Topic

The Machine-Learned Density of States in Multicanonical Simulations.

Case study: Neutron Activation Analysis at Ghana Research Reactor-1

Mustapha Wamakin Ali

(Graduate school of Nuclear& allied science)

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Introduction

- The **Ghana Research Reactor–1 (GHARR-1)** is a low-power nuclear research reactor located at the **Ghana Atomic Energy Commission (GAEC)** in Accra. Commissioned in 1994.

- It is a **30kW tank-in-pool, miniature neutron source reactor (MNSR)** originally supplied by China.

- It operates primarily as a training, research, and isotope-production facility.

- Ghana successfully completed the **conversion of GHARR-1's core from Highly Enriched Uranium (HEU) to Low Enriched Uranium (LEU)**, aligning the reactor with global non-proliferation standards and enhancing its long-term sustainability.

Pictures of Ghana Research

Neutron Activation Analysis (NAA)

- Neutron Activation analysis is a method for the determination of elements by conversion of stable nuclei to radioactive nuclei via nuclear reactions, and measurement of the reaction products.

- The analysis is based on the use of gamma-ray spectrometry to identify and quantify the elemental matrices.

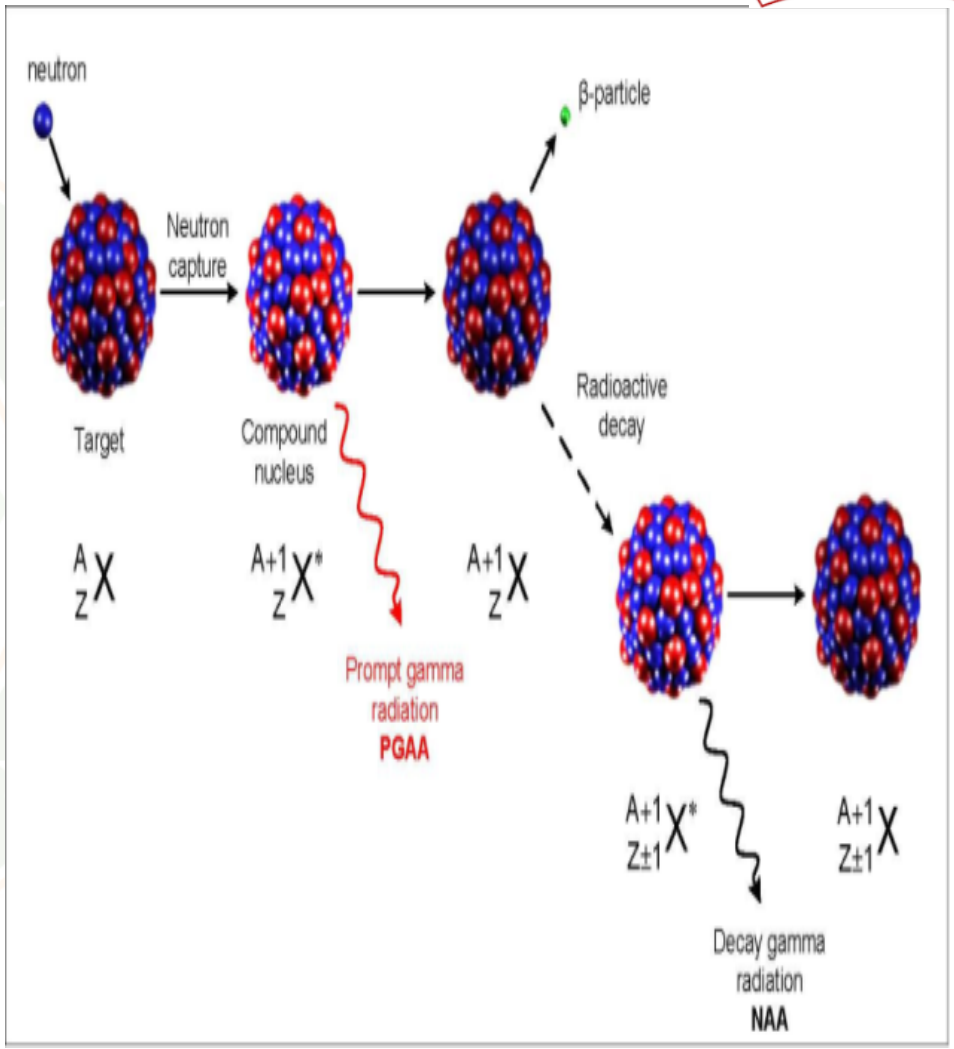
- The technique require at least 3 qualified personnel who should be able to control the counting equipment and have good knowledge of the basic principles of the technique.

The Basic Physics of NAA

- For NAA, the neutron-target interaction specially arranged procedure (process) is a special designed procedure called neutron activation.
- There are different types of neutron-atom interactions: (n, p), (n, n), (n, 2n), (n, γ), etc.

The Basic Physics of NAA

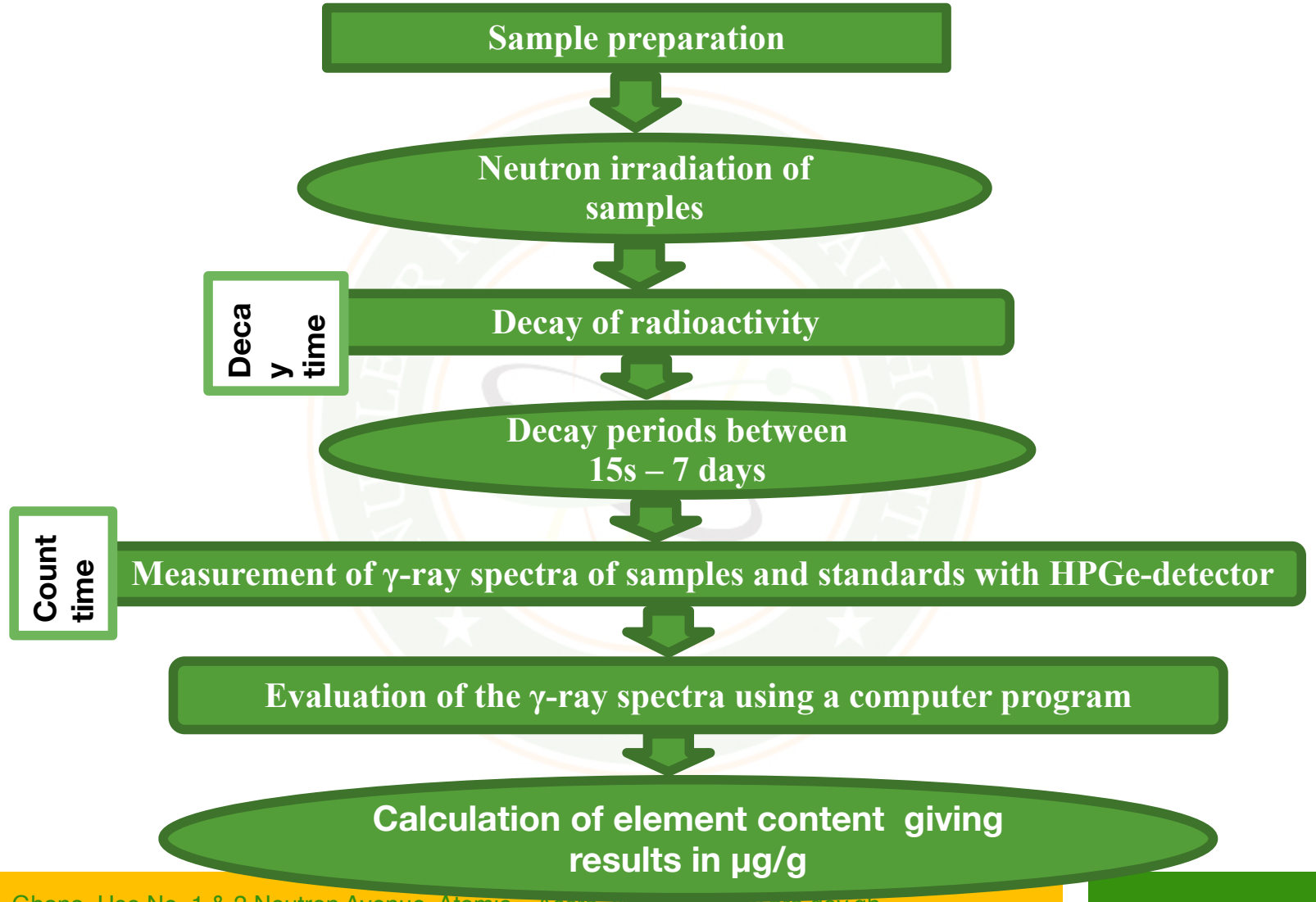
- The target capture neutron via (n, gamma) reaction.
- Creation of a compound nucleus forms an excited state.
- Compound nucleus instantaneously de-excite into a more stable configuration through emission prompt gamma rays.
- The new configuration yields a radioactive nucleus which also decays by emission of delayed gamma rays.
- Each radioactive nucleus decay with unique half-life.



NAA Advantages

- NAA is essentially considered to be a non-destructive method.
- Nondestructive. Aside from the production of some short lived activity, the sample is chemically and physically unchanged after the analysis.
- Especially effective with large solid samples (e.g. soil) that are difficult to analyze by other means. i.e., materials can be activated in any physical state: solid, liquid or gaseous.
- There is no fundamental necessity to convert solid material into a solution prior to activation.
- A multi-element technique many elements can be analyzed simultaneously.
- Most elements can be analyzed to 1 ppm and many can be analyzed in orders of magnitude below that.
- Fast turn-around time . The only processing of the sample routinely employed is drying and mixing.
- Neutron Fluence Rate (Flux) Measurements Neutron fluence rates in reactors or other neutron sources can be measured by exposing targets (e.g., metal foils) to the neutrons and measuring the induced activity.

NAA Procedure (1/3)



NAA Procedure (2/3)

- Samples are sealed in **polyethylene vials**, **quartz ampoules**, or **aluminium capsules**, depending on temperature and irradiation duration.
- Vials are thoroughly labeled with **identification codes** resistant to heat and radiation.
- Multiple samples are often placed in **sample rabbits** or holders designed for the reactor system.
- Prepared and labeled sample vials are transported from the NAA laboratory to the reactor hall using approved radiation-safe container.
- These steps are similar worldwide for miniature neutron source reactors but adapted to Ghana's research environment.

NAA Procedure (3/3)

Sample Preparation at GHARR-1:

- Sample are clean to remove surface contamination
- Big samples may be **ground** and **sieved** to obtain uniform particle size.
- The sample is weighed using an analytical balance with high precision.
- Documentation (sample ID, irradiation time, researcher name) accompanies each batch.
- GHARR-1 uses **designed irradiation sites** intended for research samples.

- These include vertical irradiation channels and pneumatic transfer systems (commonly referred to as “rabbits)

Irradiation (1/2)

Short irradiations

Lightweight capsules are placed in the **pneumatic transfer system**, which sends the sample from the laboratory end to the irradiation position using compressed air.

Long irradiations

Samples requiring longer exposures are placed in **fixed irradiation sites** using holders that keep them stable and correctly positioned.

Irradiation (2/2)

Irradiation timing

Reactor staff input the **requested irradiation time**, which depends on:

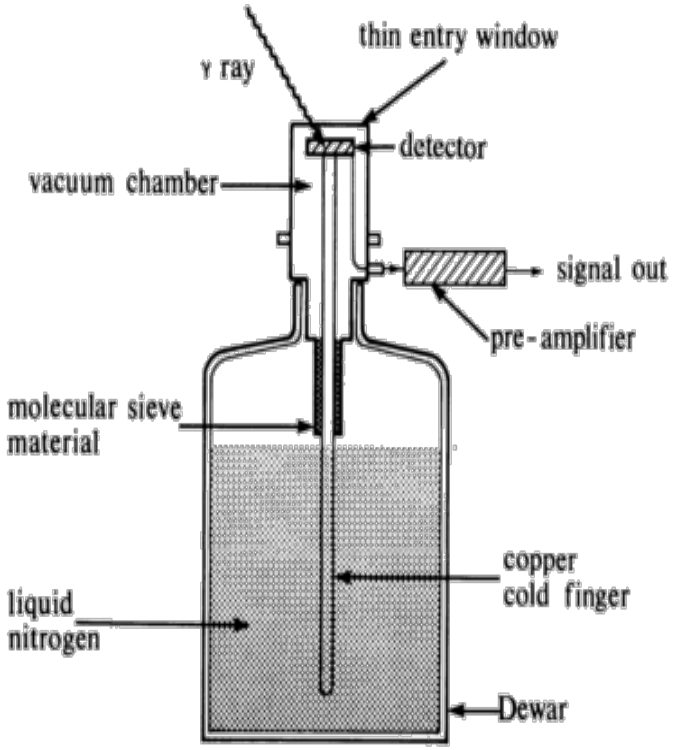
- The elements of interest
- The neutron flux environment
- The type of analysis (short-lived or long-lived isotopes)

Retrieval after irradiation

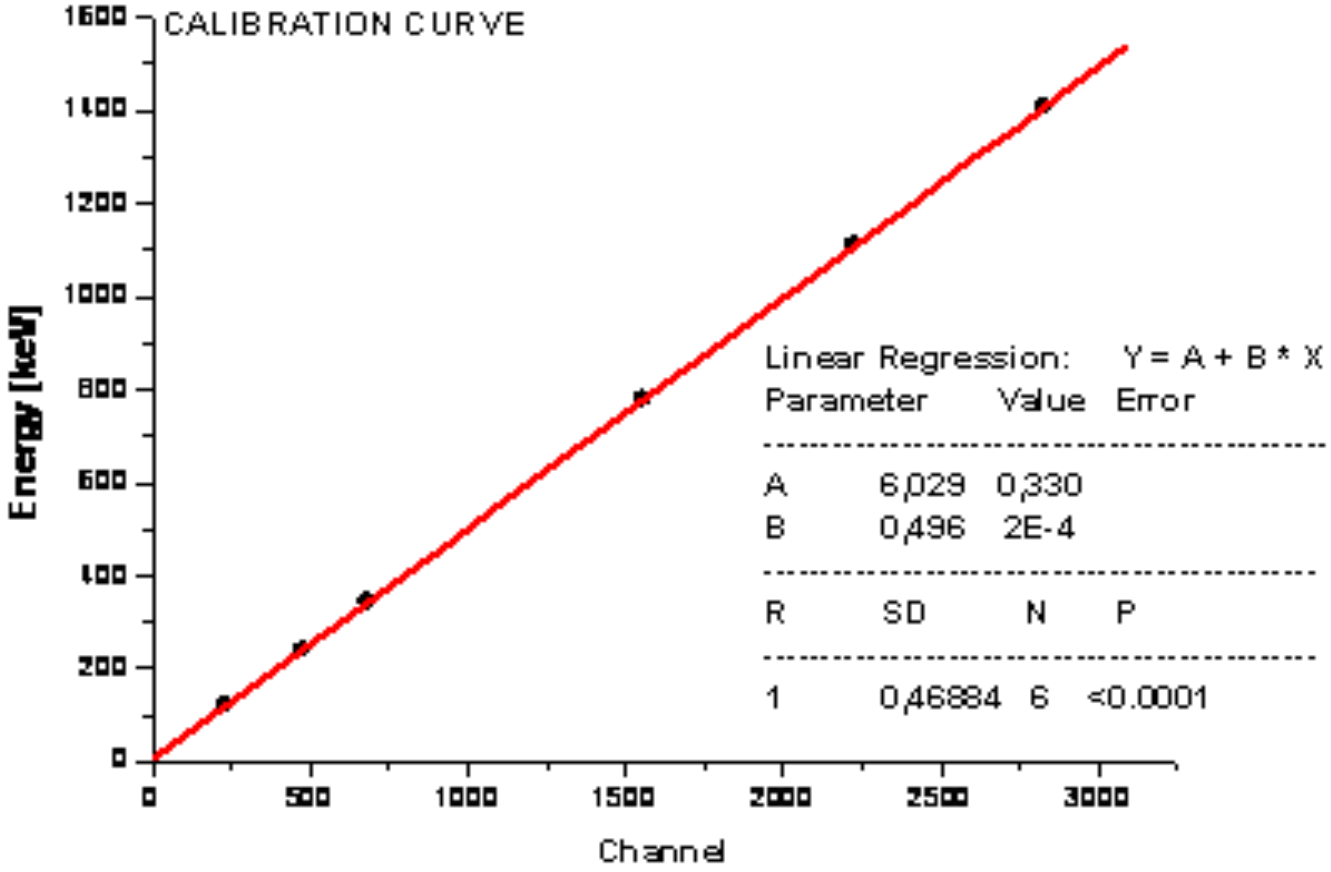
- After irradiation, the sample is safely withdrawn (either returned pneumatically or manually retrieved by trained staff).
- It is then taken to the **decay area** to allow short-lived radioactivity to stabilize.
- Once safe for handling, the sample proceeds to gamma-ray measurement.

Counting and Data analysis using γ- Spectroscopy

Detector



Detector Calibration



Machine Learning aiding NAA

Step in NAA Workflow	Traditional Challenges	ML Solutions	Improvements
Gamma-ray spectrum preprocessing	Baseline drift, noise, pile-up	Autoencoders, U-Net, Wavelet denoising + ML	Better S/N, automated baseline subtraction
Peak detection & locating	Overlapping peaks, low statistics	CNNs (1D), YOLO-style detectors, peak-finding network	>95–99 % detection rate even in low-count spectra
Nuclide identification	Complex libraries, interferences (e.g., 152Eu vs 154Eu	Random Forest, XGBoost, Deep Neural Networks on peak ratios & energies	Reduces misidentification from ~10–20 % to <1–2 %
Interference correction	Coincidental energies, Compton continuum	ML regression models trained on known interference patterns	More accurate net peak areas
Uncertainty estimation	Counting statistics only	Bayesian NNs, Monte Carlo dropout, ensemble methods	Realistic uncertainty quantification
Spectral deconvolution / unmixing	Heavily overlapping multiplets	Non-negative Matrix Factorization + NN, Physics-informed Neural Networks (PINNs)	Resolves peaks that are impossible manually

- **Choose a potential**
  Common choices:
  - TIP3P/TIP4P-like water plus compatible Na^+/acetate parameters,
  - polarizable force fields for accuracy.
- **Iteratively build MUCA weights**

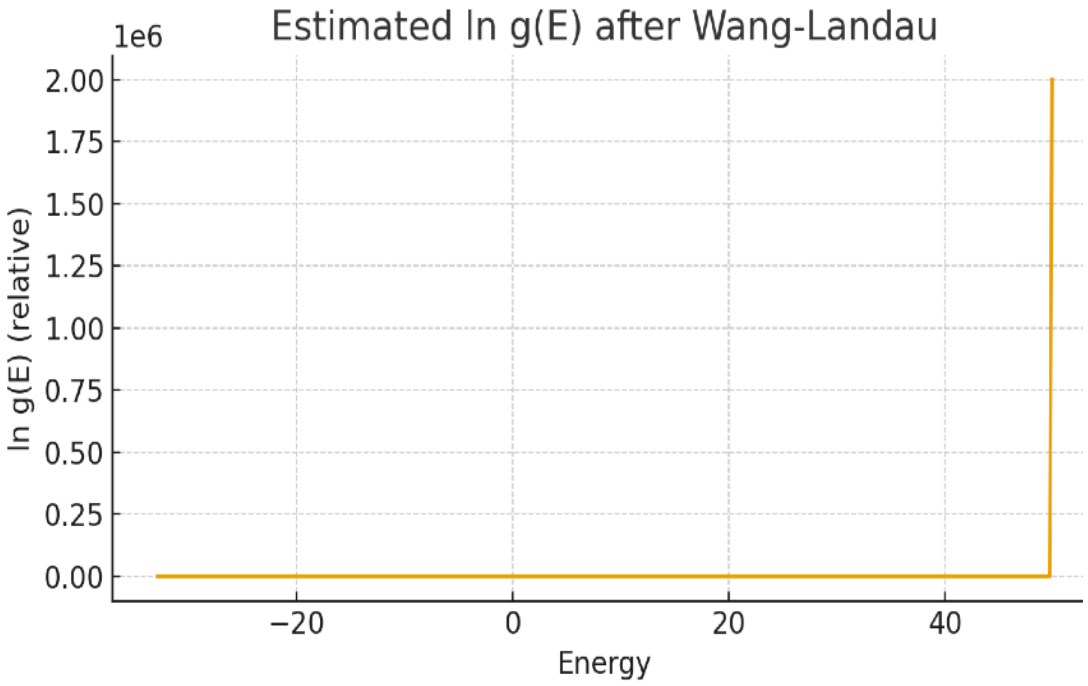
- Usually via:
  - **Wang–Landau method**,.

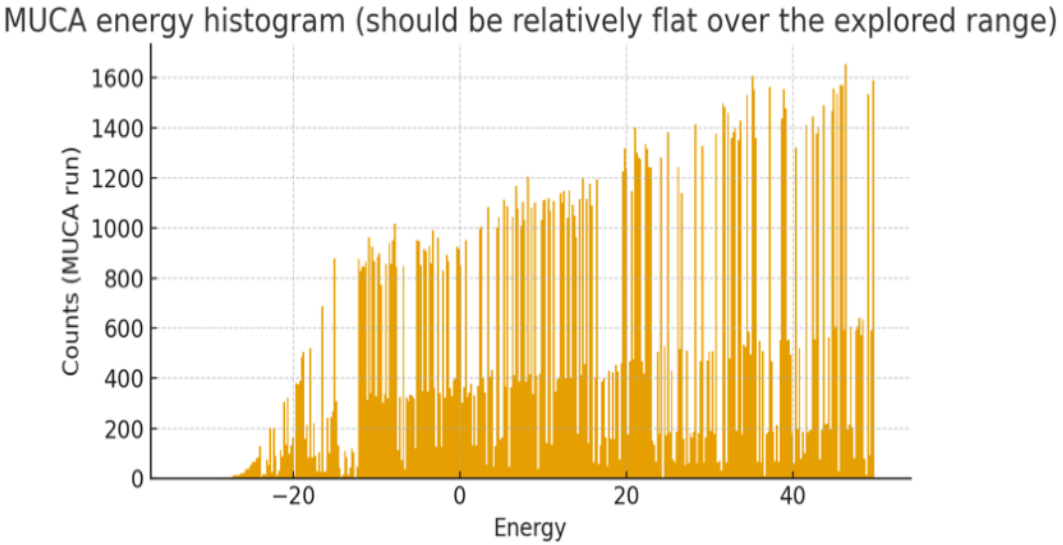
CONT.

- **Run long MUCA sampling over a wide energy range**

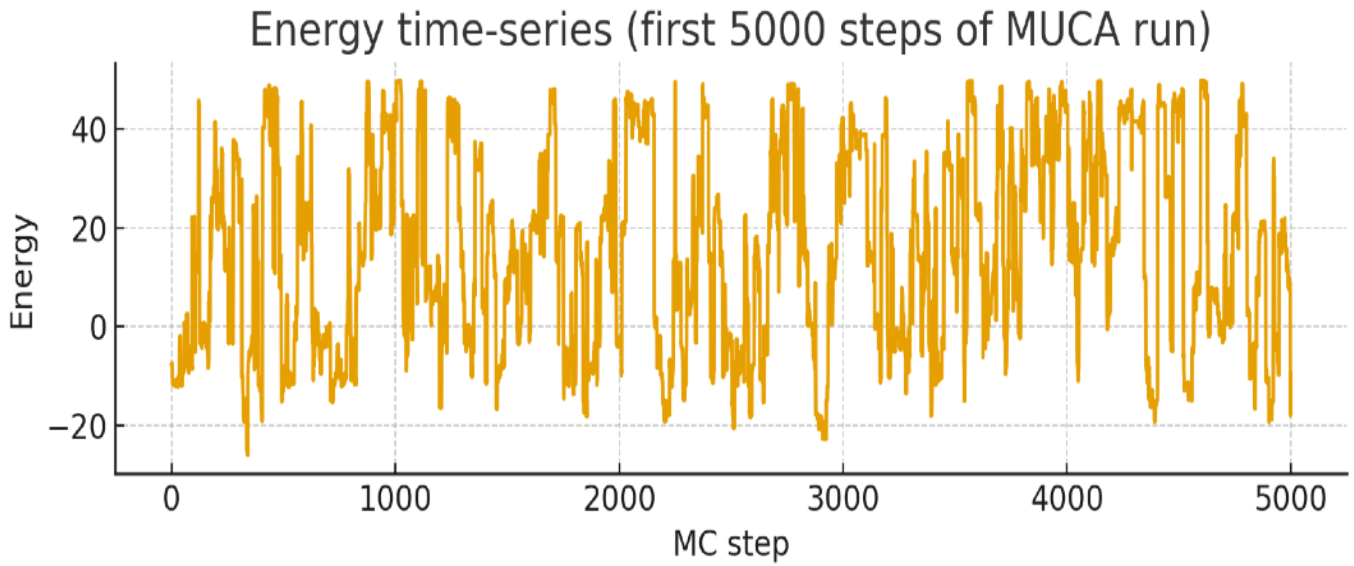
- **Reweight trajectories to obtain**
  - $C_V(T)$curves,
  - structural populations,
  - radial distribution functions at any temperature,
  - free-energy barriers for crystallization

GRAPHS


Estimated ln g(E) after Wang-Landau
1e6
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
ln g(E) (relative)
−20
0
20
40
Energy


MUCA energy histogram (should be relatively flat over the explored range)
1600
1400
1200
1000
800
600
400
200
0
Counts (MUCA run)
−20
0
20
40
Energy

CONT.



Multicanonical (MUCA) workflow on a small prototype system and saved the results.

Thank You

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