Master’s Thesis Engineering Technology 2024-2025

Analysis of the most critical configuration in nuclear fuel storage using an optimization algorithm

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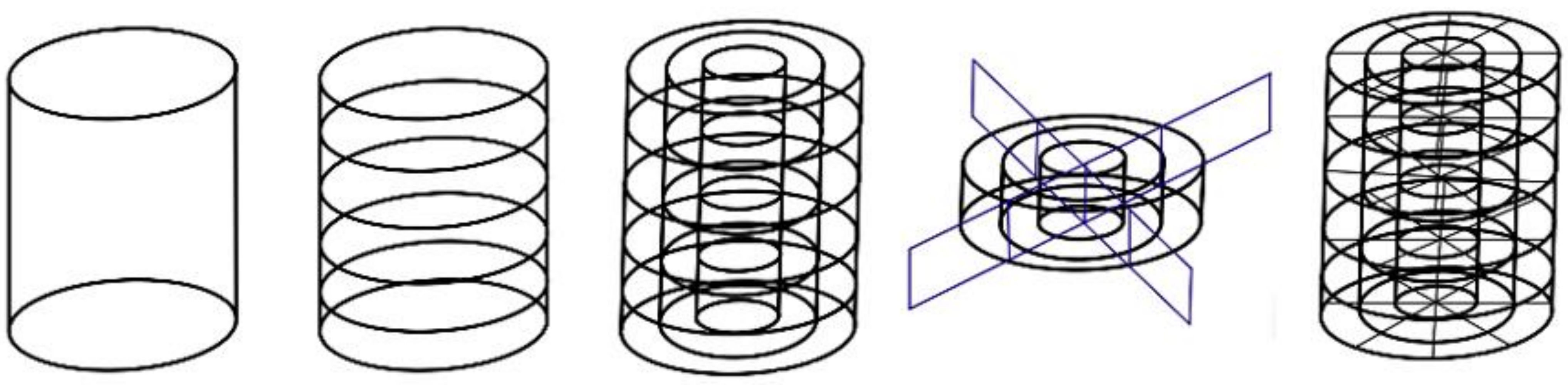
Introduction

Nuclear fission is a potent energy source but poses critical safety risks. An unintended self-sustaining chain reaction—called a **criticality accident**—can release lethal radiation. Safety depends on parameters like fissile mass, enrichment, geometry, moderation, and reflection [1].However, the **spatial distribution** of fissile material is less studied. Real-world events like precipitation or mechanical shifts can cause uneven distributions, increasing risk. This thesis explores how uranium distribution in solution **affects criticality** within cylindrical vessels—seeking to identify the **most critical configurations** based on mass and geometry.

Methodology

Vessel segmentation

To simulate non-uniform fuel distributions in **Serpent**, the cylindrical vessel must be **subdivided into many smaller regions**, each assigned a distinct material composition. This is achieved by segmenting the geometry along three axes: **axially** (into horizontal discs), **radially** (into concentric rings), and **planarly** (into wedge-shaped sectors). This approach allows for a detailed representation of complex distributions. Figure 1 shows the segmentation process.



a) Initial cylinder b) Axial segmentation c) Radial segmentation d) Planar segmentation e) Final result

Figure 1: Division of the cylinder into cells

Optimization Algorithm

A **genetic algorithm** (GA), implemented in Python, is used to identify the most critical spatial distribution of fissile material. Each solution (or “individual”) is represented by a DNA-like array that defines how uranium mass is allocated across the vessel’s cells.

For each individual, a Serpent Monte Carlo simulation is performed to evaluate the effective multiplication factor (keff) which serves as the fitness value. Based on fitness, the best-performi individuals are **selected** and combined through **crossover** to produce new “offspring.” These are then slightly altered using **mutation** techniques [2]. This evolutionary process is repeated over multiple generations to approach an optimal configuration. Figure 2 illustrates the working principle of the genetic operators in greater detail.

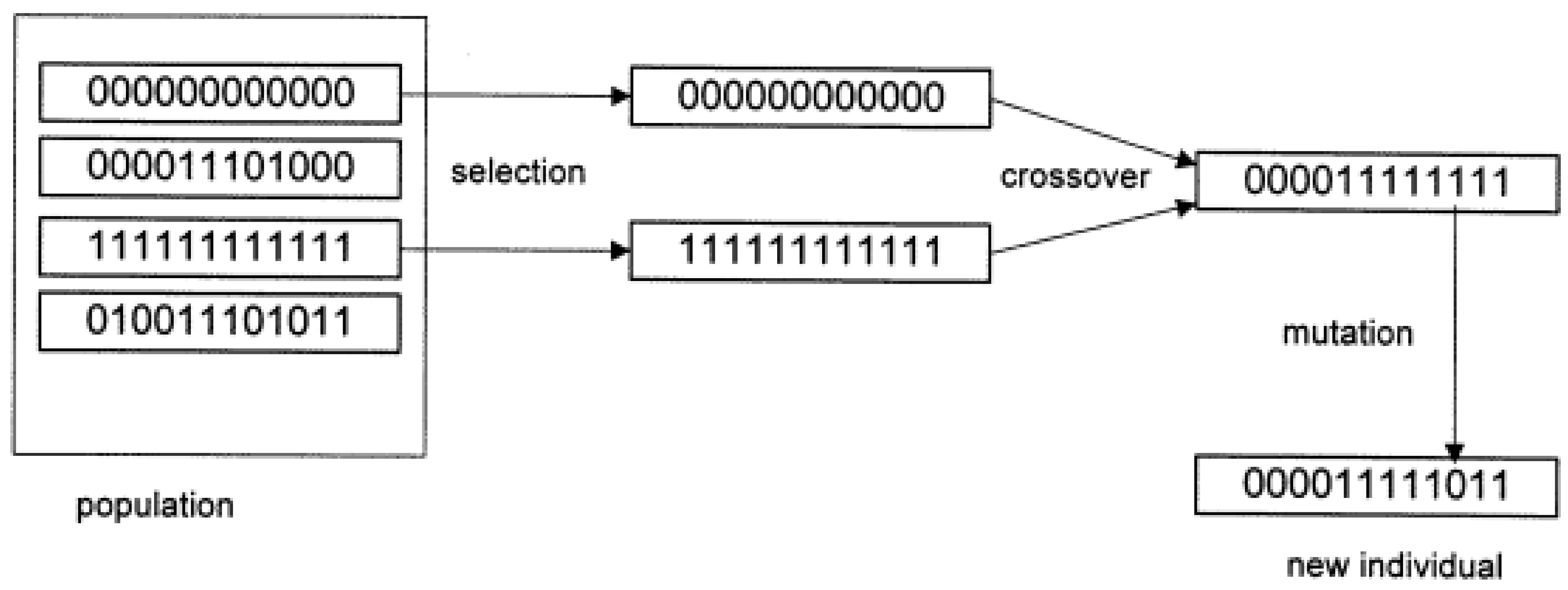


Figure 2: Genetic operators : selection, crossover and mutation [2]

In parallel, a **Bayesian Optimizer** is integrated into the algorithm. It maintains a record of previously evaluated individuals and their fitness scores, and uses this data to make informed predictions about promising new configurations via an **acquisition function**.

Biased distributions

The initial population of uranium distributions includes both random and biased configurations. Random distributions **promote diversity** and help avoid premature convergence in the optimization process. In contrast, biased configurations—such as uniform or centrally concentrated distributions—are deliberately chosen to **explore known extreme cases**. The combination of randomness and strategic bias improves the algorithm’s robustness. Figure 3 gives an overview of the distributions.

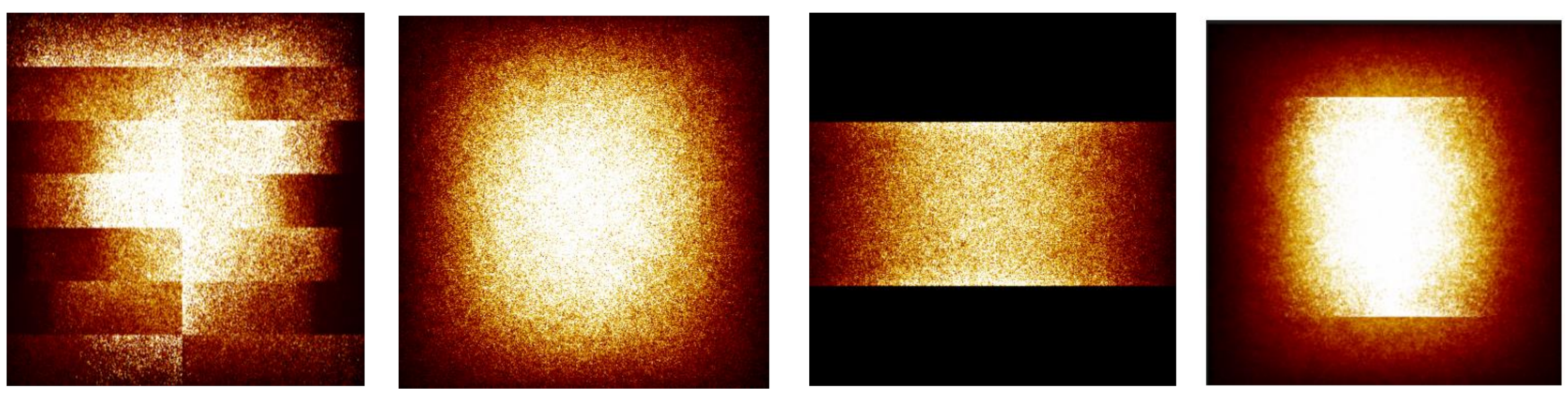
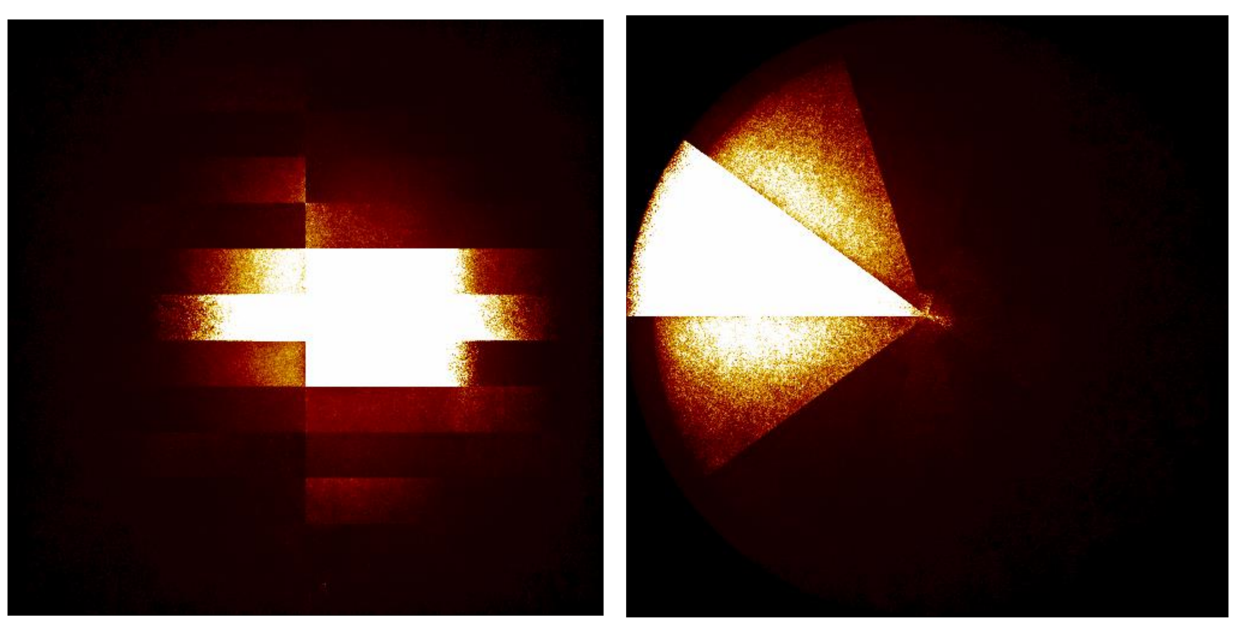


Figure 3: Lateral view of random, uniform, axially centered and concentrated distributions respectively

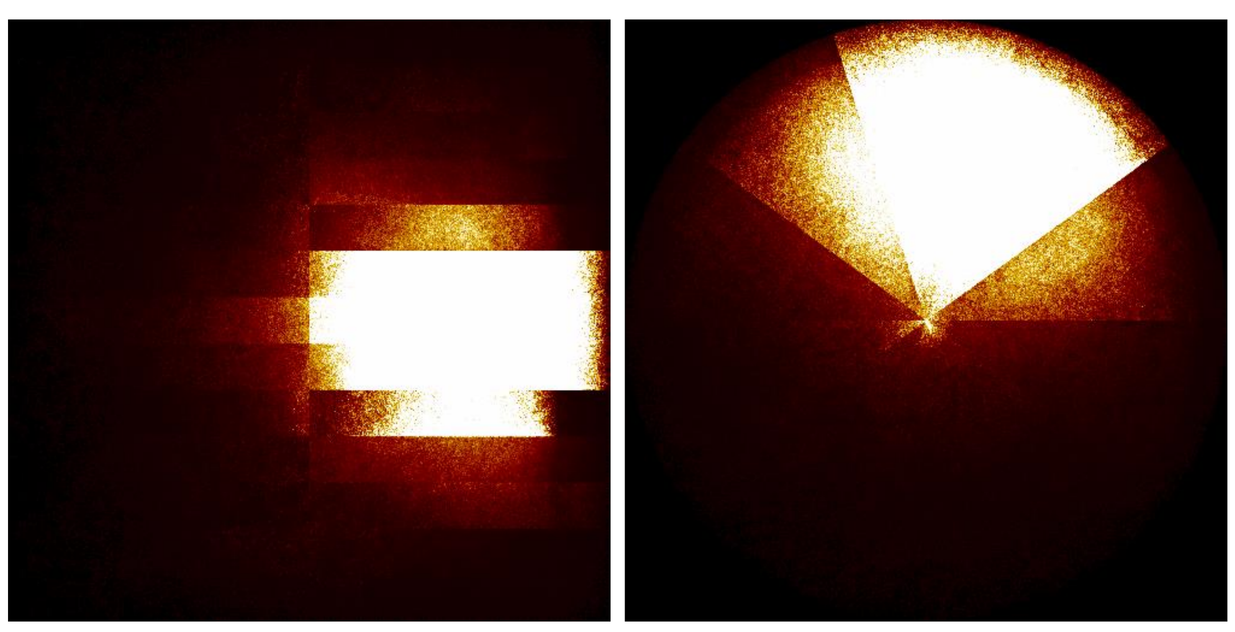
Results

Simulations using 1430 cells, 100 individuals, and 5-day wall time were performed on a **supercomputer**. The genetic algorithm found more critical distributions than initial biases in several cases. However, some runs failed to reach criticality, revealing a trade-off between **convergence speed** and **solution quality**. Geometry and uranium mass influenced the resulting distributions. Key **limitations** included small population size, high computational cost, and HPC-related issues. Figures 4 and 5 show two configurations with identical geometry but different uranium masses.



(a) Lateral view ($keff = 0.968386$) (b) Top view ($keff = 0.968386$)

Figure 4: Most critical distribution – 40cm × 70cm, 1500g, 242 gens



(a) Lateral view ($keff = 1.08485$) (b) Top view ($keff = 1.08485$)

Figure 5: Most critical distribution – 40cm × 70cm, 3000g, 180 gens

Conclusion

This study shows the potential of genetic algorithms to optimize fissile material distributions in criticality simulations. The algorithm **outperformed** initial biased inputs but did not always reach **criticality**, underscoring the need for **faster convergence** under limited resources. **Future improvements** should focus on reducing simulation time, using adaptive Serpent settings, progressive segmentation, and prior data for initialization. **Tuning algorithm** parameters like mutation rate, selection method, and Bayesian optimization may also boost performance.

Supervisors / Co-supervisors / Advisors: Prof. dr. ir. Van den Eynde Gert

[1] N. L. Pruvost and H. C. Paxton, “Nuclear Criticality Safety Guide,” Tech. Rep. LA-12808, Los Alamos National Laboratory, 1996.

[2] V. Podgorelec, J. Brest, and P. Kokol, “Power of Heterogeneous Computing as a Vehicle for Implementing E3 Medical Decision Support Systems,” *Studies in Health Technology and Informatics*, vol. 68, pp. 703–708, 1999.