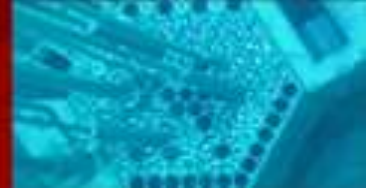


PyNIC: Python-Based Neutron Interaction Calculator for Accurate Activation Predictions in TRIGA Experiments and Student Training

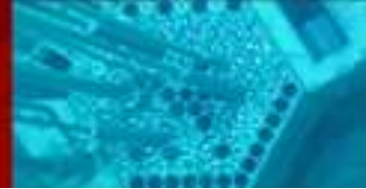
Greg Moffitt, JoCee Porter, Tatjana Jevremovic

5/25/16



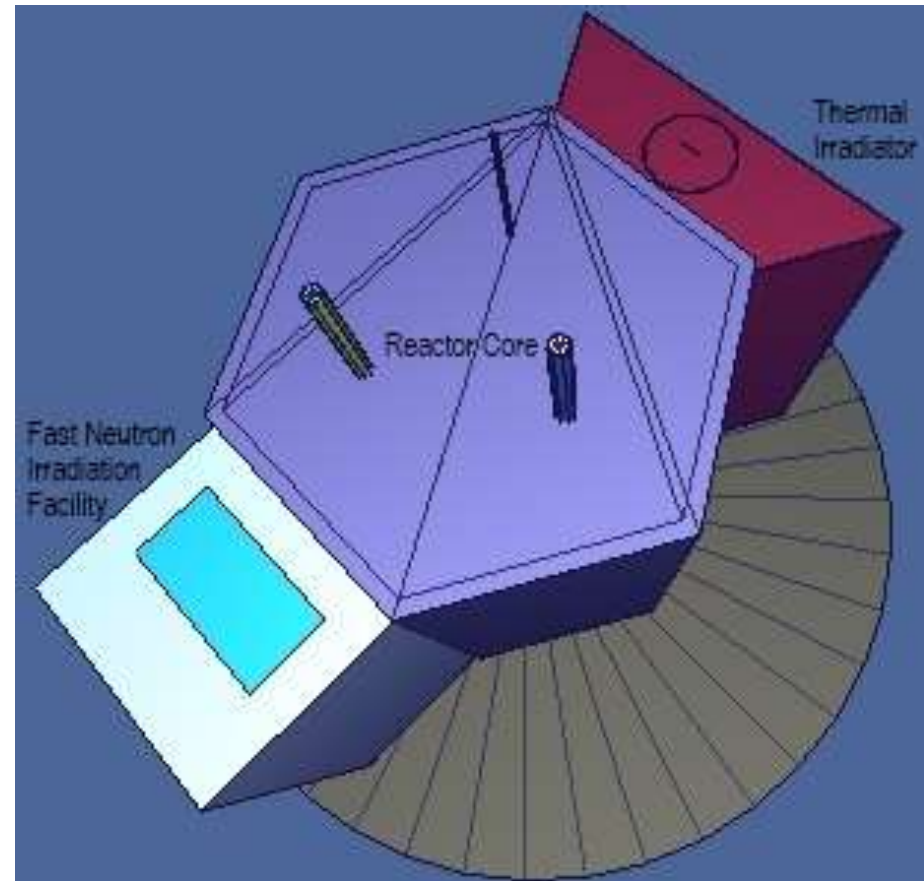
Outline

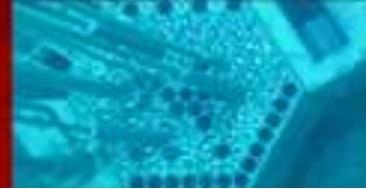
- NAA at University of Utah TRIGA Reactor
- PyNIC Layout and Use
- TRIGA Reactor Info and Irradiation ports
- MCNP6 Simulations of University of Utah TRIGA reactor
- PyNIC Code Benchmarking
- Future Work



NAA at University of Utah TRIGA Reactor

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



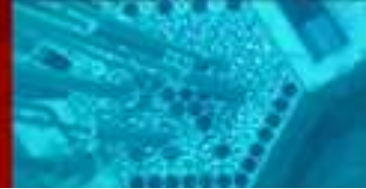


Python-Based Neutron Interaction Calculator (PyNIC)

$$A_D(t) = m \left(\frac{N_A}{A_m} \right) A_{\%} (1 - e^{-\lambda_D t_{irr}}) e^{-\lambda_D t_{decay}} \int_0^{\infty} \Phi(E) \sigma_p(E) dE$$

- Entire neutron absorption cross-section included for each built-in nuclide
- Calculates the activity
- Calculates the dose rate for γ at 1 ft
- Currently contains 240 nuclides
- Once validated, PyNIC can be applied to any neutron energy spectrum

$\Phi(E)$ – neutron flux at energy E ($n/(cm^2*s)$)
 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 Input - Irradiation Parameters

- GUI developed to facilitate the use of PyNIC by any user
 - Aids students as they prepare their own NAA irradiations (with final approval by reactor supervisor)
- User enters/selects:
 - sample mass,
 - irradiation time,
 - decay time,
 - neutron beam



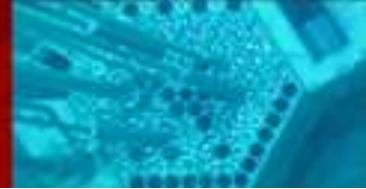
PyNIC GUI

Neutron Interaction Simulation Tool, version 1.00

Sample Mass:	<input type="text" value="0.5"/>	(g)
Irradiation time:	<input type="text" value="5"/>	(minutes)
Decay time:	<input type="text" value="1"/>	(minutes)
Multiplication factor:	<input type="text" value="1"/>	
Neutron beam:	<input type="text" value="UUTR FNIF - 1 kW"/>	

Nuclide #1:	<input type="text" value="Ti-50"/>	Percent mass abundance in sample:	<input type="text" value="50"/>	%
Nuclide #2:	<input type="text" value="Co-59"/>	Percent mass abundance in sample:	<input type="text" value="50"/>	%
Nuclide #3:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #4:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #5:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #6:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #7:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #8:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #9:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%
Nuclide #10:	<input type="text" value="none"/>	Percent mass abundance in sample:	<input type="text" value="0"/>	%

MCNPX HPGe Input nps:	<input type="text" value="1e8"/>	
HPGe count time:	<input type="text" value="10"/>	(minutes)



PyNIC: Running Calculations

Perform Calculations

Generate MCNPX HPGe Input Files

Run MCNPX HPGe Input File

Run MCNPX HPGe Instant Input File

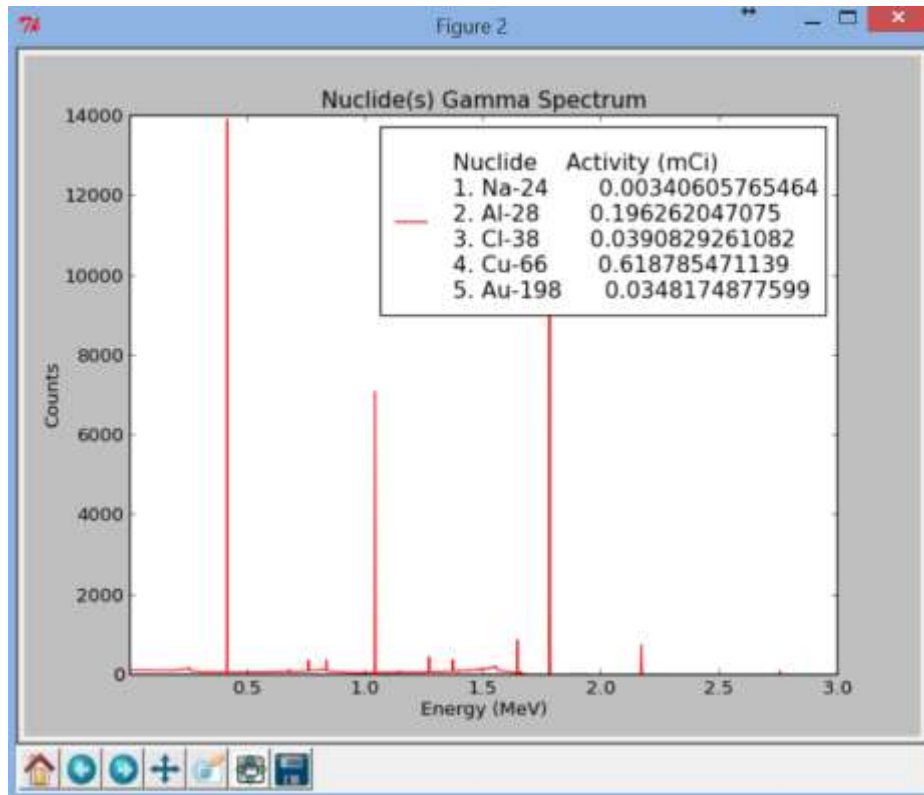
Generate HPGe Instant Report

- Perform Calculations button:
 - 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
 - Result can be used in MCNPX simulation of germanium detector response



PyNIC: MCNPX Gamma Spectrum Simulations

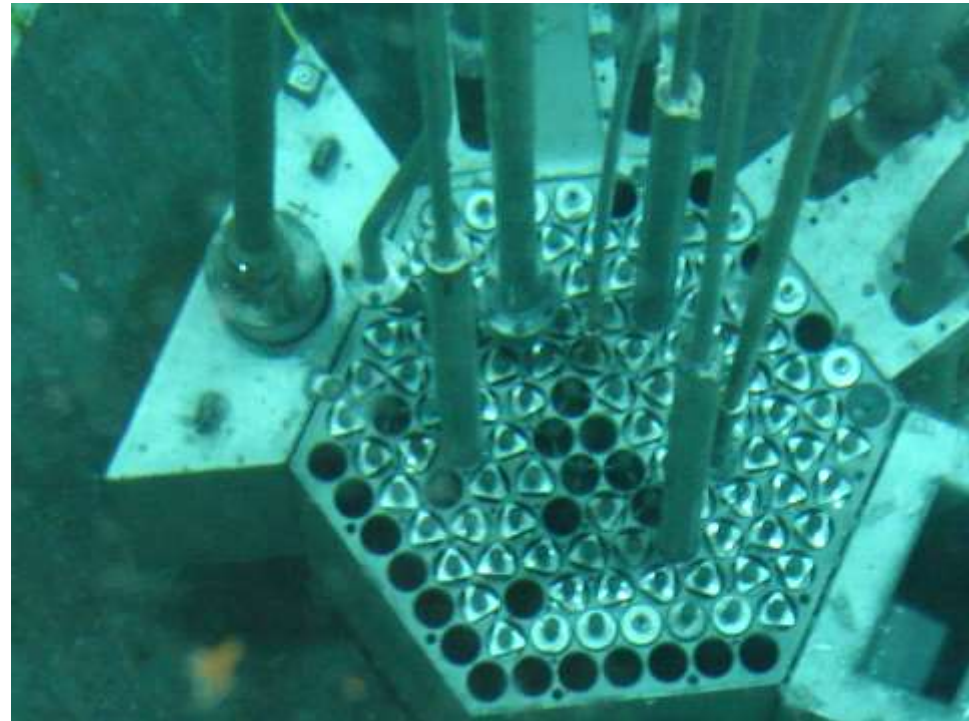
- Generate and run MCNPX HPGe detector input based on the predicted gamma emissions from the activated sample
 - Creates input file
 - Runs file (MCNPX must be installed)
 - Parses MCNPX output file and plots gamma spectrum



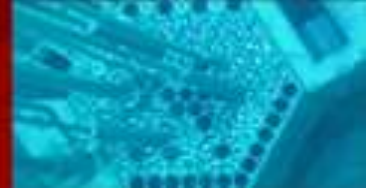


UUTR Irradiation Ports

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

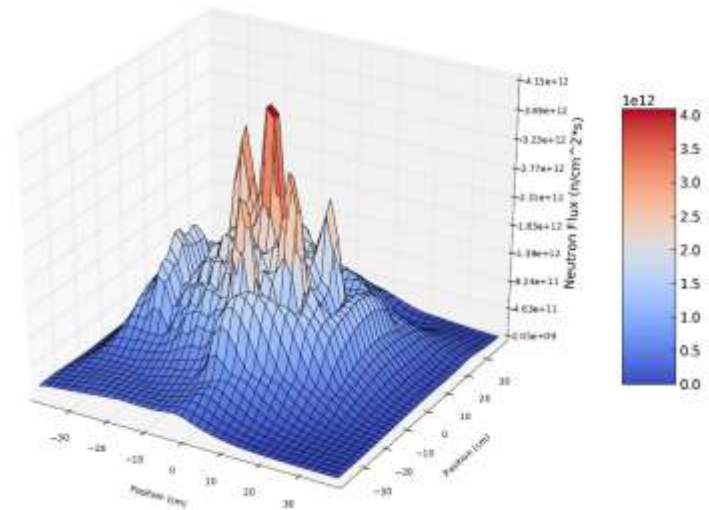


University of Utah TRIGA Reactor

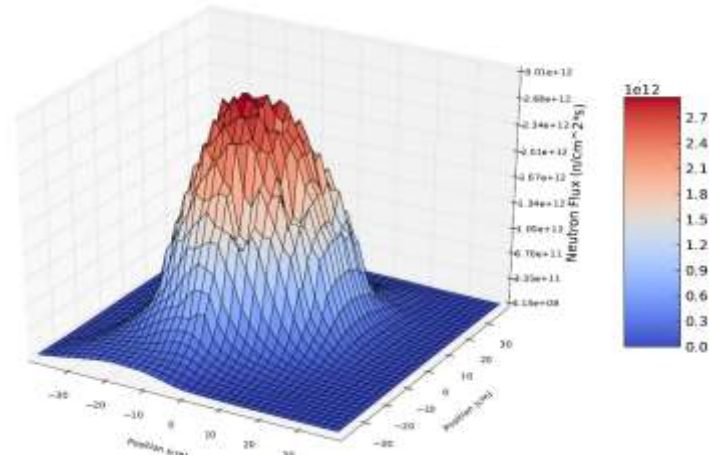


MCNPX Simulation of UUTR

- 2620 neutron fluence tally bins from 0 to 10 MeV for neutron fluence tally (F4:n)
- PyNIC can use any neutron energy bin structure
 - User can make energy bin structure as fine or as course as needed for their application



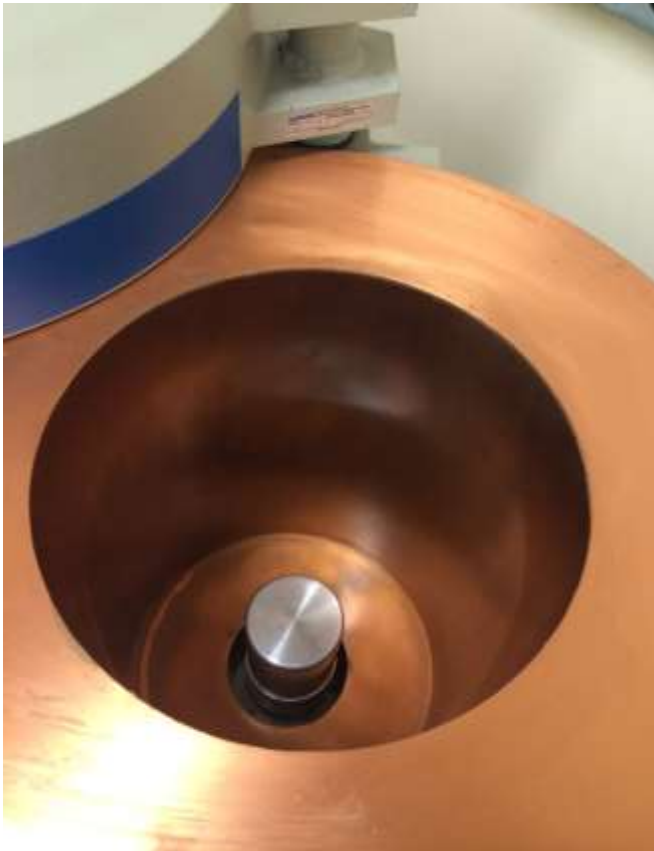
UUTR Thermal Neutron Flux



UUTR Fast Neutron Flux

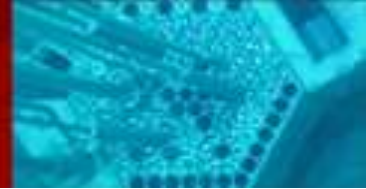


PyNIC Benchmarking



HPGe detector with Canberra lead
and copper shielding

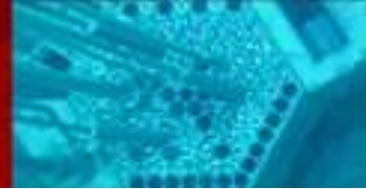
- Samples irradiated in the thermal irradiator port in the UUTR
- Materials irradiated
 - Ni wire
 - Co wire
 - Ti wire
 - W wire
- Samples counted on a HPGe detector



NAA Measurement Results

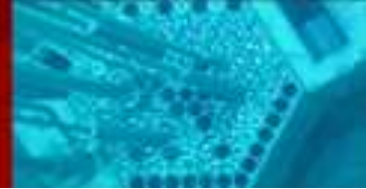
- Ni and Ti results agree with predictions within +/-8.5% for all points
- PyNIC over predicts the activity for W and Co samples by ~20-30% for most experiments

Material	Reactor Power (kW)	Measured Activity (uCi/g)	PyNIC Activity (uCi/g)	% Difference
Ni	1	0.23	0.25	7.4%
	10	2.8	3.0	8.5%
	30	7.5	7.6	1.6%
	50	13	12	-0.9%
	70	18	18	1.1%
	90	22	23	4.0%
Ti	1	3.7	3.8	-1.4%
	10	39	38	-2.8%
	30	111	114	2.0%
	50	202	189	-6.3%
	70	264	265	0.4%
	90	326	341	4.3%
W	1	1.50	1.20	24.6%
	30	136	104	30.6%
	50	75	74	2.2%
	70	106	84	26.5%
	90	136	106	27.9%
Co	1	6.7	7.7	23.1%
	50	35	39	17.7%
	90	61	70	17.0%



Future Work

- Additional NAA experiments in UUTR
- Add post calculation functionality to get starting material concentration
- Add secondary decay daughter product gamma emissions



Acknowledgements

- This research is being performed using funding received from DOE through the Integrated University Program
- Tristalee Williams
- Ryan Schow
- Steve Burnham