Genetic Algorithm-Based Optimisation of the Few-Group Structure for Lead Fast Reactors Analysis

M. Massone, N. Abrate, G. F. Nallo, S. Dulla, P. Ravetto, D. Valerio

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Motivation

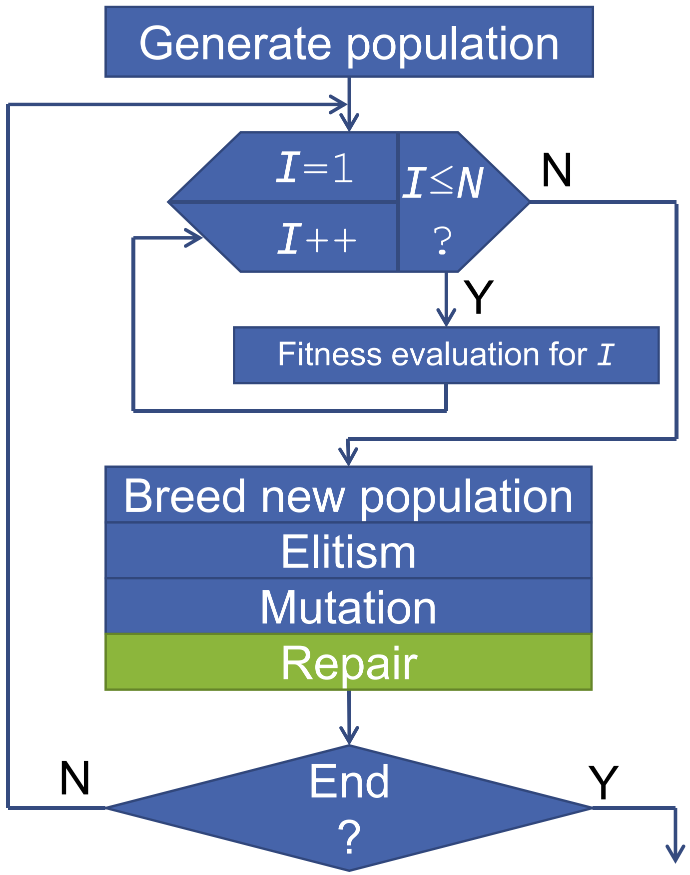
Need for accurate computational models for design safety assessment and operation	• 2-group calculation, common for LWRs, is often inaccurate for fast reactors
Full-core analyses are based on deterministic multi-group calculations	• Especially transient, coupled analyses • Only few-groups analyses are actually viable
The definition of a few-groups energy structure for a fast system is still an open problem	• Lack of a general algorithm and problem stiffness • Somewhat of an art.

Motivation

- The problem is often addressed by expert judgement
  - Criteria are vague and arbitrary
  - Aim an <u>automated</u> and <u>reproducible</u> results
- Approach the problem with Artificial Intelligence
  - Optimization algorithm
  - Access to non-obvious solutions
- The problem is sensitive to schemes
  - Each group influence the others, especially neighboring ones
  - Genetic algorithm is an excellent option for its ability to preserve schemes

The genetic algorithm (GA)

- Start from a random possible solution set (**population**)
- For each of these solutions (**individuals**), the value to optimize (**fitness**) is calculated
- Individuals are **selected** based on their fitness and they breed the next generation by **crossing-over**
- Best individuals from the old population can survive and pass to the next one (**elitism**)
- New individuals can change due to **mutation**.
- Repeat until a termination condition occurs



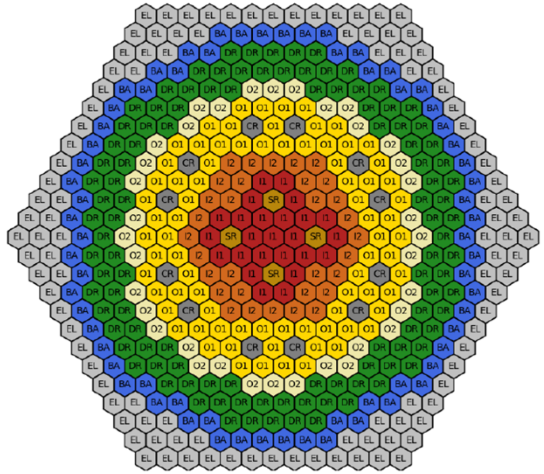
Methodology summary

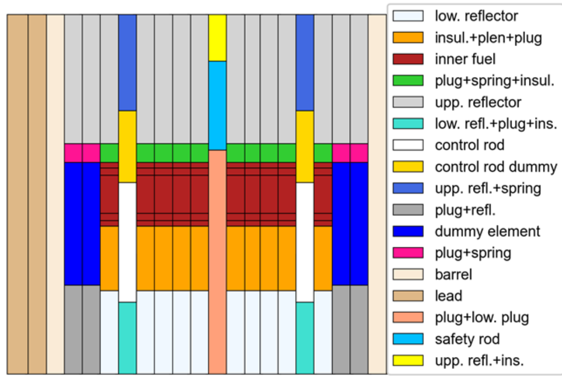
Generation of the fine-group libraries	Serpent 2 HDF format to improve data readability, memory management, consistency, flexibility *
Import these libraries into SIMMER	Development for SIMMER to read HDF libraries Cross-section processing in SIMMER skipped
Set the fitness function	Import Serpent flux and k_{eff} Objective values for optimization
Run the genetic algorithm	Results compared with the Serpent objective values Many few-groups calculations

* **M. MASSONE, N. ABRATE, G. F. NALLO, D. VALERIO, S. DULLA, P. RAVETTO, „Code-to-code SIMMER/FRENETIC comparison for the neutronic simulation of lead-cooled fast reactors", Ann. Nucl. En. 174 (2022)**

Fine-group cross section generation

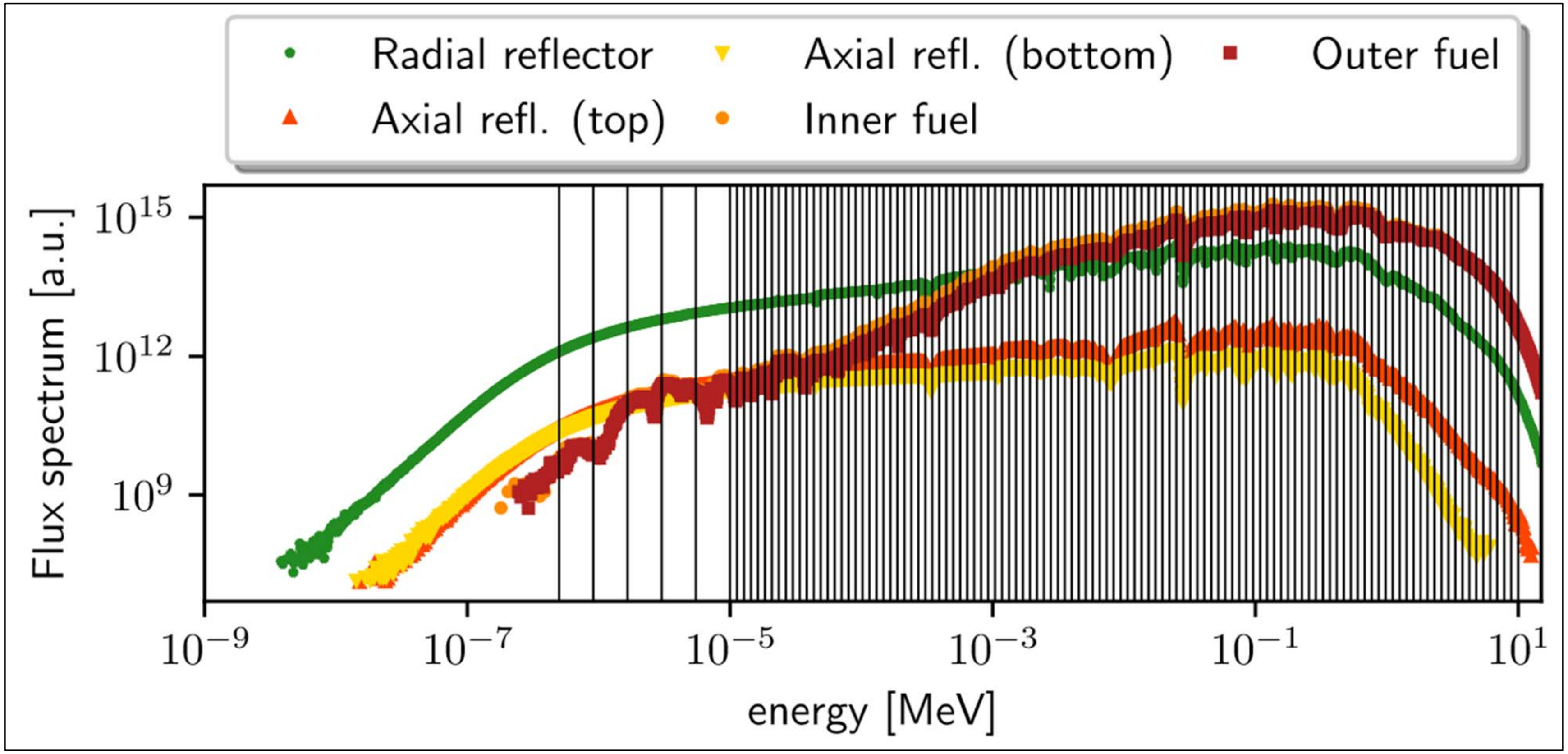
- Start from continuous-energy ENDF-B/VIII.0 libraries
- Serpent 2 model to generate:
  - Fine-group cross section library
  - Calculation of neutron flux and multiplication factor
- ALFRED core model (LEADER project)
  - Uniform temperature: 673 K
  - BoC conditions
  - Close-to-critical system ($k_{\text{eff}} = 1.00002(4)$)
- We will not be able to subdivide fine-groups
  - Large number at the beginning: 120 groups
  - 114 equally spaced (in lethargy) groups in the central spectrum zone
  - Compromise at the energy space extremes to limit statistical noise





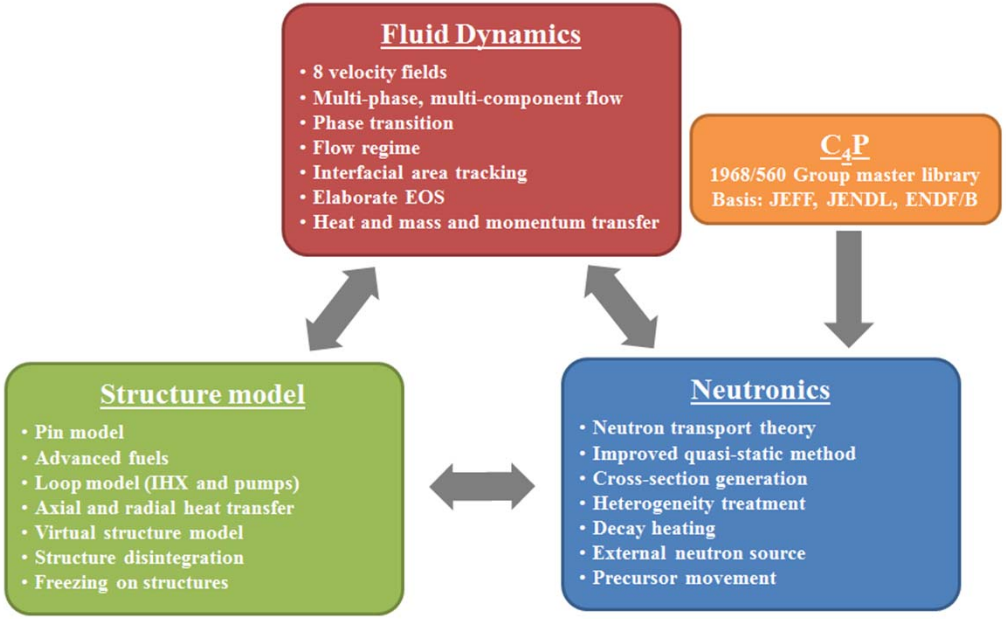
G. F. NALLO, N. ABRATE, S. DULLA, P. RAVETTO, D. VALERIO, „Neutronic benchmark of the FRENETIC code for the Multiphysics analysis of lead fast reactors.", European Physical Journal Plus 135 (2020)

Fine-group cross section library



Introduction to SIMMER

- SIMMER is a mechanistic, multi-velocity-field, multiphase, multicomponent, Eulerian fluid-dynamics code coupled with a space-dependent neutron kinetics model and a structure model.
- Developed for safety studies of liquid-metal-cooled fast reactors
  - Further developed and improved, it has been applied successfully to LWRs and general multiphase problems
- Extended to read fine libraries from Serpent and with a cross-section condensation tool



The fitness function

- The fitness function is the driving force of the algorithm
  - Its choice reflects the aim given to the GA by its designer
- Our objective: Energy discretization that best allows SIMMER to match the Monte Carlo results

$$f_{\mathrm{k}}^{I} = \left| k^{I} - k^{\mathrm{MC}} \right|$$

$$f_{\phi}^{I} = \sqrt{\sum_{g} \sum_{j} w_j \left(\phi_{g,j}^{I} - \phi_{g,j}^{\mathrm{MC}} \right)^2}$$

$$FF^{I} = \sqrt{f_{\mathrm{k}}^{I} \cdot f_{\phi}^{I}}$$

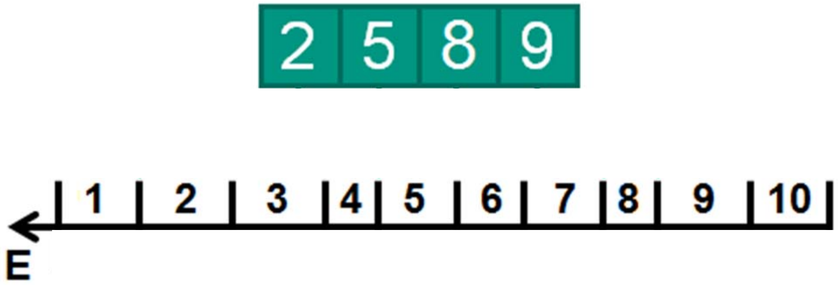
Equal weighting

$$\hat{f}_{\mathrm{x}}^{I} = 1 + \frac{f_{\mathrm{x}}^{I} - \min\limits_{S \in U} f_{\mathrm{x}}^{S}}{\max\limits_{S \in U} f_{\mathrm{x}}^{S} - \min\limits_{S \in U} f_{\mathrm{x}}^{S}} \cdot 9$$

$$FF^{I} = \sqrt{\hat{f}_{\mathrm{k}}^{I} \cdot \hat{f}_{\phi}^{I}}$$

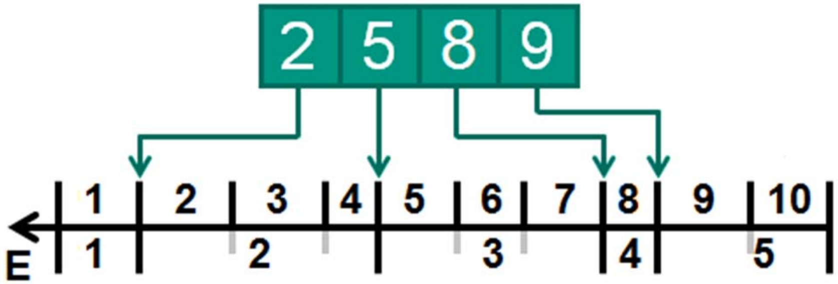
Individual representation

- The way genetic information is expressed

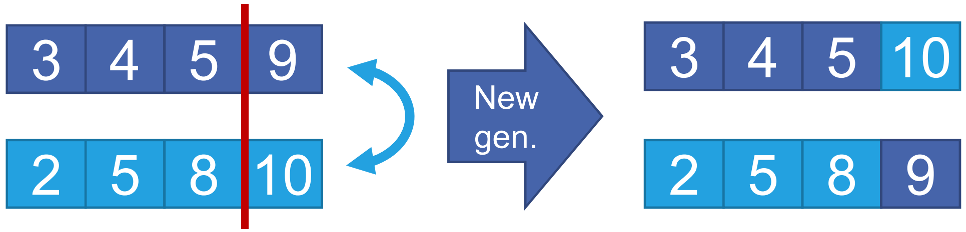


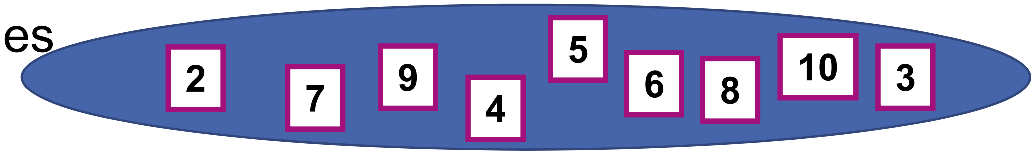
Individual representation

- The way genetic information is expressed



- Integer representation
  - Easy crossing-over
  - Limited allele pool
    - Chromosomes are combinations of alleles

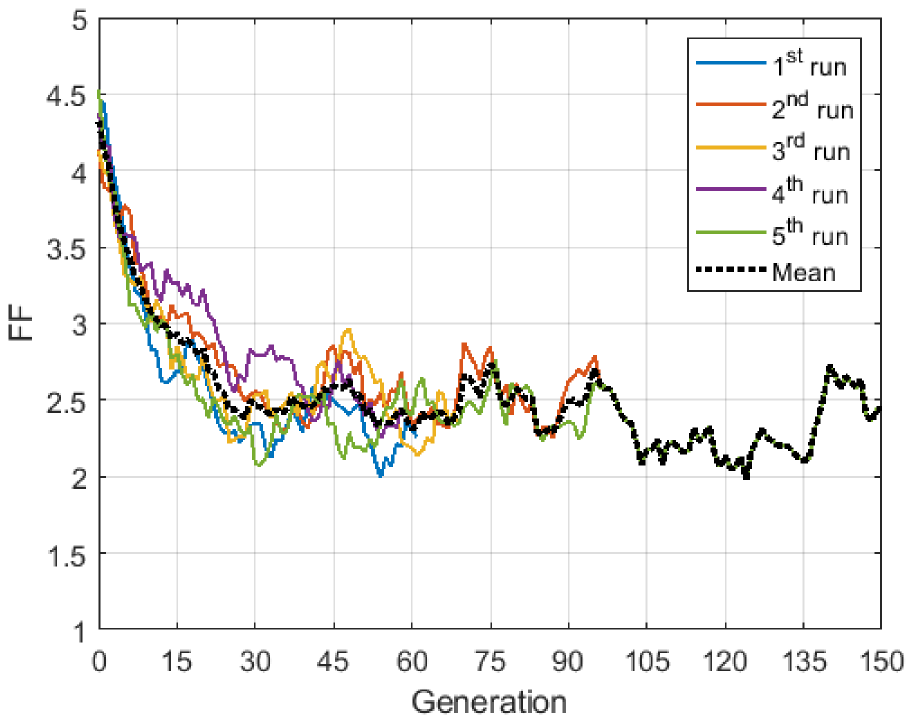




M. MASSONE, F. GABRIELLI, A. RINEISKI, "A genetic algorithm for multigroup energy structure search", *Annals of Nuclear Energy* 105, p. 369-387 (2017)

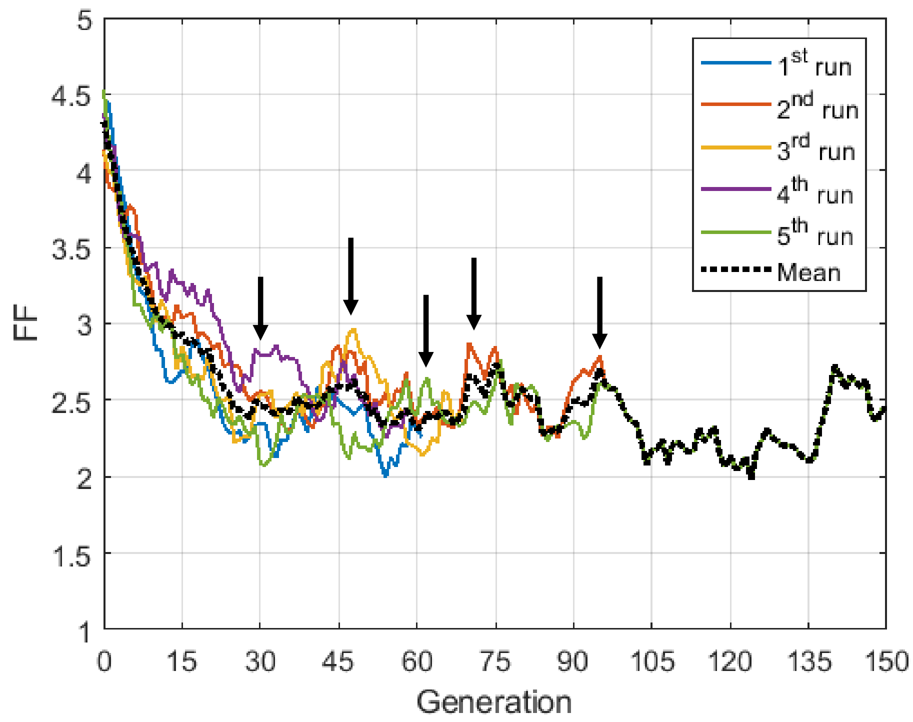
Convergence

- 5 identical runs
  - Exclude genetic drift
- Fitness improvement is concentrated in the first 30 generations
  - Later adjustments (exploitation)

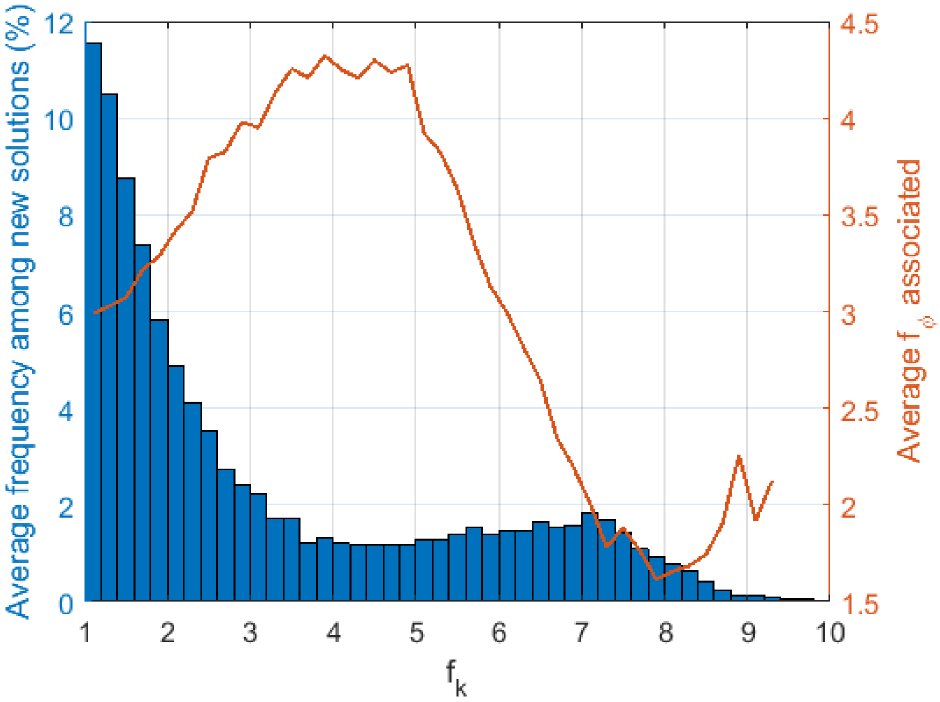


Convergence

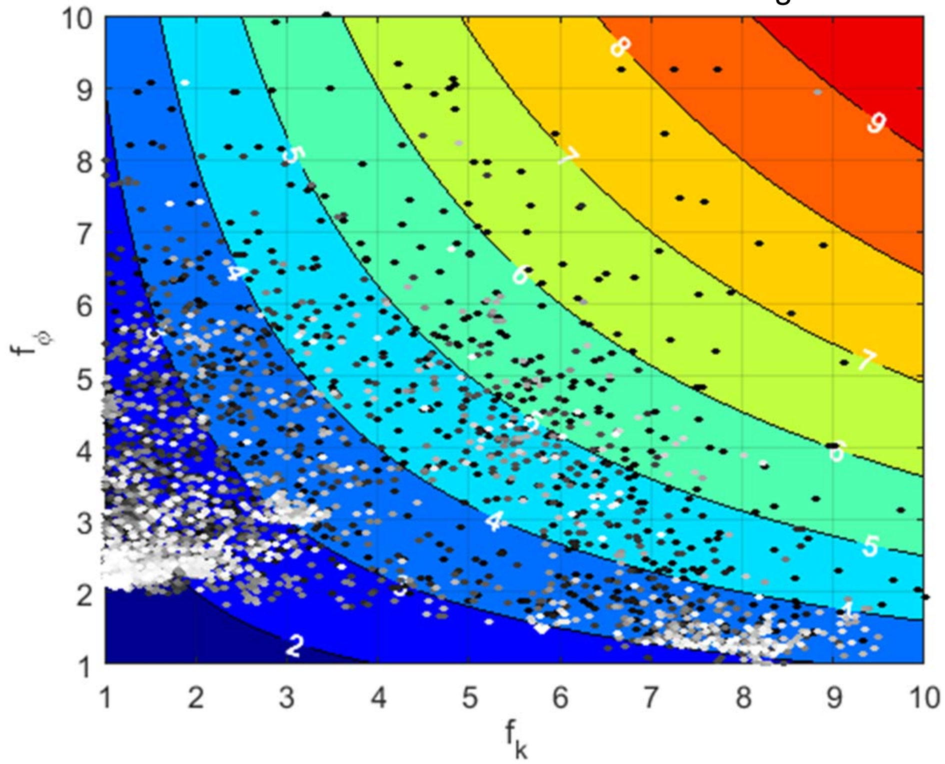
- 5 identical runs
  - Exclude genetic drift
- Fitness improvement is concentrated in the first 30 generations
  - Later adjustments (exploitation)
- Spiky pattern
  - Accommodated in few generations
  - Usual exploration of new zones
  - Definition of the fitness function: <u>the fitness is rescaled at every improvement</u>



Fitness distribution



Dots are darker for older generations



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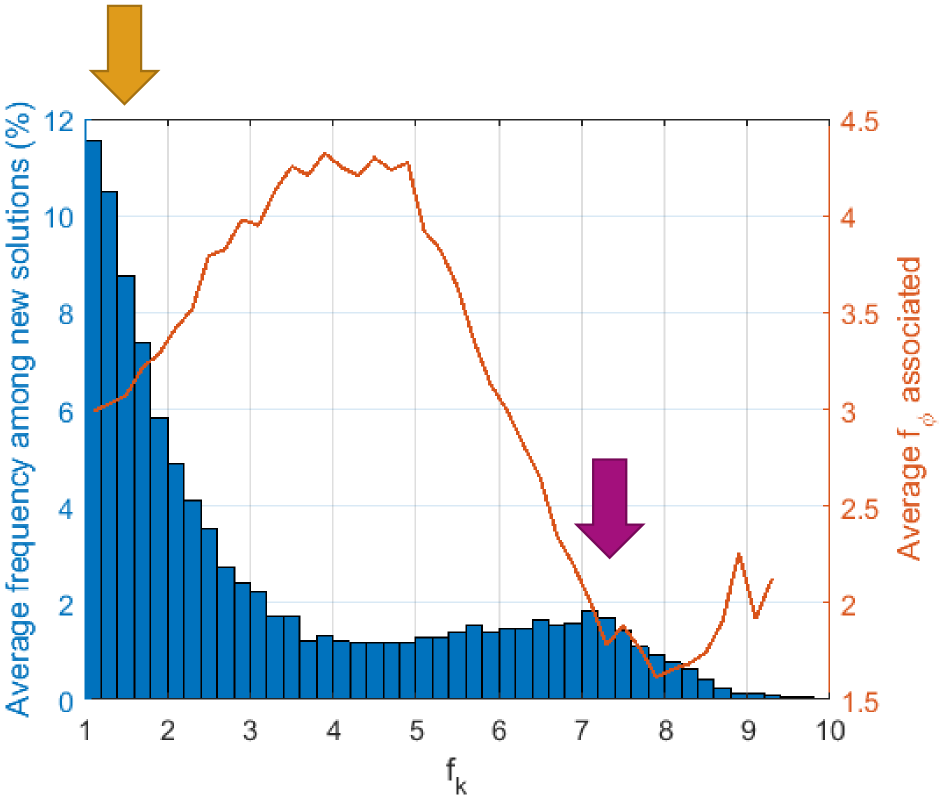
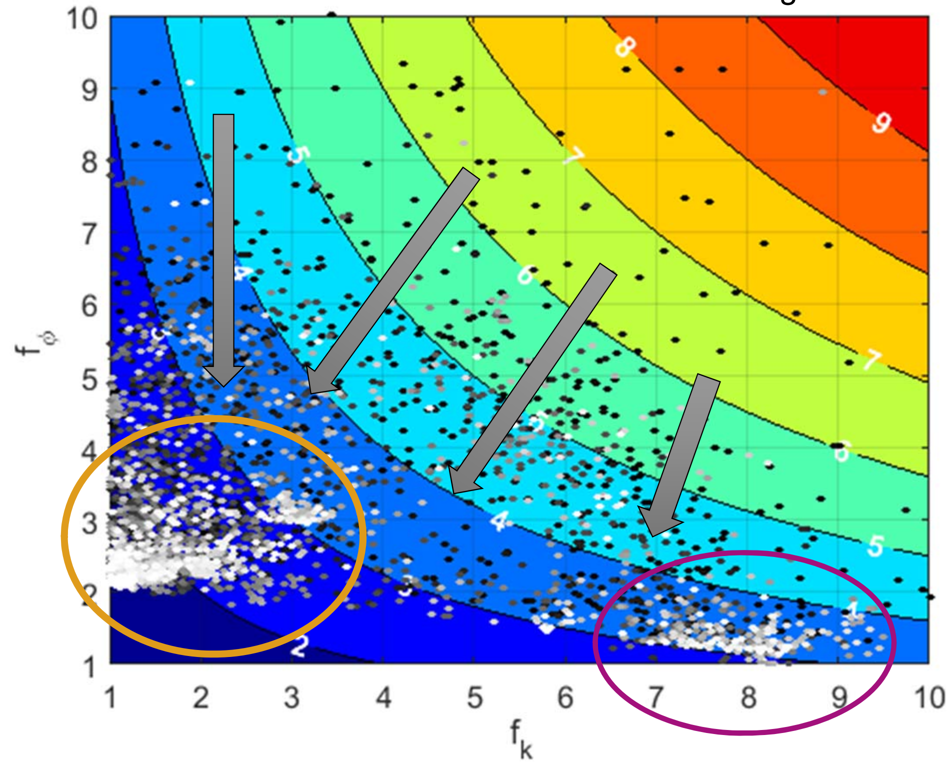
Fitness distribution





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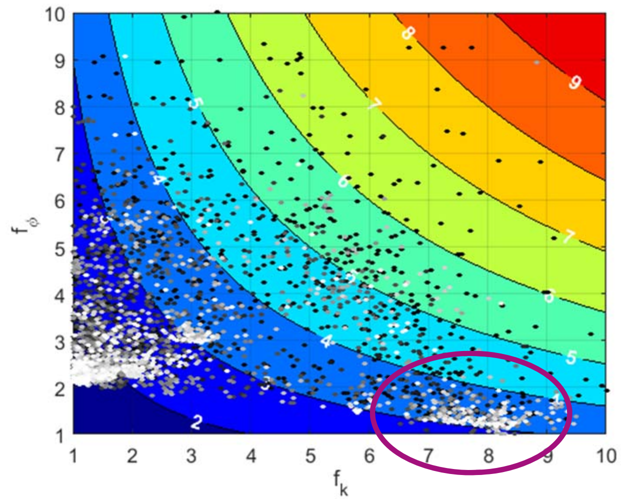
Be careful what you wish for…

- A cluster of candidate solutions with good f_{ϕ}^{I} and bad f_{k}^{I}
  - The GA found a vulnerability in the f_{ϕ}^{I} definition
  - Good score, but fail to represent the physics
  - Not necessarily bad: slower convergence, but preserve variaty in the gene pool
    - Uniformity harms the exploration capability of the GA



- Recall our objective: <u>Energy discretization that best allows SIMMER to match the Monte Carlo results</u>
  - That's what we get!

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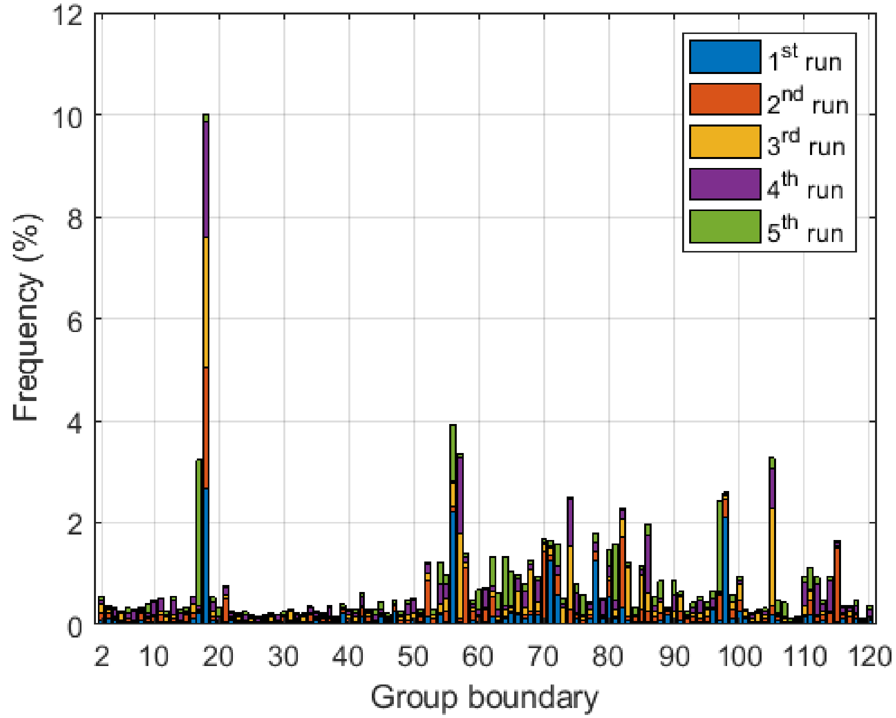
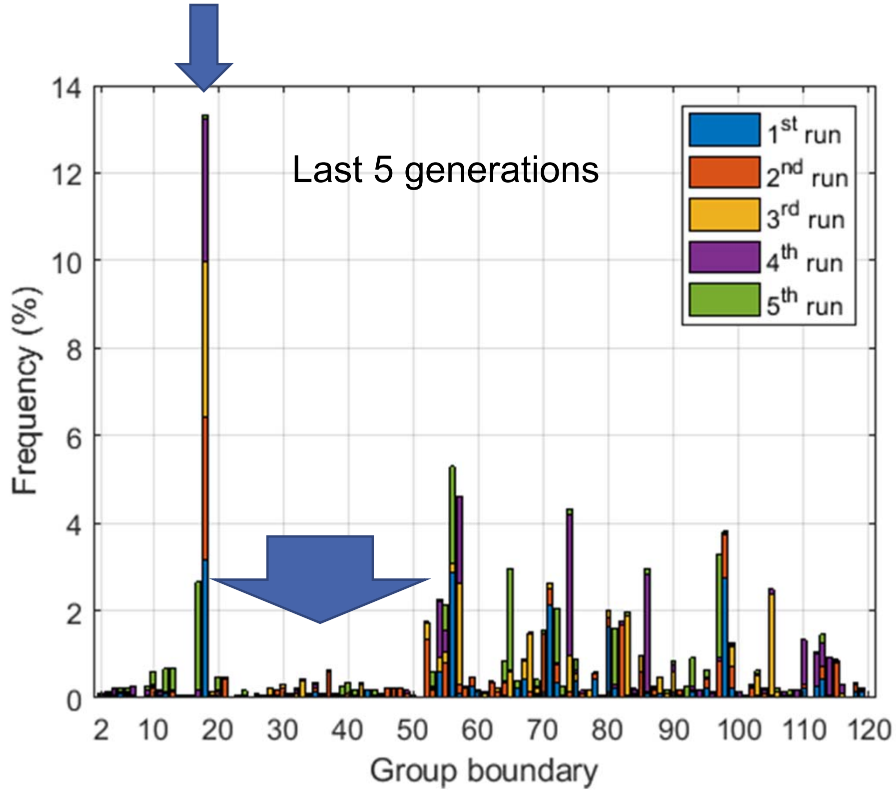
Traits success and extinction

- Positive traits tend to survive, negative ones do not last.

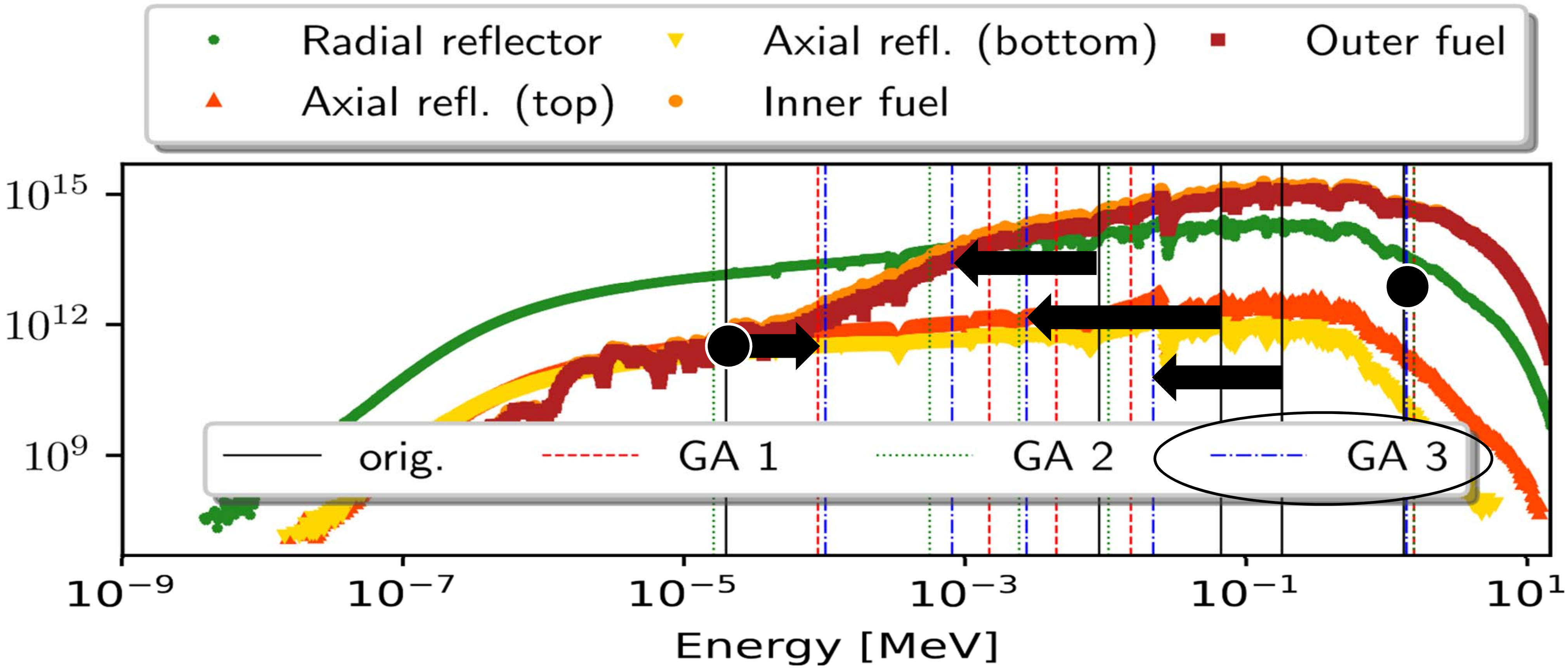


Successful alleles

- Positive traits tend to survive, negative ones do not last.
- All simulations agree in a first energy boundary at 1.4-1.6 MeV
  - Tail of the fission spectrum
- Large empty region
  - Energy groups are a scarce resource
  - They are better invested in other zones of the spectrum



Structures comparison



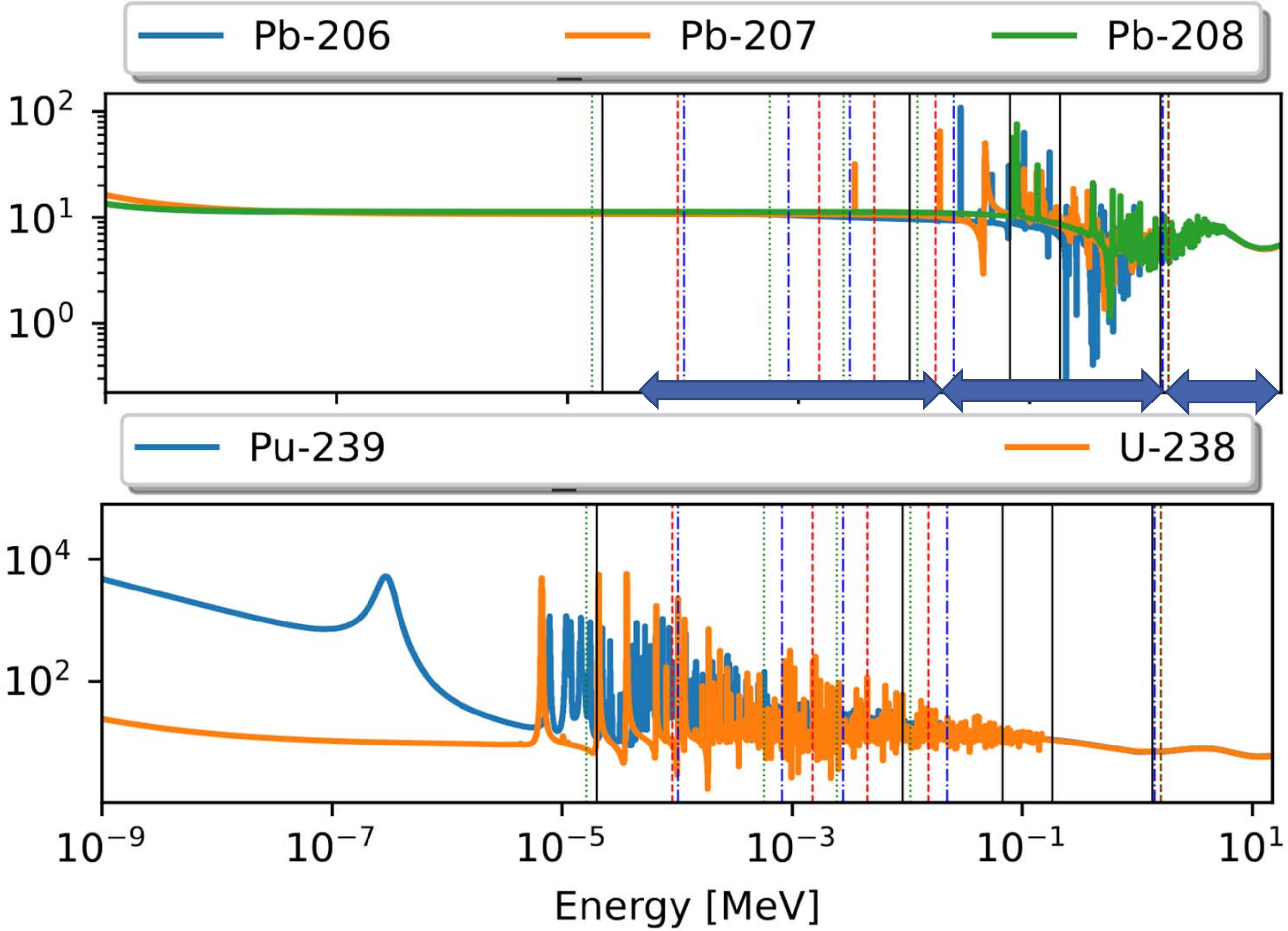
Rationalization

Group 2
Pb resonances

Group 6
Low energy

A low energy group must exist also for fast cores

Rarely more than one



Group 1: Fission production

Group 3, 4, (5)
U and Pu resonances

High frequencies observed around 200 eV: the limit for the major Pu resonances

Conclusion and perspectives

- In the framework of FR development (especially for accidental transients) the energy structure problem plays an important role.
- We have employed a genetic algorithm for the condensation of fine-groups libraries generated with Serpent 2.
- The SIMMER code has been used for the few-groups calculations.
- The fitness function has been chosen such that the SIMMER transport solver matches the Monte Carlo results.
- The GA finds satisfactory solutions for the given objectives.
  - Accurate results in terms of both multiplication factor and flux distribution.
- The results can be reasonably interpreted in light of the underlying physics.

Conclusion and perspectives

Study the impact of the initial number of fine-groups	
Different fitness functions	Adjoint flux weighting Feedback effects
Consider transient case	Multiple temperatures and conditions
Leave the GA free to choose the number of groups	Model the trade-off accuracy/computational time/convergence trend
Increase the procedure flexibility	Standalone GA framework for nuclear applications

Thank you for your attention!

Politecnico di Torino

Karlsruhe Institute of Technology

Questions?

Energy structures

Original

2.000×10^{1}	1.353	1.832×10^{-1}	6.738×10^{-2}	9.119×10^{-3}	2.000×10^{-5}	1.000×10^{-11}

GA optimized

2.000×10^{1}	1.5979	1.5341×10^{-2}	4.5172×10^{-3}	1.5031×10^{-3}	9.0313×10^{-5}	1.000×10^{-11}
2.000×10^{1}	1.5979	1.0630×10^{-2}	2.4512×10^{-3}	5.6521×10^{-4}	1.6308×10^{-5}	1.000×10^{-11}
2.000×10^{1}	1.4140	2.2138×10^{-2}	2.7700×10^{-3}	8.1565×10^{-4}	1.0206×10^{-4}	1.000×10^{-11}

Hyperparameters

- Population size: 80
- Tournament selection
  - 30 tournaments
  - Probability parameter: 0.15
- Mutation rate: 15%
- Elitist selection: 5%
- Termination conditions
  - Maximum number of generations: 150
  - 30 generations without improvements
  - Time limit: 10^5 s