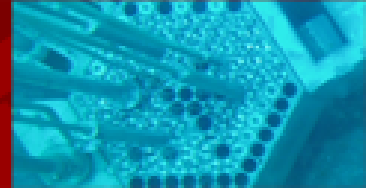


PyNIC: Python-Based Neutron Interaction Calculator

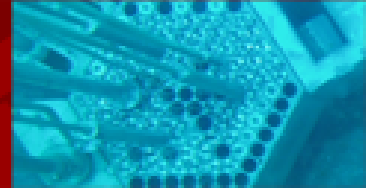
Greg Moffitt

8/7/14



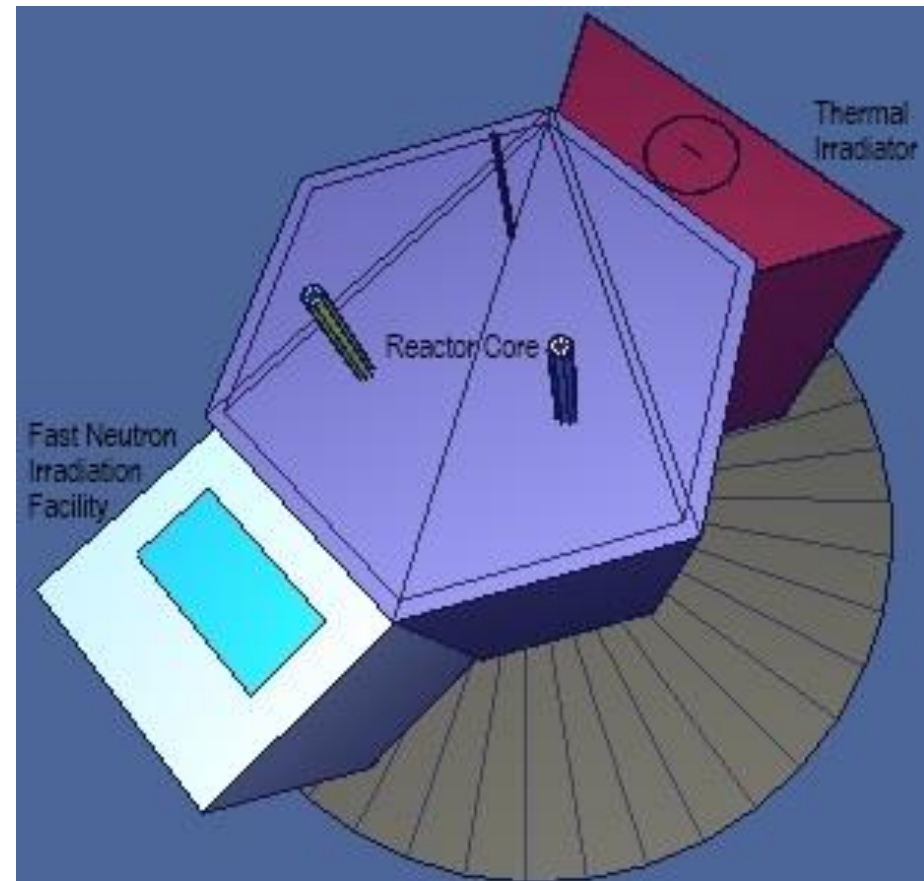
Outline

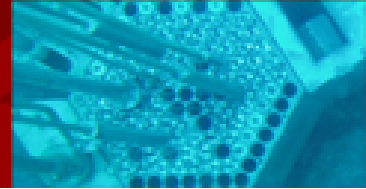
- Development of NAA Pre-calculator
- PyNIC code
- TRIGA Reactor Info and Irradiation ports
- MCNP6 Simulations of University of Utah TRIGA reactor
- PyNIC Code Benchmarking
- Future Work



Development of a NAA Pre-calculator

- Neutron activation analysis (NAA) is performed in the University of Utah TRIGA reactor (UUTR) for a wide range of samples
- Accurate pre-calculations leads to safe irradiations where dose is limited and activities are maintained in a range for counting on HPGe detectors





Python-Based Neutron Interaction Calculator (PyNIC)

$$A_D(t) = \varphi(\sigma_p)m \left(\frac{N_A}{A_m} \right) A_{\%} (1 - e^{-\lambda_D t_{irr}}) e^{-\lambda_D t_{decay}}$$

- Entire neutron absorption cross-section included for each built-in nuclide
- Calculates the activity across the entire neutron energy spectrum of a neutron source
- Calculates the dose rate of an irradiated sample from gamma rays at 1 ft
- Currently contains 240 nuclides
- Once validated, PyNIC can be applied to any neutron energy spectrum

φ – neutron flux ($n/(cm^2*s)$)

σ_p – radiative capture cross section of parent isotope (cm^2)

m – mass of sample (g);

N_A – Avogadro's number;

A_m – atomic mass (g/mole),

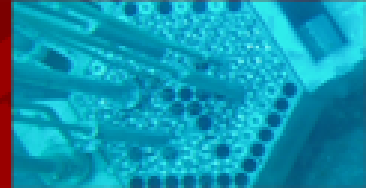
$A_{\%}$ – atomic abundance ratio

t_{irr} – irradiation time (sec)

t_{decay} – decay time (sec)

$A_D(t)$ – activity of daughter isotope (Bq)

λ_D – decay constant of daughter isotope (s^{-1})



PyNIC GUI: Irradiation Parameters

- GUI developed to facilitate the use of PyNIC by any user regardless of programming experience
 - Allows students to prepare their own NAA irradiations with final approval by reactor supervisor
- User enters/selects sample mass, irradiation time, decay time, and neutron beam

Neutron Interaction Simulation Tool, version 1.00

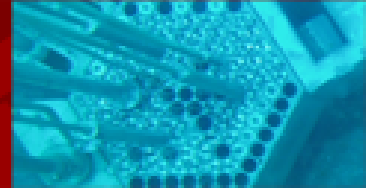
Sample Mass: 0.5 (g)

Irradiation time: 5 (minutes)

Decay time: 1 (minutes)

Neutron Beam:

- UUTR FNIF - 1 kW
- UUTR FNIF - 10 kW
- UUTR FNIF - 90 kW
- UUTR TI - 1 kW
- UUTR TI - 10 kW
- UUTR TI - 30 kW
- UUTR TI - 50 kW
- UUTR TI - 70 kW
- UUTR TI - 90 kW
- UUTR CI - 90 kW



PyNIC GUI: Sample Nuclide Selection

- User selects the nuclides present in the sample
 - Selects up to 10 different nuclides
- User enters the percent mass abundance of each nuclide

74 tk

Neutron Interaction Simulation Tool, version 1.00

Sample Mass: 0.5 (g)

Irradiation time: 5 (minutes)

Decay time: 1 (minutes)

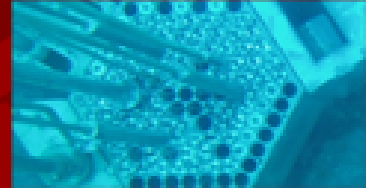
Neutron Beam:

- UUTR FNIF - 1 kW
- UUTR FNIF - 10 kW
- UUTR FNIF - 90 kW
- UUTR TI - 1 kW
- UUTR TI - 10 kW
- UUTR TI - 30 kW
- UUTR TI - 50 kW
- UUTR TI - 70 kW
- UUTR TI - 90 kW
- UUTR CI - 90 kW
- none

Nuclide #1:

- H-1
- H-2
- He-3
- Li-6
- Li-7
- Be-9
- B-10
- B-11
- C
- none

Percent mass abundance in sample: 100 %



PyNIC: Running Calculations

Perform Calculations

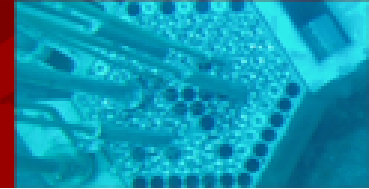
Generate MCNPX HPGe Input Files

Run MCNPX HPGe Input File

Run MCNPX HPGe Instant Input File

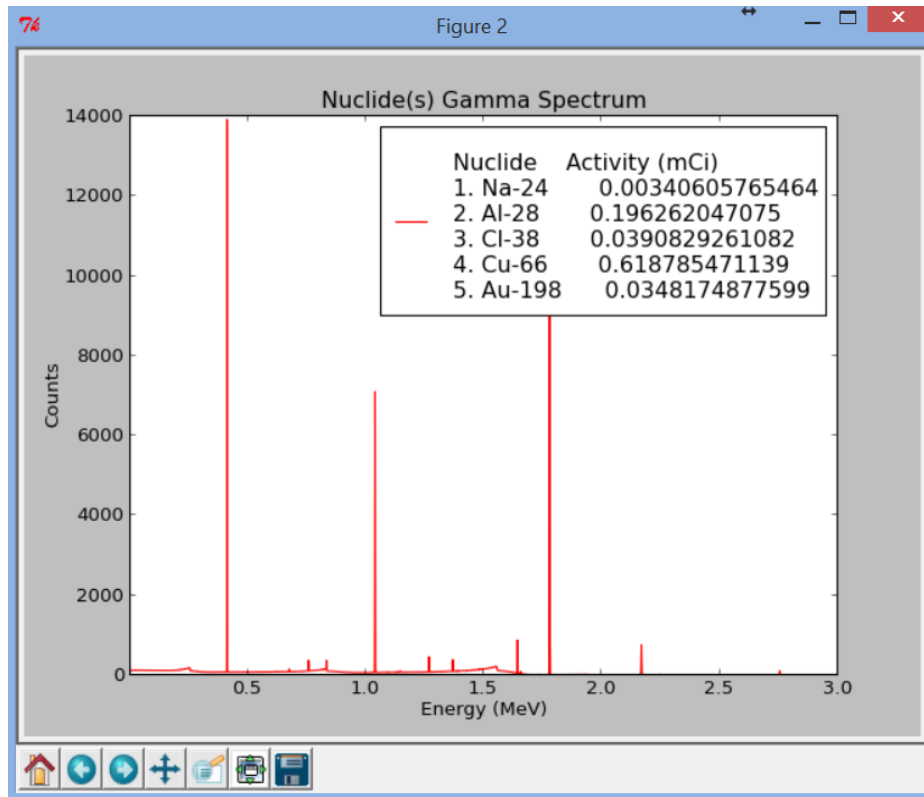
Generate HPGe Instant Report

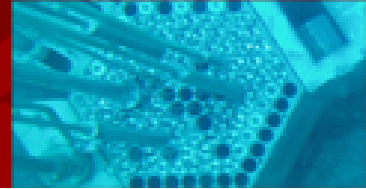
- The “Perform Calculations” button calculates the activity and dose rate for the user specified irradiation parameters and nuclides
 - Prints activity and dose rate calculations to command prompt
 - Generates a report of activity, dose rate, 5 most abundant gamma emissions from daughter product decay, prompt gamma emission rates and gamma ray energies



PyNIC: MCNPX Gamma Spectrum Simulations

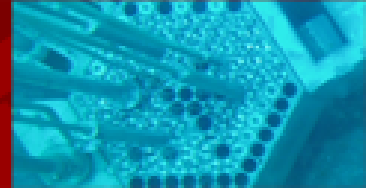
- The remaining buttons are for generating and running an MCNPX HPGe detector input based on the predicted gamma emissions from the activated sample
 - Creates input file
 - Runs file (MCNPX must be installed)
 - Parses MCNPX output file and plots gamma spectrum





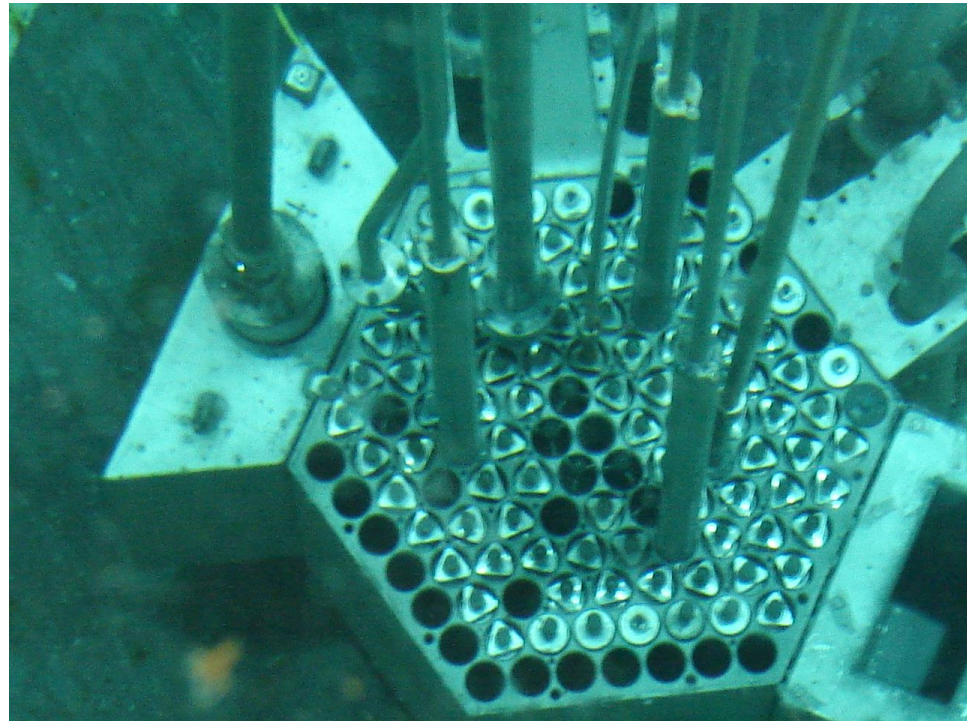
Additional Features of PyNIC

- Prompt-gamma emissions from radiative neutron capture programmed into PyNIC for select nuclides
- Inelastic scattering gamma emission data programmed in for select nuclides
- Fission gamma emission data for ^{235}U , ^{238}U , and ^{239}Pu
- Applications in the simulation of neutron interrogation of materials such as explosives or special nuclear material
- No benchmarking for prompt-gamma emissions currently being performed – future work

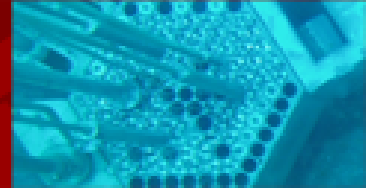


UUTR Irradiation Ports

- UUTR has 4 irradiation ports
 - Central Irradiator (CI)
 - Pneumatic Irradiator (PI)
 - Thermal Irradiator (TI)
 - Fast Neutron Irradiator Facility (FNIF)
- Reactor licensed to operate up to 100 kW
- TI flux of $7.3 \times 10^{11} \text{ n}/(\text{cm}^2 \cdot \text{s})$ (as simulated in MCNP6)

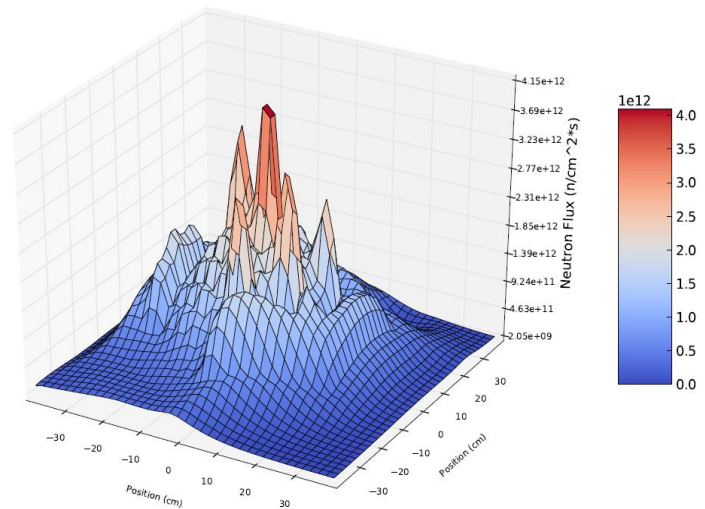


University of Utah TRIGA Reactor

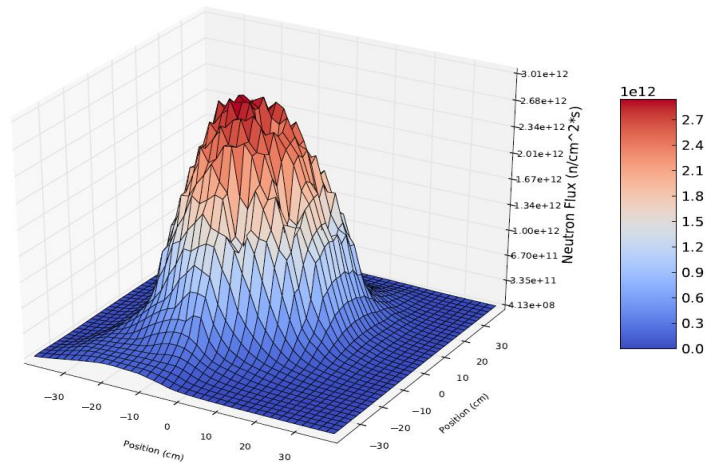


MCNP6 Simulation of UUTR

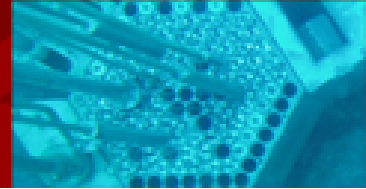
- The neutron energy spectrum and fluence simulated in MCNP6
- 2620 tally bins from 0 to 10 MeV for neutron fluence tally (F4:n)
- PyNIC has a neutron cross-section processor that can handle any neutron energy bin structure
 - User can make energy bin structure as fine or as course as needed



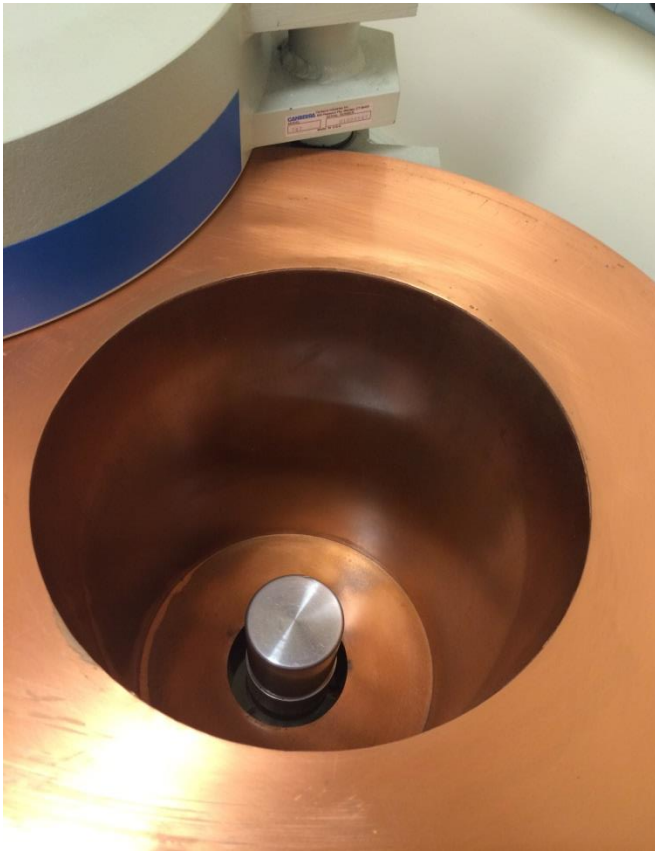
UUTR Thermal Neutron Flux



UUTR Fast Neutron Flux

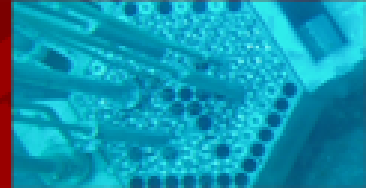


PyNIC Benchmarking



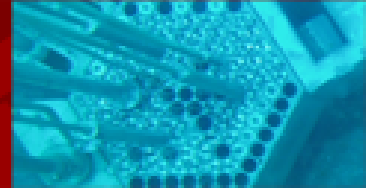
HPGe detector with Canberra lead
and copper shielding

- Benchmarking being performed through NAA experiments performed in the thermal irradiator port in the UUTR
- Materials irradiated
 - Pure nickel wire samples
 - NIST coal fly ash standard
 - NIST Montana soil standard
- Samples counted on a HPGe detector



Future Work

- Additional NAA experiments in UUTR
- Add ability to perform post calculations to get starting material concentration
- Validate for prompt gamma analysis
- Add secondary decay daughter product gamma emissions



Acknowledgements

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- Tristalee Williams
- Ryan Schow
- Steve Burnham