Shielding calculations with Markov chains and genetic algorithms

Konstantin Batkov[1]
Stuart Ansell[1]
Phil Bentley[2]
Leonid Kurakhtenkov

[1]MAX IV Laboratory, Lund University, Lund, Sweden
[2]European Spallation Source, Lund, Sweden

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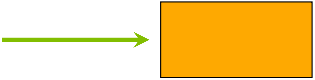
Outline

Outline

How to stop a beam?

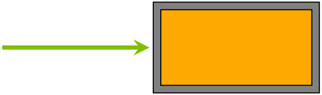
- $\sim$ few GeV electrons,
  - but does not really matter
- Imagine how you would do it . . .

Motivation
How to stop a beam?



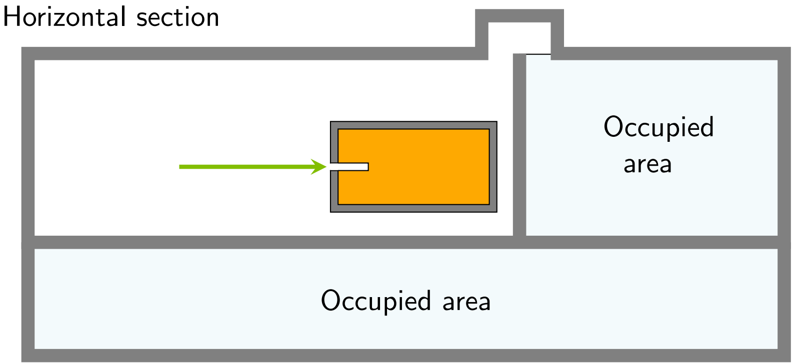
Probably:

- Use a heavy material block to stop γ
  - but keep in mind its Z to reduce (γ,n)



Probably:

- Use a heavy material block to stop γ
- Surround it with something light to slow down fast neutrons
  - to increase $\sigma(\mathrm{n},\gamma)$

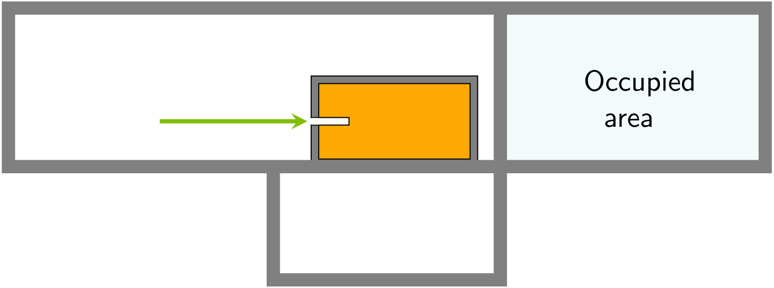


Probably:

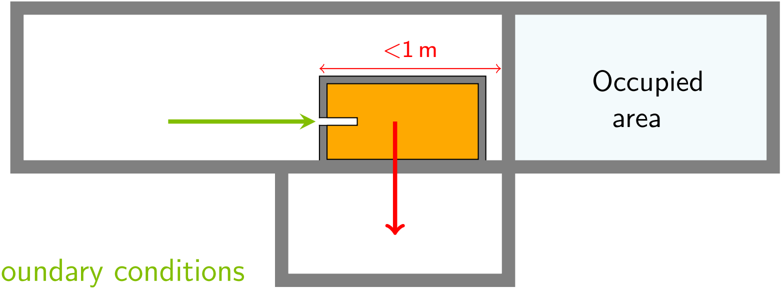
- Use a heavy material block to stop γ
- Surround it with something light to slow down fast neutrons
- Optimise dimensions to reduce dose rates where needed

- Sounds easy?
- Challenge comes from the **boundary conditions**:
  - beam dumps are normally **large and heavy**
  - but this one should be **small and light**

Vertical section



Vertical section



Boundary conditions

- Limit **dose rates** in the occupied areas
  - both forward and lateral
- Fit within the horisontal **space** (1 m)
- Minimise **weight** (load on the floor)
- Minimise **cost** and **complexity**

Multi-dimensional optimisation

- Parameter space
  - Dimensions
  - Materials
    - either heterogeneous or homogeneous

Multi-dimensional optimisation

- Parameter space
  - Dimensions
  - Materials
    - either heterogeneous or homogeneous
- Monte Carlo runtime
  - Single configuration: $\sim$4 h on 100 cores ← slow
    - with aggressive variance reduction

⇒ Can't explore large parameter space

Simplification needed

Outline

Inspiration

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RESEARCH ARTICLE

MEDICAL PHYSICS

An iterative prediction method for designing the moderator used for the boron neutron capture therapy

Ruiqin Zhang[1,2] | **Yangyi Yu**[1,2] | **Zhi Zhang**[1,2] | **Yigang Yang**[1,2]

[1] Department of Engineering Physics, Tsinghua University, Beijing, People's Republic of China

[2] Key Laboratory of Particle & Radiation Imaging, Tsinghua University, Ministry of Education, Beijing, People's Republic of China

Correspondence
Yigang Yang, Department of Engineering Physics, Tsinghua University, Beijing, People's Republic of China.
Email: yangyigang@mail.tsinghua.edu.cn

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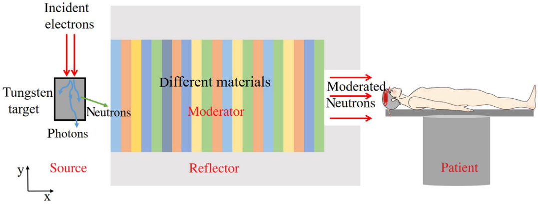
Abstract

Purpose: To conduct research related to slow neutrons, fast neutrons must be mode-rated and shifted to the desired energy region.

Methods: In this research, an iterated prediction method, in which the neutron transportation properties of all materials were characterized by a reflection matrix, ***R***, and a transmission matrix, ***T***, was proposed to bypass a time-consuming Monte Carlo simulation and predict the performance of the moderator, including the epithermal neutron flux and the dose of fast neutrons and gamma rays, used for boron neutron capture therapy (BNCT). To find the optimal solution in the huge parameter space, a genetic algorithm combined with transmission and reflection matrices was utilized.

Results: The results showed that a 70-loop iteration was able to find a design for the moderator of BNCT with almost 80% higher epithermal neutron flux per kilowatt than that of the empirically optimized moderator that was previously reported in the literature. Compared with the Monte Carlo method, this method had the advantage of reducing the calculation time and statistical errors.

Inspiration

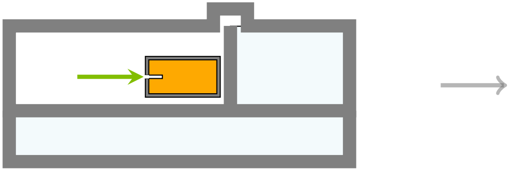


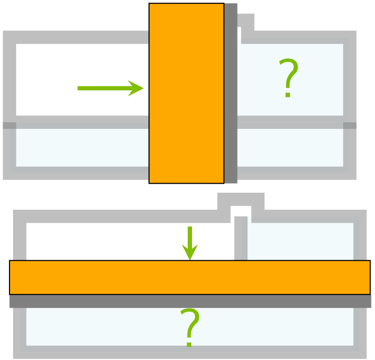
[R. Zhang et al]

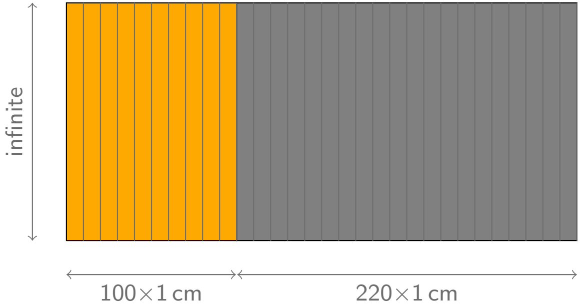
- The paper describes a methodology of 1D neutron transport with **transmission matrices**
  - and optimisation of the moderator layout with **genetic algorithms**
- We extended it to transport **arbitrary number of particle types** including conversion between particle types
  - and improved accuracy utilising the **Markov chain process**

Outline

The radiation transport is simplified by performing it along a single direction at a time







- The material is split by thin layers
- For each material, its Green's functions are pre-calculated with Monte Carlo (needs to be done once)

Green's functions — definition

If one knows the solution $G(x, x')$ to a δ-function

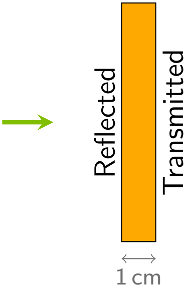
$$\hat{L}(x)\, G(x, x') = \delta(x - x')$$

then one can fold them to build the solution

$$u(x) = \int f(x')\, G(x, x')\, dx'$$

for a general source term

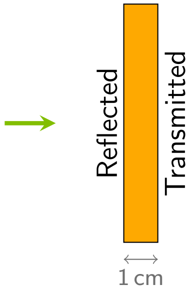
$$\hat{L}(x)\, u(x) = f(x)$$

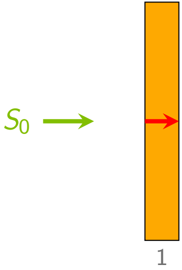


Green's functions — calculation

1. Bin the **energy range** of interest
2. Bin the **angular range** $[-\pi, \pi]$
3. For each incident **particle type, energy and angle** calculate double **differential spectra** of reflected and transmitted particles with Monte Carlo
4. Use these spectra to build **reflection** and **transmission** matrices for each particle type, i.e. for neutrons and photons:
   - $R_{n\to n}$, $R_{n\to\gamma}$, $R_{\gamma\to n}$, $R_{\gamma\to\gamma}$
   - $T_{n\to n}$, $T_{n\to\gamma}$, $T_{\gamma\to n}$, $T_{\gamma\to\gamma}$

- Matrix shape: $(N_E \cdot N_\Omega) \times (N_E \cdot N_\Omega)$

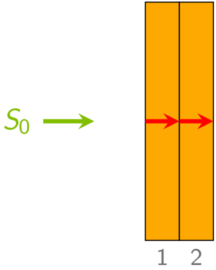




Solution for 1 layer

- $S_1 = S_0 \times T_1$

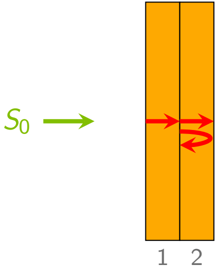
- S_i — spectra exiting layer i (and entering layer $i + 1$)
  - S_0 — source term (mixed particle spectra allowed)
- T_i — layer i transmission matrix
- R_i — layer i reflection matrix



Solution for 2 layers

- $S_1 = S_0 \times T_1$
- $S_2 \approx S_1 \times T_2$

- S_i — spectra exiting layer i (and entering layer $i+1$)
  - S_0 — source term (mixed particle spectra allowed)
- T_i — layer i transmission matrix
- R_i — layer i reflection matrix

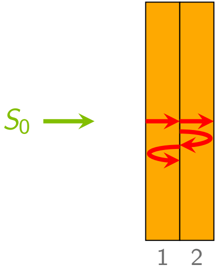


Solution for 2 layers

- $S_1 = S_0 \times T_1$
- $S_2 \approx S_1 \times T_2 + S_1 \times R_2$

- S_i — spectra exiting layer i (and entering layer $i + 1$)
  - S_0 — source term (mixed particle spectra allowed)
- T_i — layer i transmission matrix
- R_i — layer i reflection matrix

Transmission matrices
Solution



Solution for 2 layers

- $S_1 = S_0 \times T_1$
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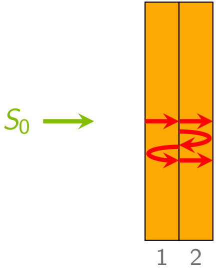
Transmission matrices
Solution



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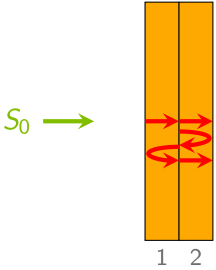
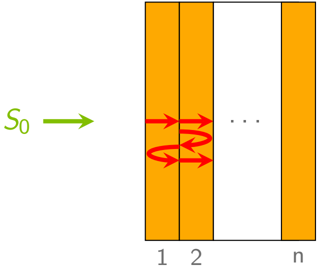
Transmission matrices
Solution



Solution for 2 layers

- $S_1 = S_0 \times T_1$
- $S_2 \approx S_1 \times T_2 + S_1 \times R_2 \times R_1 \times T_2$
  $+$ higher order reflections

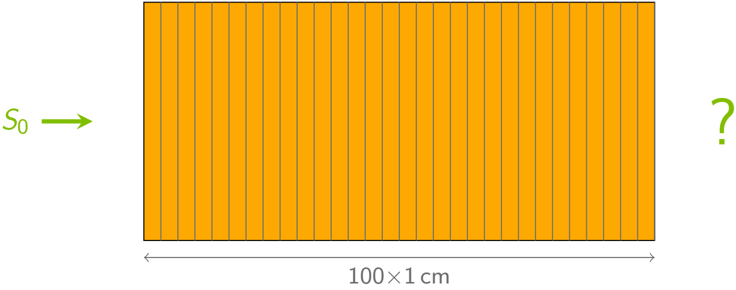
- S_i — spectra exiting layer i (and entering layer $i+1$)
  - S_0 — source term (mixed particle spectra allowed)
- T_i — layer i transmission matrix
- R_i — layer i reflection matrix



Solution for n layers

- $S_1 = S_0 \times T_1$
- $S_2 \approx S_1 \times T_2 + S_1 \times R_2 \times R_1 \times T_2$
  $+$ higher order reflections
- $S_n \approx \dots$

- S_i — spectra exiting layer i (and entering layer $i+1$)
  - S_0 — source term (mixed particle spectra allowed)
- T_i — layer i transmission matrix
- R_i — layer i reflection matrix



- Incident beam: 3 GeV electrons
- Material: Concrete
- Thickness: 1 m (100 layers)
- Transported particles: n, γ, $e^{\pm}$, $\mu^{\pm}$
- Energy: 130 bins between 1 meV and 5 GeV
- Emission angles: 18 bins between $-\pi$ and π

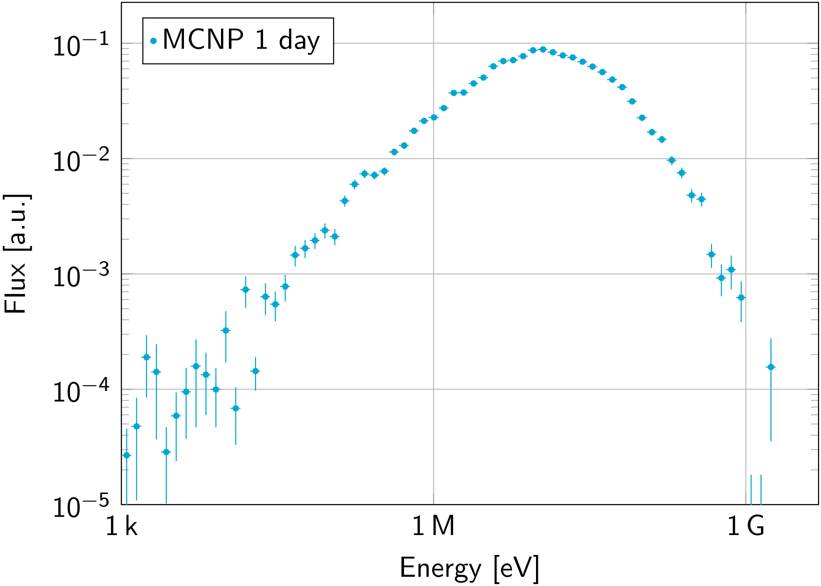
Matrix shape:

$130 \cdot 18 \Rightarrow$

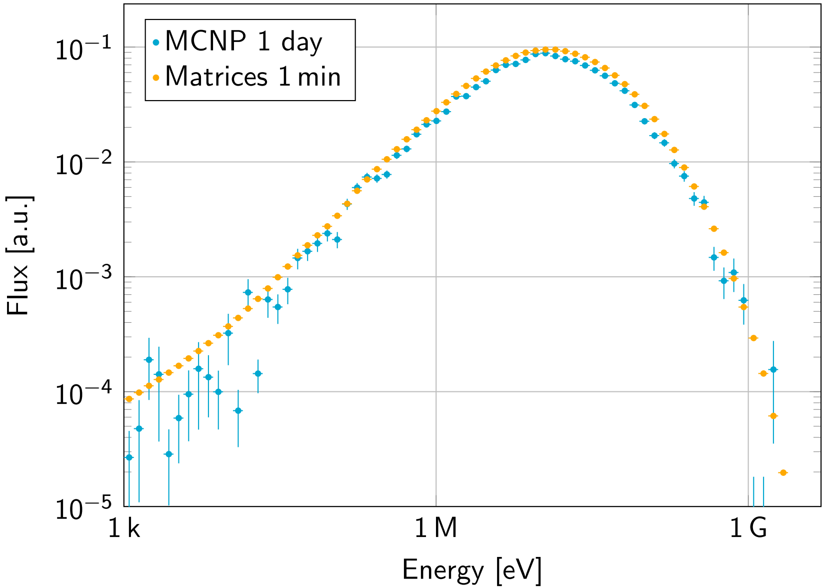
2340×2340

Photons

Transmission matrices
Results — Photons

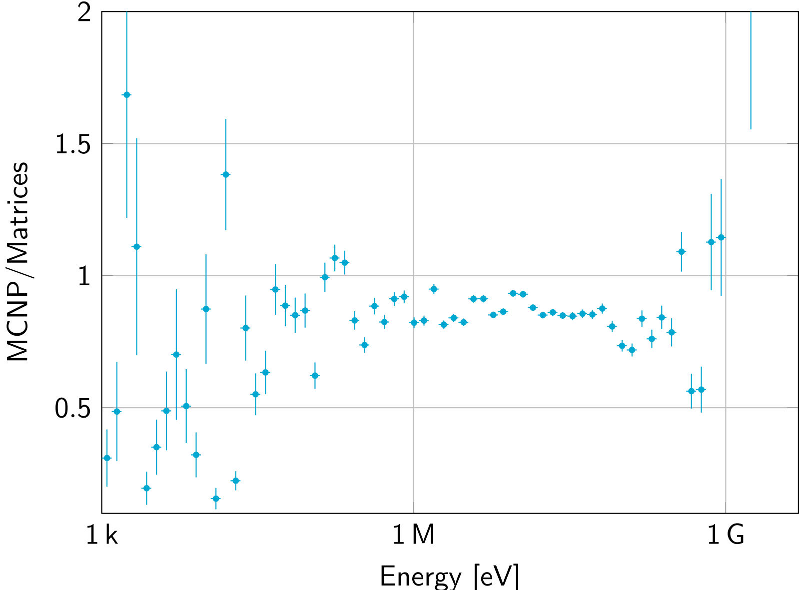


Transmission matrices
Results — Photons



Transmission matrices

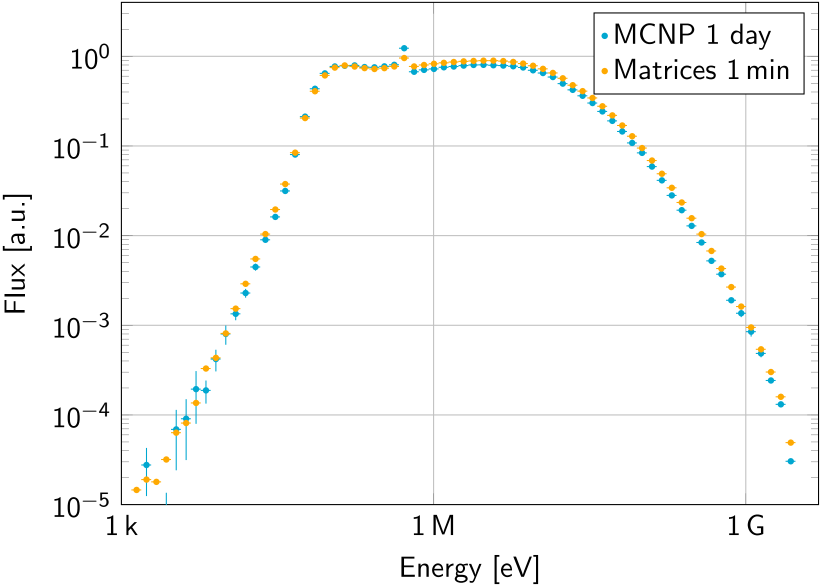
Results — Photons



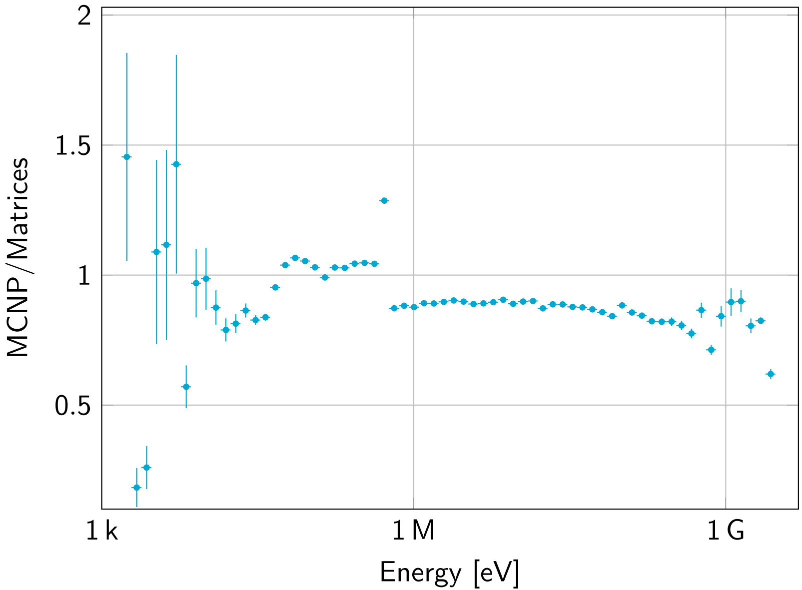
Electrons

Transmission matrices

Results — Electrons



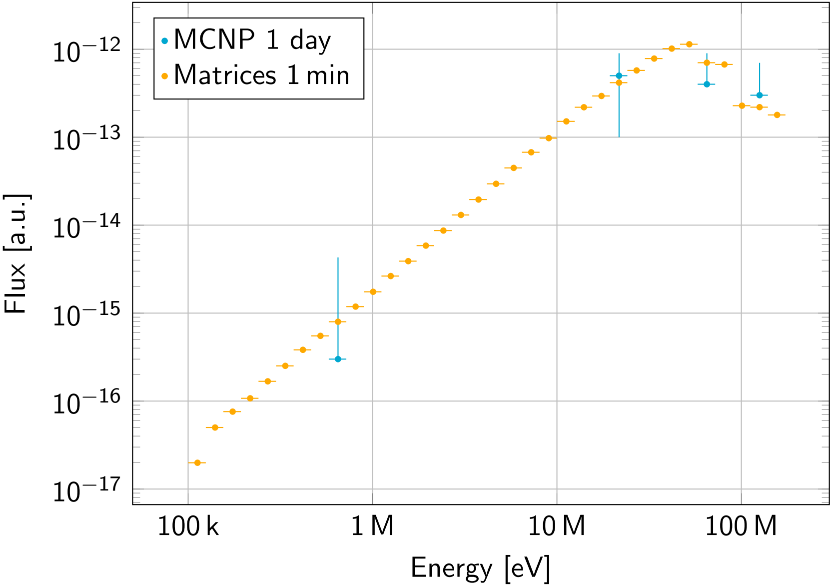
Transmission matrices
Results — Electrons



Muons

Transmission matrices

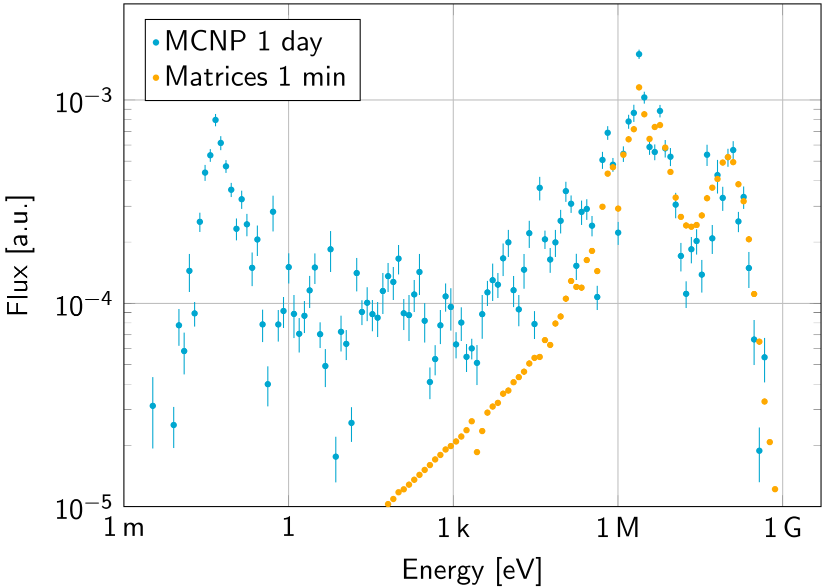
Results — Muons



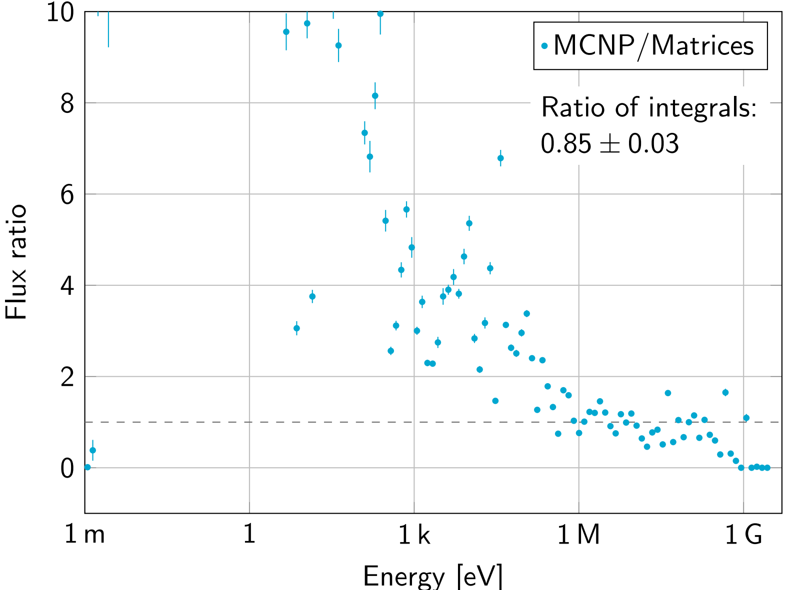
Neutrons

Transmission matrices

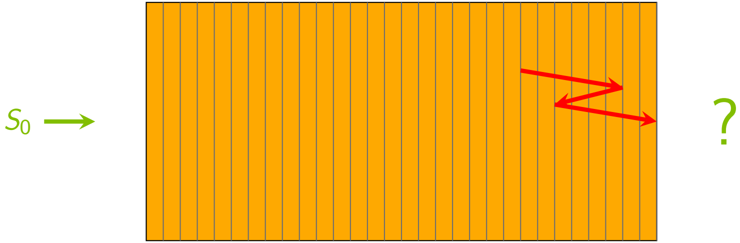
Results — Neutrons



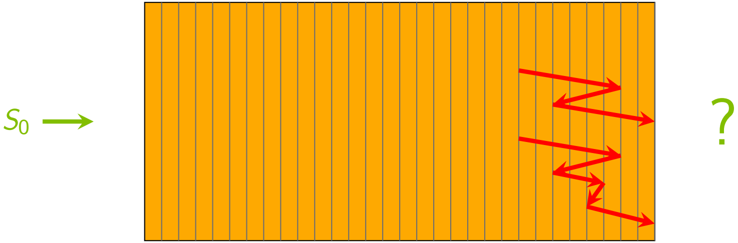
Transmission matrices
Results — Neutrons



Motivation for using Markov chains to improve neutron spectrum



Motivation for using Markov chains to improve neutron spectrum



Outline

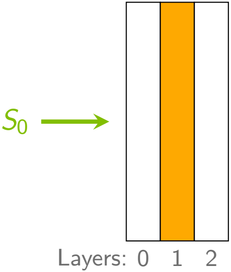
Future depends on today but not on yesterday

Typical examples

- Brownian motion
- Poisson processes
- Stock market
- Google's PageRank
- Monopoly game
  - search: "Dominating Monopoly using Markov chain"

Markov chains
Block matrix definition for 1 layer

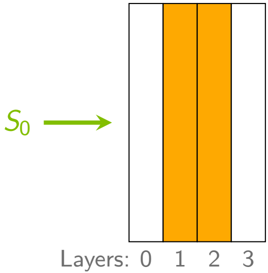
	0	1	2
0	[0]	[E]	[0]
1	[R_1]	[0]	[T_1]
2	[0]	[0]	[0]



- Matrix shape: $((N_{layers} + 2) \cdot N_E \cdot N_\Omega \cdot N_{particle\ types}) \times ((N_{layers} + 2) \cdot N_E \cdot N_\Omega \cdot N_{particle\ types})$

Markov chains
Block matrix definition for 2 layers

	0	1	2	3
0	[0]	[E]	[0]	[0]
1	[R_1]	[0]	[T_1]	[0]
2	[0]	[R_2]	[0]	[T_2]
3	[0]	[0]	[0]	[0]

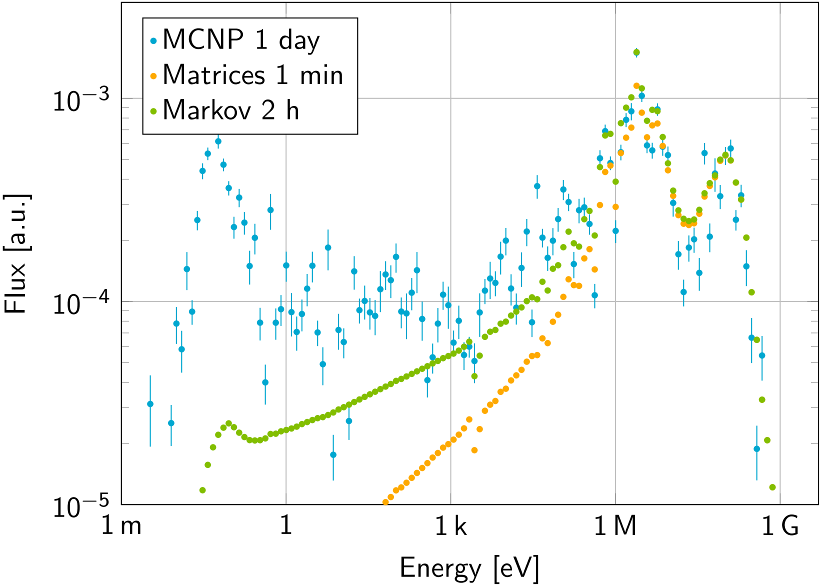


- Matrix shape: $((N_{layers}+2)\cdot N_E \cdot N_\Omega \cdot N_{particle\ types}) \times ((N_{layers}+2)\cdot N_E \cdot N_\Omega \cdot N_{particle\ types})$

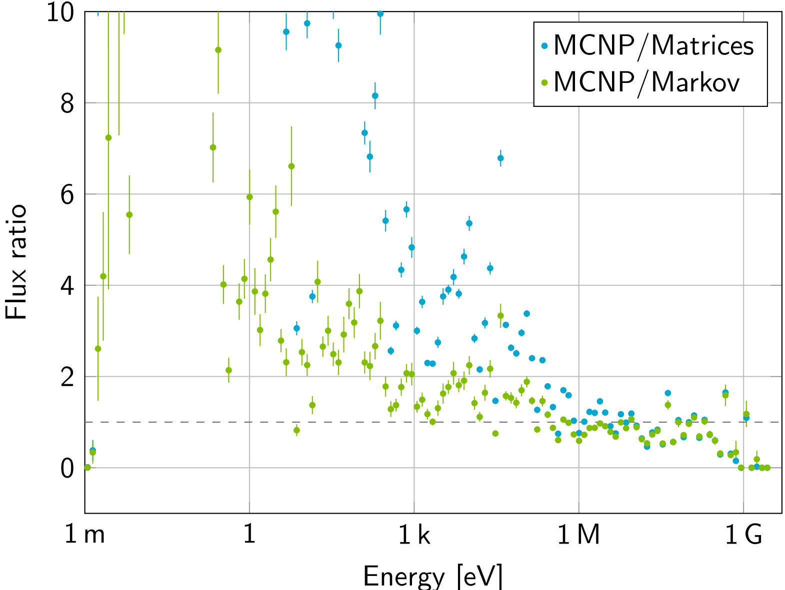
$$S_n \leftarrow S_0 \times (M_n)^k$$

- S_0 — source term (mixed particle spectra allowed)
- S_n — spectra exiting n layers
- $(M_n)^k$ — Markov chain matrix for n layers in the power of k
  - The value of k defines the reflection orders to be included in the result
  - The process quickly converges $\Rightarrow$ k does not need to be large

Markov chains
Results — Neutrons

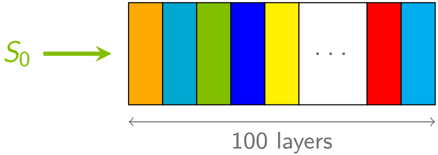


Markov chains
Results — Neutrons



Outline

- At this point we can quickly calculate particle spectra beyond thick shielding
- This allows us to test many heterogeneous beam dump configurations in 1D



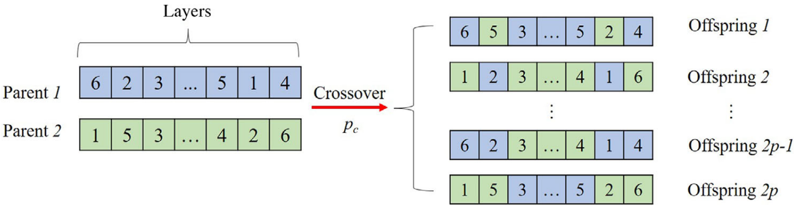
- How many configurations to test?
  - Number of layers: n=100
  - Number of materials, e.g. k=7

    ⇒ **brute force is still too time expensive**

Genetic algorithms
Quick introduction

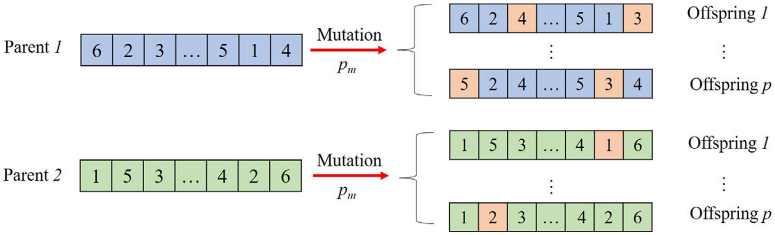
- Genetic algorithms implement natural selection principles
  - Crossover
  - Mutation
- They induce evolution of population to a state that maximises the specified figure-of-merit
- We can define a figure-of-merit to reflect our boundary conditions:
  - Dose rate
  - Size
  - Mass
  - Cost
  - Complexity

Genetic algorithms
Quick introduction — Crossover



[R. Zhang et al]

- p_c — crossover probability
- Elements of both parents are randomly exchanged to form a new offspring



[R. Zhang et al]

- p_m — mutation probability
- The offspring inherits the elements of its parent but some randomly chosen elements are randomly changed

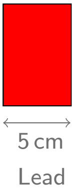
Outline

Results
Materials

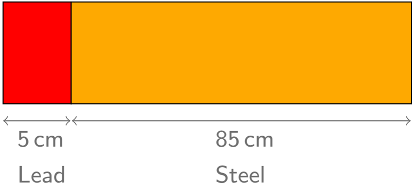
- Steel
- Lead
- Tungsten
- Concrete
- Boron carbide (B_4C)
- Water
- Polyethylene

Optimised beam dump layout

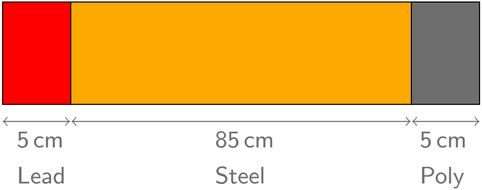
Results
Optimal beam dump configuration



Results
Optimal beam dump configuration

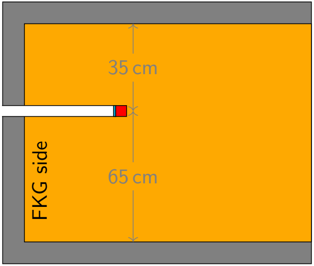


Results
Optimal beam dump configuration

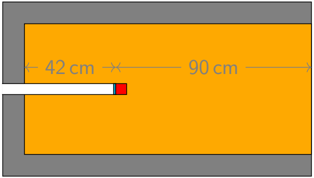


Almost the same as our initial guess!

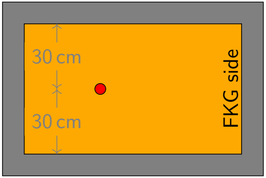
Final geometry (fine-tuned with FLUKA)



(a) Horizontal section



(b) Vertical section



(c) Vertical section

- Kapton tape: ∼0.1 cm thick.
- Lead: 3 cm radius, 5 cm length.
- Steel: S235JR.
- Borated polyethylene: 5 cm thick.

Results
Final geometry (as built without Polyethylene)

Outline

MAG — an open source tool for 1D shielding calculations:
https://github.com/kbat/mag

Solver

```
$ mag-solve -layers 5 Lead 100 Concrete 5 Poly
            -source e 3e3
```

Dose rates [pSv/primary]:
e: 1.13
n: 0.04
γ: 1.42
μ: 1.49e-11
total: 2.56

+ data file with spectra for each particle type

MAG — an open source tool for 1D shielding calculations:
https://github.com/kbat/mag

Optimiser

```
$ mag-optimise -nlayers 100 -source e 3e3
```

- Optimises a slab made of 100 layers filled with materials from the existing database
- Arbitrary figure-of-merit can be specified
- Complex sources are supported

Applications

- Simple shielding calculations
  - e.g. non-neutron applications
  - e.g. for non-FLUKA users
- General particle transport through matter
- Layer/mesh-based variance reduction generation

References

Zhang R, Yu Y, Zhang Z, Yang Y.
An iterative prediction method for designing the moderator used for the boron neutron capture therapy
Med Phys. 2022; **49**:598–610.
https://doi.org/10.1002/mp.15339
2022