good way to think about such a tally is a Lego Block, an example one seen in Figure 6.

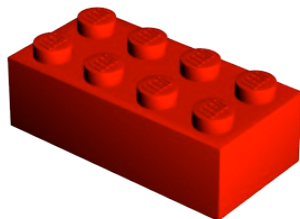


Figure 6: Mesh tallies can be thought of as Lego blocks.

The block itself, most of which are rectangular, is the tally. It is defined in 3 dimensions, again with x, y and z coordinates. The connectors that link up the Lego blocks are the bins, where the particles will actually be counted. The sizes and positions of these bins must also be specified. An example FMESH tally is defined below:

```
FMESH14:N geom=XYZ origin=-15, 105, -15
      imesh 15 iints 100
      jmesh 106 jints 1
      kmesh 15 kints 100
      OUT=COL
```

The above example defines the following parameters for the volumetric tally. The tally will be an FMESH one, counting only the neutrons. Its location and dimensions are defined in x, y and z coordinates. The origin of the tally is at $(x, y, z) \rightarrow (-15, 105, -15)$. The x direction of the tally will be split into 100 bins and will start at 15cm from the origin. The y direction will start at 106cm from the origin and will have 1 bin. Finally, the z direction will start at 15cm from the origin, and have 100 bins. At the end, the output is specified to be collimated - meaning that the results will be split into their coordinate groupings. The example output is seen below:

⁵There are a total of 11 types of tallies available in MCNP, all of which are listed in the manual or the primer.

X	Y	Z	Result	Relative error
95.500	-24.833	-24.833	2.67541E-03	5.18589E-01
95.500	-24.833	-24.500	8.02861E-03	4.72413E-01
95.500	-24.833	-24.167	1.60623E-02	3.91226E-01
95.500	-24.833	-23.833	9.61243E-03	3.83485E-01
95.500	-24.833	-23.500	1.24564E-02	3.95931E-01

Through these two types of simulations, two versions of the GOFr reactor were designed. Although the versions share similarities on a basic level, the materials and results differ vastly.

3 Methods and Materials

GOPR was designed incrementally, slowly testing each improvement to the design at each step, to ensure the inner workings of the reactor were understood and minimizing errors in optimization. Initially, core behavior and criticality in response to enrichment, core alloy material, and size were determined. After that, moderating materials and the interaction with the shell was tested and a rough design was decided upon, that was to be optimized. As a benchmark, a more conventional version was created that retained some of the concepts GOFR was intended to leverage for greater flux. In both, success was measured by a critical core and a FMESH tally located in the beam port of the reactor. A general geometry for GOFR was developed and coded into MCNP after significant geometric calculations and was changed only slightly after testing.

3.1 Core and Moderator

After considering several variations of reactors, initially GenIV power reactors and then various research sources, it was decided to use standard low enriched uranium (LEU), due to its characteristics of being well studied and relatively simple to refine and use. As a benchmark, 80% enriched uranium was used, chosen to be under the weaponization threshold of 90% but still highly enriched. This choice allowed for the comparison of designs by giving a clear goal for criticality and flux. Furthermore, LEU fuel of 20% enrichment, and two half uranium and half alloy core compositions were tested. Initially, naked cores were tested to see the exact influence of size on the criticality and to further compare the improvements made by any additions. First was the moderating material, the material that encased the core and filled out the space between the core and the reflecting shell. It was not yet certain if the geometric approach would work, so a variety of moderators were examined. Water was very good at reducing the energy of the neutrons enough to raise the criticality but would be a hindrance to the geometric approach as it relied on neutrons traveling largely undisturbed. For that purpose, aluminum performed well, only slightly altering the criticality. Vacuum performed the best in keeping the

criticality constant as it showed no interaction with neutrons, which was a result used as another benchmark. These results are consistent with the data from NIST on neutron scattering lengths and were already largely factored into design considerations. These simulations are to confirm that the models and effects used in the design of GOFR were well founded in reality, using MCNP as a surrogate for reality.

As a result of these simulations, it was decided that GOFR would use aluminum as the moderating filling and the conventional-style reactor would use water. The use of water in this case is consistent with the majority of research oriented reactors. Next was the shell material. A brief and oversimplified test of possible materials was done, in which a sphere of the reflector material was placed around the core and the criticality was compared. A thickness was arbitrarily chosen such that significant neutrons would not escape. Graphite was then chosen for further development, rather than beryllium, zirconium hydride, water, or heavy water for both criticality and geometric design considerations.

A rough volume to enrichment relationship was used to decide how enriched the uranium would be and still be critical. It was decided to adhere to the general standard of having sub-20% enrichment to maximize flux while maintaining safety but did not go as low as some reactors do. Using this minimum volume of LEU, alloys and geometries could be explored without too much iteration in running MCNP code. For the conventional style reactor, a cube, side length of $l = 30\text{cm}$, was used and its enrichment, 15%, was determined by this value. For GOFR, a sphere made of 50% uranium at just below the 20% limit, 19.9%, the radius had to be $r = 25\text{cm}$ to achieve criticality upon introduction of the shell.⁶

3.2 Shell

The surrounding shell and its geometry has three purposes:

1. Increasing criticality. The generated neutrons that manage to escape the core do not need to be wasted. By sending more back into the core, the reactor can fission

⁶For a full listing of tables and results, see section 4

more than would be expected as if it was a larger, more intrinsically critical piece of uranium.

2. Neutron reflection. The neutrons that are generated do not need to continue radiating isotropically. By biasing how neutrons travel in the reactor, more of the generated neutrons can pass through the beam port, giving off a flux much higher than a similarly powerful reactor.
3. Thermal regulation. Any heat generated by the fission reactions in the core is transported out to the shell where it can be more easily regulated. The exact workings and optimizations for this are outside the scope of the project but some discussion is given in section 6.

Increasing Criticality

Any material upon which neutrons scatter can be used for moderation and reflection to this end. The only requirements are that the core be surrounded and that there is no path out of the reactor, especially if scattering is elastic. As long as more neutrons hit the core that otherwise would not have, the criticality will increase, and even more neutrons will be produced.

Neutron reflection

Neutrons do not behave like light and reflecting them is not as simple. However, with certain materials and angle, reflection is largely elastic and therefore reflected neutrons follow a general trajectory with a higher incidence along the central path. Therefore, neutrons will differ from light in terms of path mostly in a rather tight distribution around this central path. This general logic was used when designing GOFR. Initially, a parabolic reflector was considered as it is a common optical tool. It would take a radiant source located at the focal point and direct its now collimated beam forward. That would be perfect, if the reactor were small and the irradiation window was much larger, because it turns an isotropic source into a linear one and collimates the beam, as seen in Figure

7. Unfortunately, such a large irradiation window and reactor size would not fit the application.

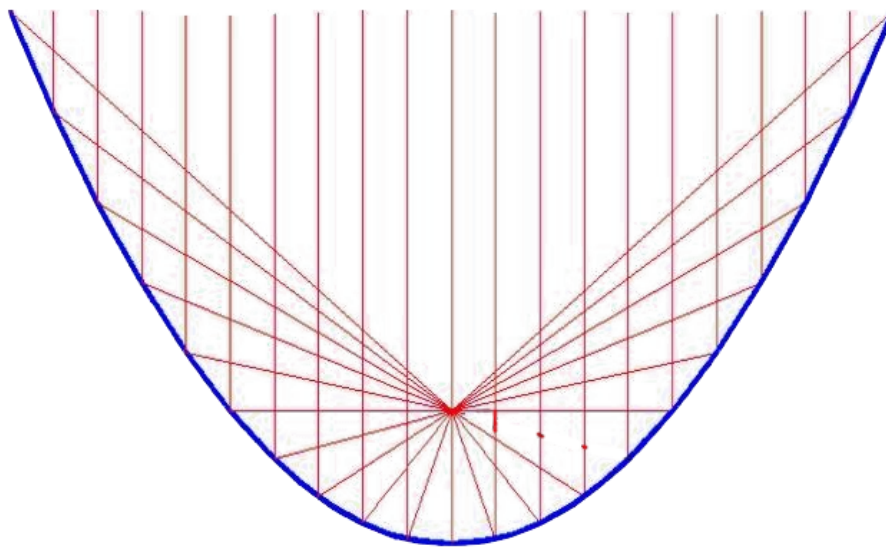


Figure 7: Parabolic reflector

Next a sphere was considered, as its surface is perfectly perpendicular at every radial line and that is exactly the use case with increasing criticality. However, this does nothing to promote a mass exodus of neutrons and creating a high flux beam. This is where deviation from conventional reactor design started. In the conventional reactor, the core was placed against one side of the shell and the beam port where the core met the shell. This allowed for most of the generated neutrons to support continuing fission while a significant amount were shuttled out of the reactor, as seen in Figure 8.

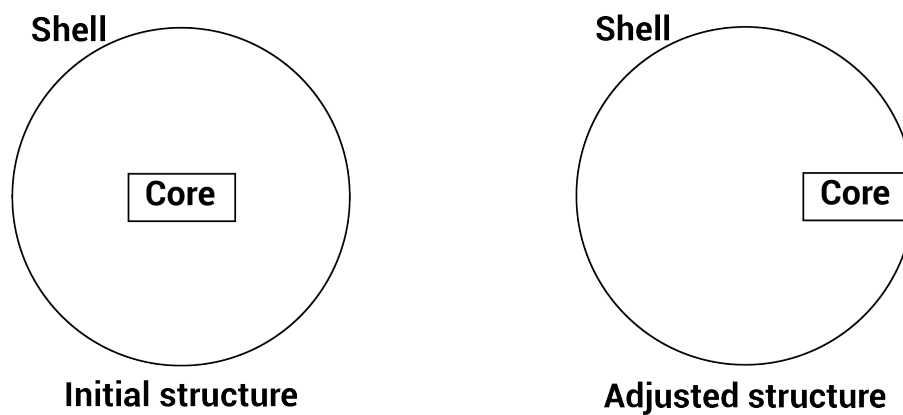


Figure 8: Core and shell structures of Conventional Reactor

For GOFR, it seemed that the answer was in the geometry of the reflector. To that

end, an ellipsoidal reflector was developed, the size and shape based upon data from the tests on the core composition. An ellipsoid has two focal points, and anything radiating isotropically from one, irradiates the other perfectly uniformly, as seen in Figure 9.

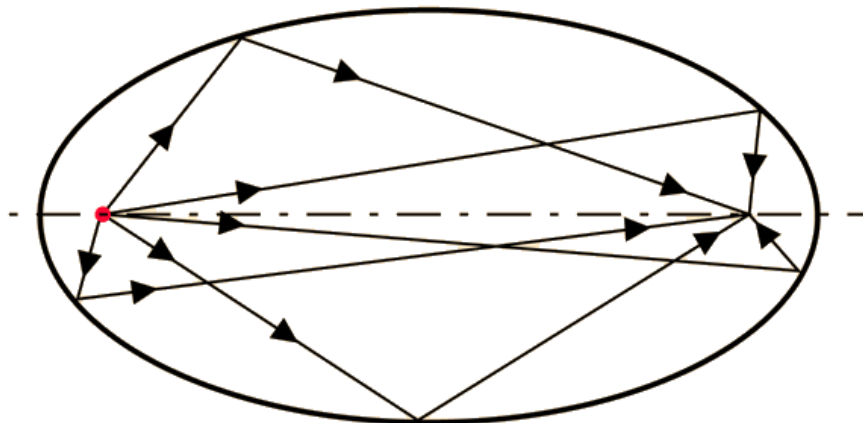


Figure 9: Ellipsoidal reflector

Since the aim was to maximize neutrons leaving the reactor, an ellipsoidal shell was not the entire solution. To accomplish that, a conical reflector was fitted to the midpoint of the ellipsoid, its surface angle matching the path of any neutrons that reflect off of the ellipsoidal reflector at the junction of the two surfaces. This ensured that the focal point of the neutron radiation was inside the beam port, ensuring that the majority of the generated neutrons would escape the reactor. The conical reflector further ensured that enough neutrons would return to the core by acting as a conventional reflector. This geometric concept is illustrated in Figure 10.

Particle interaction

Thermal regulation is outside the scope of this project but aluminum conducts heat very well and would conduct heat away from the core and deposit it in the shell, where coolant can be pumped on or through the shell. This allows the core to function at higher wattage without damage and thus create higher neutron flux. By running water over the shell's surface and through cavities or pipes inside the shell, heat can be extracted efficiently. More discussion is given in Chapter 6.

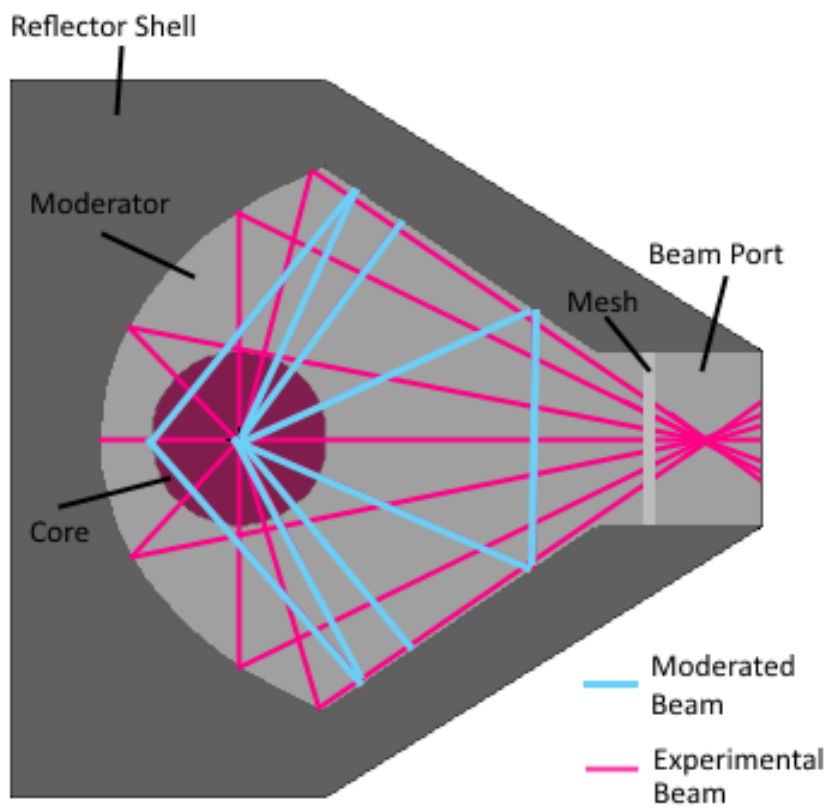


Figure 10: GOFR concept design

3.3 Beam Port and Tally

In both designs, the neutrons were directed towards the beam port, a hole in the shell in which a collimator can be inserted. The raw beam was recorded and analyzed by means of a FMESH tally, which counted the neutrons passing through the beam port and their direction. From this, the beam behavior and raw flux can be calculated. This can then be compared to existing sources and the feasibility of this design can be ascertained and gauged.

4 Results

4.1 Criticalities

The main goal of GOFR was to test the feasibility of a geometric approach to research reactors and to fit the resultant reactor into the size of a room. This dimensional criteria was where calculations started. Various sizes of cubes, for ease of visualization, were tested, to get a sense of how criticality scaled with size and how large the final core would be. From the below table, it is seen that criticality rises linearly with volume. Since a self sustaining reaction requires a k-coefficient of $k = 1$ that is what was tested for. It also shows the maximum moderated potential of each core because the many meters of water completely stopped all neutron activity outside its bounds.

Table 1: U-235 core trials

Composition	cc of U-235	Moderator	k-coefficient
U-235	1000	Vacuum	0.74311
U-235	1000	Water	1.26001
U-235	8000	Vacuum	1.30614
U-235	8000	Water	1.49408
U-235	27000	Vacuum	1.64085
U-235	27000	Water	1.76348

Table 1 suggests that a volume greater than a thousand cube centimeters of U-235 is needed for sustained fission, unless heavily moderated, but eight thousand is excessive. These initial results provide a good place to start experimenting with lower enrichments and different alloys. First, a conventionally designed reactor was designed, to provide an initial criticality and flux value. Different core sizes and enrichments were tried, submerged in water, in a graphite flask. A 15% enriched uranium core of 30 square centimeters was decided upon.

Four cores were devised to test things further. The first two were differently enriched uranium cores, 80% and 20%, designated HEU and LEU, respectively. The last two are alloys of half LEU and a metal, zirconium hydride and aluminum. These are designated as $UZrH_4$ and UAl , respectively. A sphere of $r = 10cm$ was assumed, as spheres should better utilize generated neutrons and the volume of a sphere increases rapidly with radius.

Table 2: Conventional Reactor variations

Composition	Side length (cm)	cc of U-235	k-coefficient
20% enriched Uranium	10	200	0.85447
20% enriched Uranium	20	1600	1.02792
20% enriched Uranium	30	5400	1.15384
20% enriched Uranium	60	43200	1.40225
15% enriched Uranium	60	32400	1.27469
15% enriched Uranium	40	9600	1.15583
15% enriched Uranium	30	4050	1.06625

The intention was to make the core go critical with the optimized shell and the core alloys.

Table 3: Core criticality testing, $r = 10cm$

Composition	cc of U-235	k-coefficient
HEU	3351.03	1.04706
LEU	837.76	0.51117
$UZrH_4$	418.87	0.28084
UAl	418.87	0.27939

Table 3 shows that with half the uranium, UAl at 54.66% of the criticality of the LEU core. $UZrH_4$ performs at 54.94%. Both clearly do something but $UZrH_4$ does more of it. The underlying theory is that the hydrogen in the $UZrH_4$ moderates the energy of the neutrons so that they cause more fissions. This capture is delicate and a rise in temperature that is too high will let neutrons escape the core and force a lower power level. This is the intended function, which is why $UZrH_4$ is included, despite only a slight improvement.

Table 4: Core+Moderator criticality testing, $r = 10cm$

Composition	cc of U-238	k-coefficient
HEU	3351.03	1.19440
LEU	837.76	0.59913
$UZrH_4$	418.87	0.34255
UAl	418.87	0.34051

The scattering lengths of various moderator materials was studied and it was determined that aluminum would have the smallest interaction with the neutrons while if scatter occurred, it would be elastic. Criticality rose more than expected with the addition of the aluminum moderator in Table 5. There also seems to be a growing disparity

between UAl and $UZrH_4$, which is a positive indication of the passive safety features from using $UZrH_4$.

Table 5: Final criticality testing

Composition	cc of U-238	k-coefficient
HEU	3351.03	1.28998
LEU	837.76	0.67885
$UZrH_4$	418.87	0.44506
UAl	418.87	0.44983
$UZrH_4$ @ 25cm	6544.98	1.00546

It was at this point the GOFR shell design was completed confirmed to be, at least geometrically, optimally configured to send as many neutrons as possible through the beam port. The geometry was coded into MCNP, and the aforementioned cores were put into it and then tested for criticality. Since only the HEU was critical, and it seemed that all cores had reached a plateau in criticality, the $UZrH_4$ was run at $r = 25$ to get it to the point where it could sustain itself. Since criticality had been achieved, it was time for the FMESH tally. A grid of tallies throughout the beam port recorded the number of neutrons passing through.

Table 6: Flux comparison

Reactor	Average Flux (n/cm^2)	Maximum Flux (n/cm^2)	Beam Area (cm^2)
UMass Lowell FNI	$1.390 * 10^{11}$	$9.200 * 10^{12}$	900
Graphite Flask	$8.877 * 10^{12}$	$1.692 * 10^{13}$	900
GOFR Design	$1.963 * 10^{13}$	$5.048 * 10^{13}$	1963

The two reactors had higher flux than the Lowell Research Reactor, as seen in Table 6. These values were calculated for a reactor operating at a power level of 1 MW. Each fission of U-235 releases 202.5 MeV of energy, so by dividing a megawatt by that value, it returns the fissions per second. Each fission results in 2.4 neutrons released on average so multiplying the number of fissions by the average number of generated neutrons per fission returns the total neutrons generated each second in the reactor core. After summing the neutrons that passed through the beam port and dividing by the total neutrons generated in that simulation, a ratio is obtained that indicated the number of neutrons that enter the beam port for every generated neutron. Applying that to the number of

neutrons generated each second in the core returns an absolute number of neutrons that will pass through the beam port every second. Dividing that by the cross sectional area of the beam port results in the flux of the reactor. Thus, the flux was obtained and listed in Table 6.

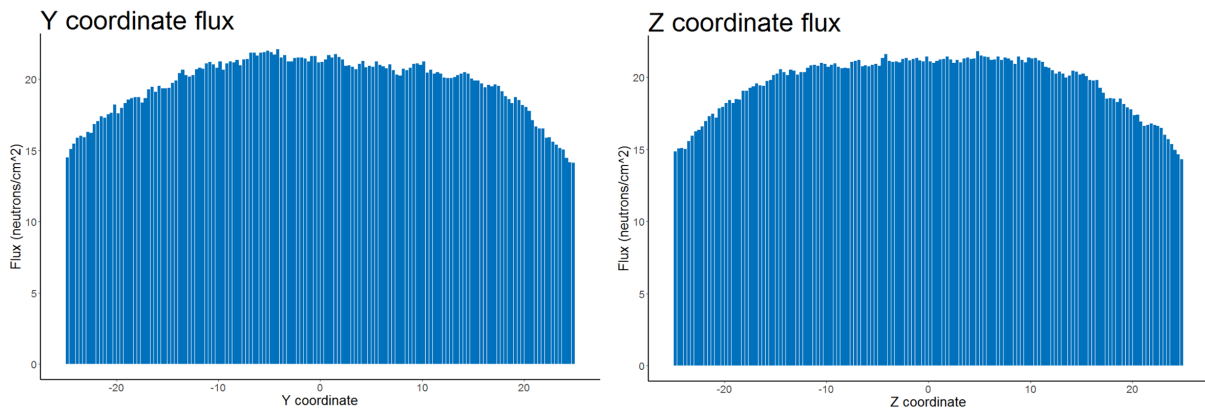


Figure 11: GOFr neutron flux distribution

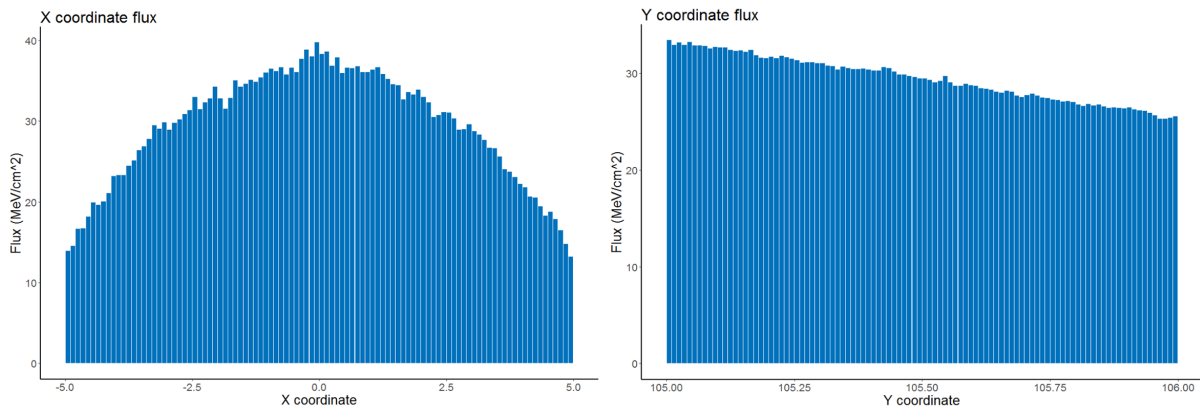


Figure 12: Conventional reactor neutron flux distribution

The beam intensity is characterized and shown visually in Figure 11 and Figure 12, of GOFr and the conventional reactor. This shows that, in addition to having a higher flux, GOFr also has a more uniformly distributed neutron flux, and bigger beam, when compared to the conventional reactor.

4.2 Reactor designs

The conventional reactor, the graphite flask of water, design is shown below in Figure 13. GOFR, the novel reactor design that was geometrically optimized for high neutron flux is seen below that, in Figure 14.

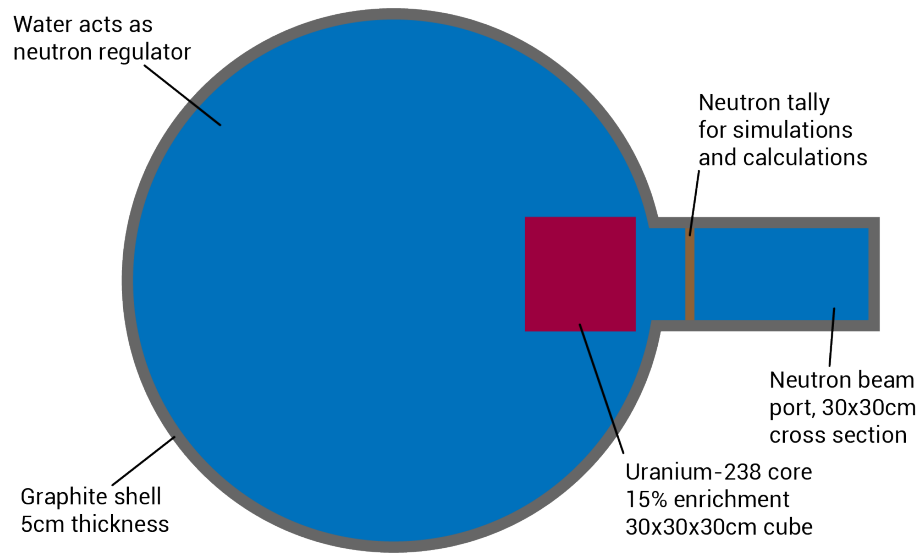


Figure 13: Conventional graphite flask design

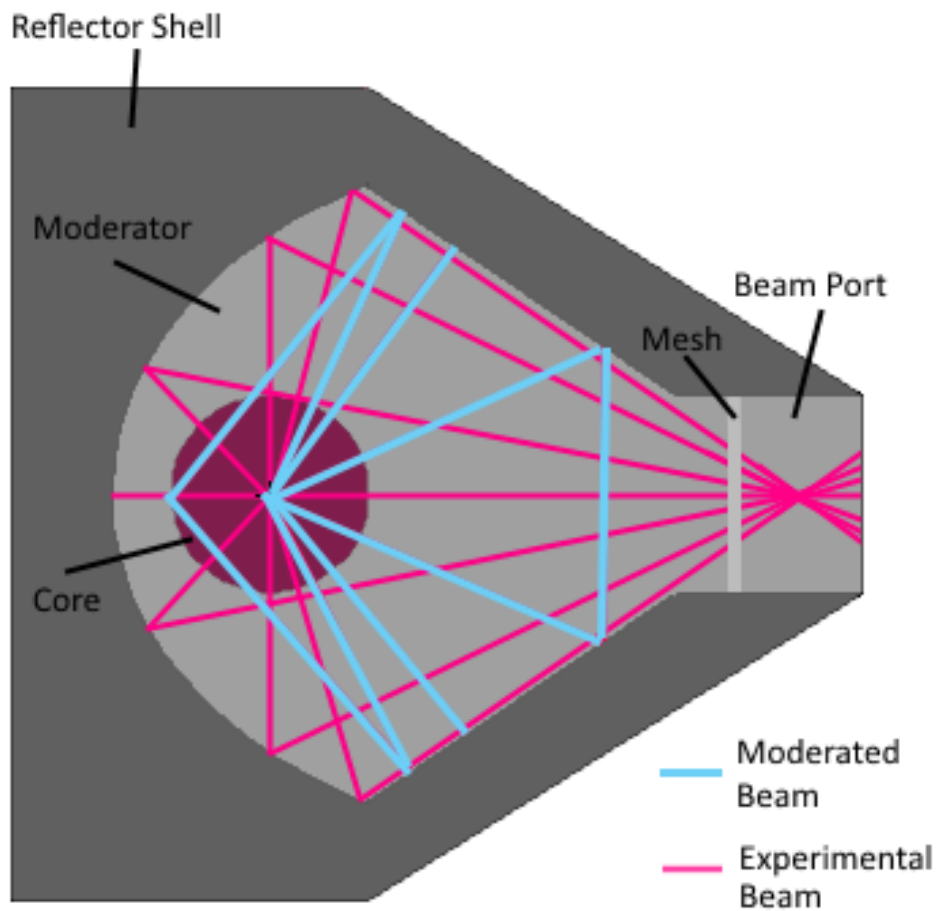


Figure 14: GOFr design

5 Conclusion

The goal of this project was to design a reactor concept that would generate a high neutron flux in a small form factor, something that could fit in a room optimistically. The flux of GOFR exceeds other research reactors, by a factor of a 180 compared to the UMass Lowell reactor. The final dimensions of GOFR are about 2 meters on all sides. The size of the Lowell reactor is not publicly available but it is a swimming pool type reactor, which range from about 60 to 365 cubic meters. GOFR is 8 cubic meters, which means that it could fit in the bedroom of a rundown Brooklyn apartment, with a twin bed, and lots of shelf space if no city statutes are violated and the room is somewhat squarish. By those metrics, the goal was reached.

Cooling is not yet accounted for, and that will add not insignificant volume, but that should be able to be done compactly enough that it still retains its appeal. The flux is somewhat artificially high due to not being collimated but that should not meaningfully decrement the neutron flux. The primary utility and value of this design is the somewhat novel approach to generating a high neutron flux, which was proven to be useful and consequential.

The design can be used in a variety of labs due to its small size, lower cost, and competitive neutron flux. This will fill the niche of cheap, affordable neutron sources for smaller research labs with limited funds or space and allow research into various kinds of neutron imaging, relieving the pressure on larger neutron sources and allowing for rapid experimental development. Research will be done by more people and more quickly. Furthermore, this could aid in medical isotope production, and perhaps even provide small amounts of power.

6 Future work

There are many areas where this project could be extended or improved. Those are, but not limited to, simulation of a collimator, better characterization of the beam, thorium conversion, thorium breeder conversion, better alloys in the core, analysis of the core behavior, thermal simulation and regulation, cost analysis, actual nuclear engineering, and building the reactor.

6.1 Collimation and Characterization

The beam produced currently has a slightly higher intensity in the center, if measured at the focal point, and is uniform if measured far enough away from the focal point. However, the vector of travel of the neutrons is not parallel and, if a lower energy beam is desired, there is no way to modulate the neutron energy. These discrepancies in trajectories can be remedied by a collimator. It will thermalize and collimate the beam, making it useful for imaging. This, however, needs to be simulated to ensure that the benefits of this design of reactor are sustained and the resultant beam is useful.

6.2 Core Advancements

This reactor core, specifically the use of zirconium hydride, was inspired by the TRIGA reactors. However, in this case, the alloy seemed to have made little difference in the performance of the reactor, which was surprising. Further research into what is happening and ensuring that the benefits are realized is important to maximize the utility of this reactor. Furthermore, the amount and type of alloy to use was a bit difficult to determine and requires more research to be done optimally.

Converting the fuel used to thorium would be a good advancement on this reactor as it would be consistent with the ideals of GenIV reactor design. Furthermore, if this thorium reactor could be used to breed more thorium, that would be an efficient use of resources and have applications in broader areas.

6.3 Engineering Concerns

Engineering is outside the scope of this project but a few concerns were kept in mind during the design of GOFR. The aim was for GOFR to passively reduce criticality as the temperature reached unsafe levels. Therefore, for sustained high level power, adequate cooling is needed for optimal behavior. To that end, the design hoped to use the aluminum to quickly and efficiently transport heat from the core to the graphite shell. In the shell, there would be a matrix of pipes for coolant to flow through and/or coolant would flow over the surface of the shell, conducting heat away. The cooling system in mind during the project was a compact magnetic refrigeration system, using a gallium alloy in a magnetic field to magnetocalorically cool the reactor. The energy for this could potentially be subsidized by the heat of the reactor itself. Alternatively, since this reactor is meant to be housed in a relatively small space on a academic campus, this could augment HVAC systems as a source of heat and energy. The main idea of the project is to not waste neutrons. This would be a poetic expansion into not wasting energy from neutrons.

Furthermore, this was not designed by nuclear engineers. There are many concerns, caveats, regulations, and other such things that we are wholly ignorant to. This requires thorough and extensive development by people that are more qualified with software more powerful than a Monte Carlo simulation done on overly simplistic models. There are wear, thermal expansion, refueling, safety, cooling, and cost considerations to evaluate and address. This is only the beginning of a long process.

Hopefully, one day, this will be realized in an actual reactor and be used by scientists to make the world a better place.

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Appendix

Appendix 1

c Example program source code

c Cell block

1 2 -1.7 -10 imp:N=1 \$ Inside of cube

2 1 1 (10 -20) imp:N=1 \$ Space around cube, inside graveyard

3 0 20 imp:N=0 \$ Graveyard definition

c Surface block

10 RPP -5 5 -5 5 -5 5 \$ Cube, centered at origin, 10cm side length

20 SO 100 \$ 100cm radius sphere, defines graveyard

c Material block

c M1 is water

c M2 is graphite

M1 1000 2

8000 1

M2 06012 1