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Title: Low-fidelity MCNP Integral Experiment Model Optimization

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Low-fidelity MCNP Integral Experiment Model Optimization

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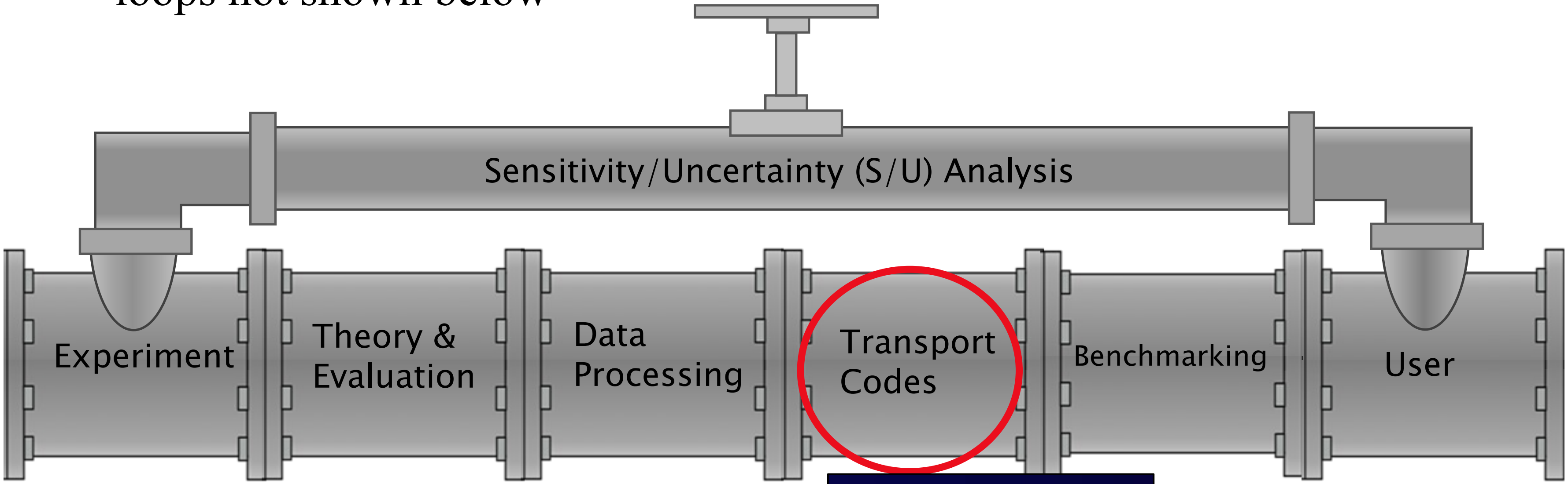
Los Alamos National Laboratory

2024 MCNP® User Symposium

LA-UR-24-XXXXX

Nuclear Data Pipeline

- The nuclear data pipeline is a visualization of the process of how measured and theorized quantities are verified, validated, and processed into a format accessible to nuclear data users
- United States nuclear data library ENDF/B-I was released in June 1968!
- Many tools and approaches have been developed to traverse the pipeline in the most efficient way possible – this process involves many feedback loops not shown below



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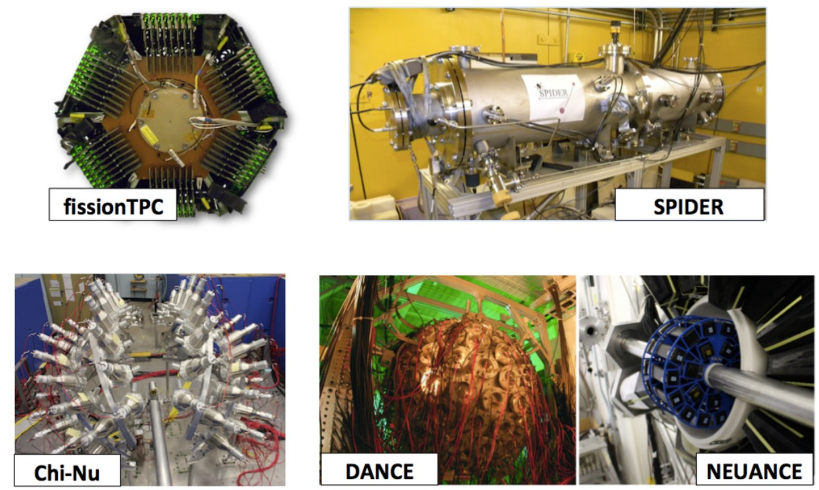
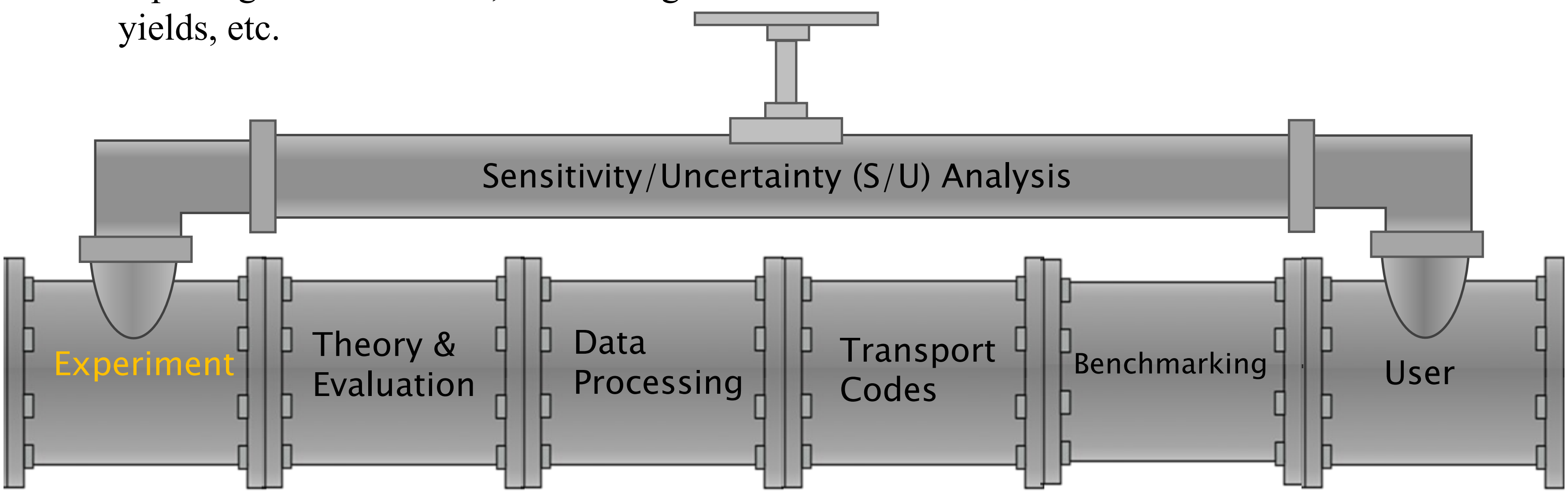
D. Brown, "Nuclear Data Pipeline," *Workshop for Applied Nuclear Data Activities* (2023)

Nuclear Data Pipeline: Experiment

- Experimental measurements are used to constrain nuclear data uncertainties as much as possible and test evaluated files in our physics codes
- Measurement types:
  1. Differential
  2. Integral
- **Differential measurements** include neutron cross section measurements as a function of incident neutron energy, capture gamma cascades, fission fragment yields, etc.

Los Alamos Neutron Science Center (LANSCE)





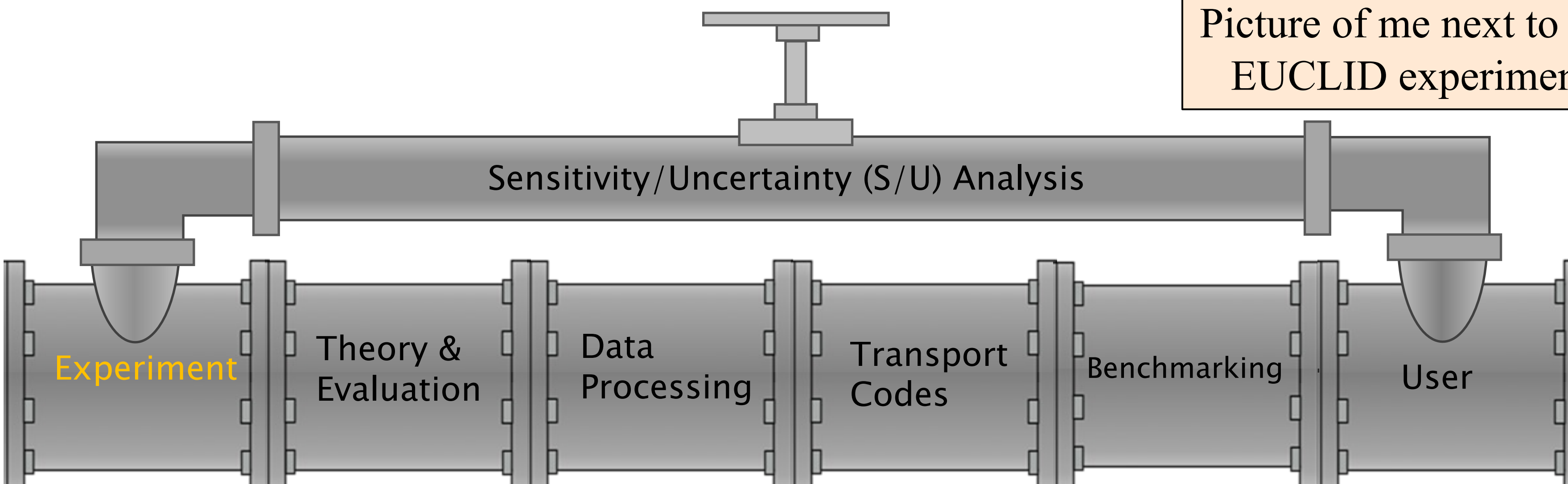
P. Lisowski et al., "The Los Alamos Neutron Science Center," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 562 (2006)

Nuclear Data Pipeline: Experiment

- Measurement types:
  1. Differential
  2. Integral
- **Integral measurements** include nuclear criticality experiments (measure multiplication of the system to infer effective neutron multiplication factor k_{eff}) and shielding measurements

National Criticality Experiments Research Center (NCERC)

Picture of me next to the EUCLID experiment



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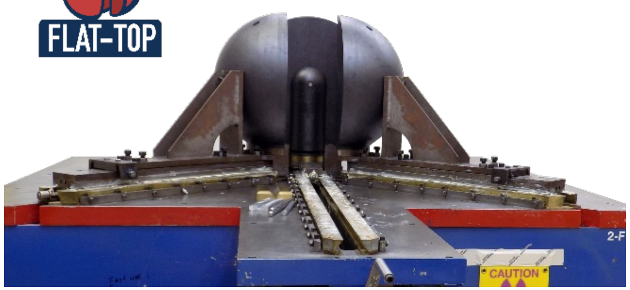
"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* 195 Supplement 1 (2021)

Nuclear Criticality Experiments

- The National Criticality Experiments Research Center (NCERC) is the only general-purpose criticality experiments facility in the United States
- 4 Critical Assembly Machines:



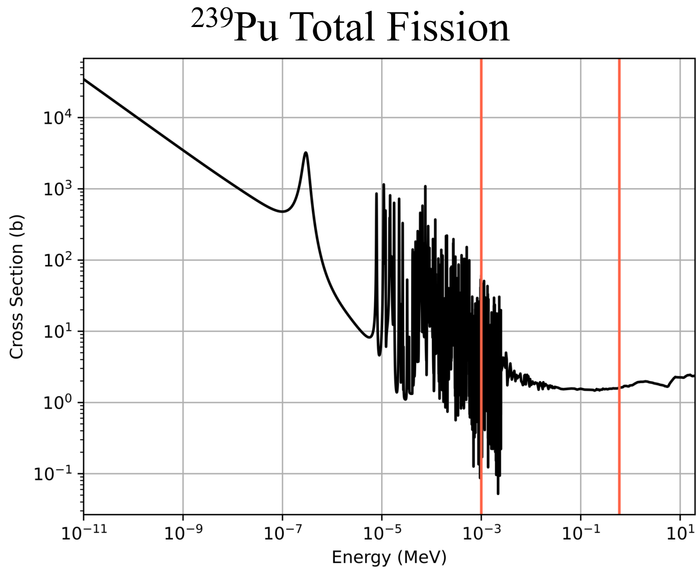
"National Criticality Experiments Research Center (NCERC): The First 10 Years of Operation," *Nuclear Science and Engineering* 195 Supplement 1 (2021)

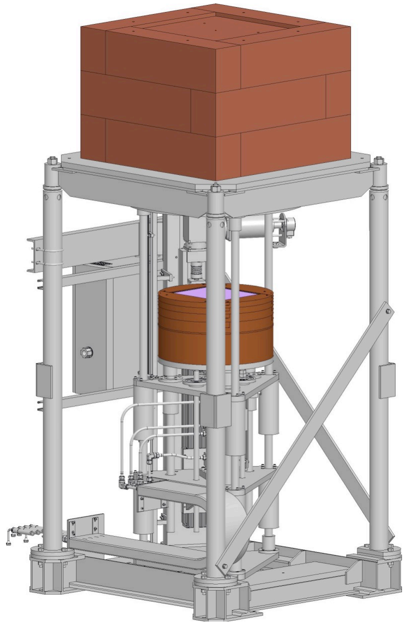
PARADIGM Project

- **PARADIGM** stands for **PAR**allel **A**pproach of **D**ifferential and **I**nte**G**ral **M**easurements

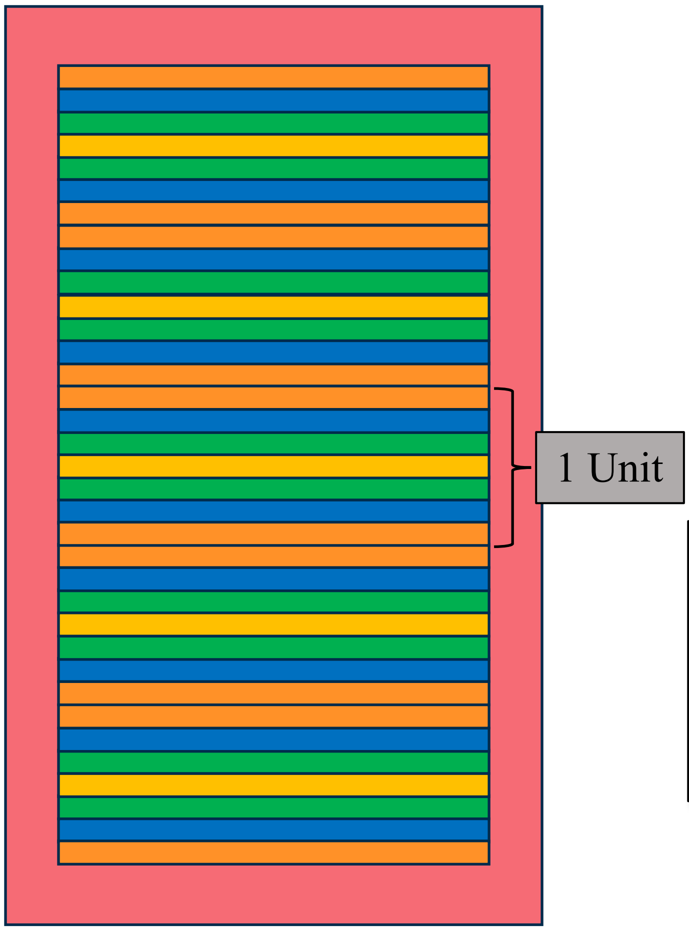
Goal: Reduce ^{239}Pu nuclear data uncertainty in the intermediate-energy range using new nuclear data theory, differential measurements, integral measurements, and statistical analysis

- Simultaneous design of criticality experiment, normally referred to as an "integral experiment," and differential measurement using machine learning decreases amount of time for initial steps of nuclear data pipeline
- "Intermediate-energy range" is normally defined in textbooks from ~1 eV to 100 keV – the energy range of interest for this work is focused specifically on 1 keV to 600 keV
- The work in this talk will focus on optimization of integral experiment design





Low-fidelity MCNP Model



Modeling Approach:

(1) Define a unit of materials, geometry (e.g., rectangular/cylindrical), reflector, and total number of units *N*

(2) Set up cell and surface cards for 1 unit and then repeat *N* times – RPP/RCC Surface Cards

(3) Determine fuel regions for KSRC points (*k*-eigenvalue calculation)

(4) Set up data cards (i.e., KCODE, KSRC, KOPTS, tally cards, KSEN)

5.3.4.2 RPP: Rectangular Parallelepiped

RPP *xmin xmax ymin ymax zmin zmax*	
xmin xmax	Termini of box sides normal to the x axis.
ymin ymax	Termini of box sides normal to the y axis.
zmin zmax	Termini of box sides normal to the z axis.

5.3.4.4 RCC: Right Circular Cylinder

RCC *vx vy vz h1 h2 h3 r*	
vx vy vz	The (x, y, z) coordinates at the center of the base for the right circular cylinder.
h1 h2 h3	Right circular cylinder axis vector, which provides both the orientation and the height of the cylinder.
r	Radius of cylinder.

J. Kulesza et al., "MCNP® Code Version 6.3.0 Theory & User Manual," (2022), LA-UR-22-30006.

Low-fidelity MCNP Model

```
c
c CELL Cards
c
1 11 -3.97 -100    imp:n=1
2 13 -1.7 -101    imp:n=1
3 19 -2.37 -102    imp:n=1
4 90 -15.1435 -103    imp:n=1
5 19 -2.37 -104    imp:n=1
6 13 -1.7 -105    imp:n=1
7 11 -3.97 -106    imp:n=1
8 11 -3.97 -107    imp:n=1
9 13 -1.7 -108    imp:n=1
10 19 -2.37 -109    imp:n=1
11 90 -15.1435 -110    imp:n=1
12 19 -2.37 -111    imp:n=1
13 13 -1.7 -112    imp:n=1
14 11 -3.97 -113    imp:n=1
15 11 -3.97 -114    imp:n=1
16 13 -1.7 -115    imp:n=1
17 19 -2.37 -116    imp:n=1
18 90 -15.1435 -117    imp:n=1
19 19 -2.37 -118    imp:n=1
20 13 -1.7 -119    imp:n=1
21 11 -3.97 -120    imp:n=1
22 11 -3.97 -121    imp:n=1
23 13 -1.7 -122    imp:n=1
24 19 -2.37 -123    imp:n=1
25 90 -15.1435 -124    imp:n=1
26 19 -2.37 -125    imp:n=1
27 13 -1.7 -126    imp:n=1
28 11 -3.97 -127    imp:n=1
29 11 -3.97 -128    imp:n=1
30 13 -1.7 -129    imp:n=1
31 19 -2.37 -130    imp:n=1
32 90 -15.1435 -131    imp:n=1
33 19 -2.37 -132    imp:n=1
34 13 -1.7 -133    imp:n=1
35 11 -3.97 -134    imp:n=1
36 11 -3.97 -135    imp:n=1
37 13 -1.7 -136    imp:n=1
38 19 -2.37 -137    imp:n=1
39 90 -15.1435 -138    imp:n=1
```

...

```
96 19 -2.37 -195    imp:n=1
97 13 -1.7 -196    imp:n=1
98 11 -3.97 -197    imp:n=1
99 1018 -8.96 -198
           +100 +101 +102 +103 +104 +105 +106 +107 +108 +109
           +110 +111 +112 +113 +114 +115 +116 +117 +118 +119
           +120 +121 +122 +123 +124 +125 +126 +127 +128 +129
           +130 +131 +132 +133 +134 +135 +136 +137 +138 +139
           +140 +141 +142 +143 +144 +145 +146 +147 +148 +149
           +150 +151 +152 +153 +154 +155 +156 +157 +158 +159
           +160 +161 +162 +163 +164 +165 +166 +167 +168 +169
           +170 +171 +172 +173 +174 +175 +176 +177 +178 +179
           +180 +181 +182 +183 +184 +185 +186 +187 +188 +189
           +190 +191 +192 +193 +194 +195 +196 +197 imp:n=1
100 0 +198 imp:n=0
```

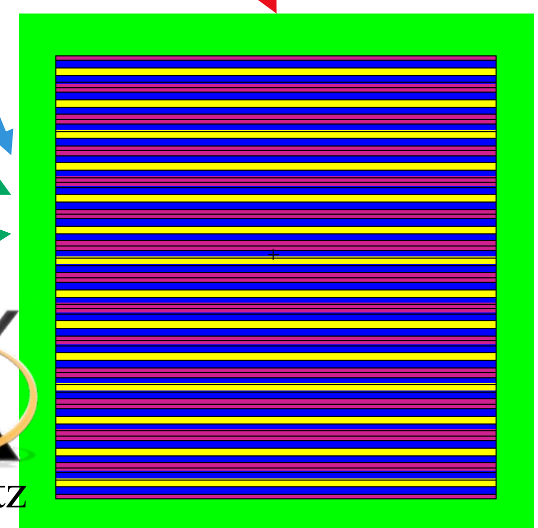
```
c
c SURFACE Cards
c
100 rpp 0 30.48 0 25.4 0 1.2753
101 rpp 0 30.48 0 25.4 1.275301 1.426601
102 rpp 0 30.48 0 25.4 1.426602 1.532602
103 rpp 0 30.48 0 25.4 1.532603 1.968603
104 rpp 0 30.48 0 25.4 1.968604 2.074604
105 rpp 0 30.48 0 25.4 2.074605 2.225905
106 rpp 0 30.48 0 25.4 2.225906 3.501206
107 rpp 0 30.48 0 25.4 3.501207 4.776507
108 rpp 0 30.48 0 25.4 4.776508 4.927808
109 rpp 0 30.48 0 25.4 4.927809 5.033809
110 rpp 0 30.48 0 25.4 5.03381 5.46981
111 rpp 0 30.48 0 25.4 5.469811 5.575811
112 rpp 0 30.48 0 25.4 5.575812 5.727112
113 rpp 0 30.48 0 25.4 5.727113 7.002413
114 rpp 0 30.48 0 25.4 7.002414 8.277714
115 rpp 0 30.48 0 25.4 8.277715 8.429015
116 rpp 0 30.48 0 25.4 8.429016 8.535016
117 rpp 0 30.48 0 25.4 8.535017 8.971017
118 rpp 0 30.48 0 25.4 8.971018 9.077018
119 rpp 0 30.48 0 25.4 9.077019 9.228319
120 rpp 0 30.48 0 25.4 9.22832 10.50362
121 rpp 0 30.48 0 25.4 10.503621 11.778921
122 rpp 0 30.48 0 25.4 11.778922 11.930222
123 rpp 0 30.48 0 25.4 11.930223 12.036223
124 rpp 0 30.48 0 25.4 12.036224 12.472224
125 rpp 0 30.48 0 25.4 12.472225 12.578225
126 rpp 0 30.48 0 25.4 12.578226 12.729526
127 rpp 0 30.48 0 25.4 12.729527 14.004827
128 rpp 0 30.48 0 25.4 14.004828 15.280128
129 rpp 0 30.48 0 25.4 15.280129 15.431429
130 rpp 0 30.48 0 25.4 15.43143 15.53743
131 rpp 0 30.48 0 25.4 15.537431 15.973431
132 rpp 0 30.48 0 25.4 15.973432 16.079432
133 rpp 0 30.48 0 25.4 16.079433 16.230733
134 rpp 0 30.48 0 25.4 16.230734 17.506034
135 rpp 0 30.48 0 25.4 17.506035 18.781335
136 rpp 0 30.48 0 25.4 18.781336 18.932636
137 rpp 0 30.48 0 25.4 18.932637 19.038637
```

...

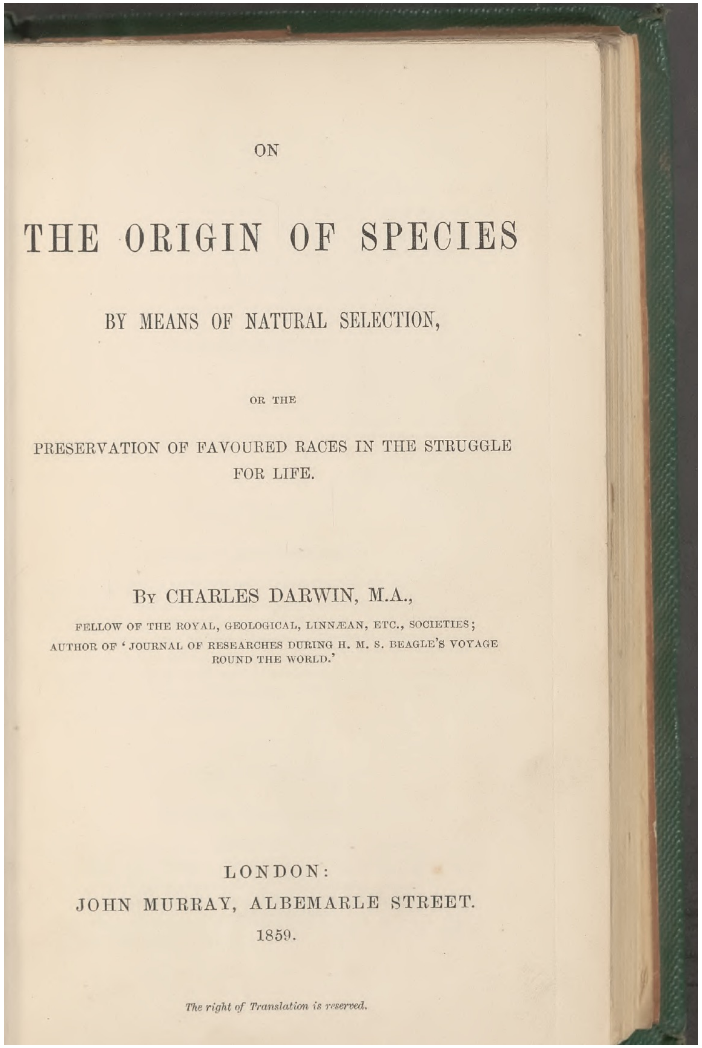
```
c
c DATA Cards
c
kcode 1e3 1 100 600
kopts kinetics = yes
ksrc    15.24 12.7 0.913502
        15.24 12.7 2.740507
        15.24 12.7 4.567512
        15.24 12.7 6.394517
        15.24 12.7 8.221522
        15.24 12.7 10.048527
        15.24 12.7 11.875532
        15.24 12.7 13.702537
        15.24 12.7 15.529542
        15.24 12.7 17.356547
        15.24 12.7 19.183552
        15.24 12.7 21.010557
        15.24 12.7 22.837562
        15.24 12.7 24.664567
f4:n  3 8 13 18 23 28
       33 38 43 48 53
       58 63 68 T
E4 0.001 .6 20
KSEN14 XS ISO = 94239.00c RXN = 18 ERG = 0 0.001 .6 20
m11       8016    -0.469474    $ Aluminum Oxide (Al2O3), 3.97 g/cc
          8017    -0.000190
          8018    -0.001086
         13027    -0.529251
```

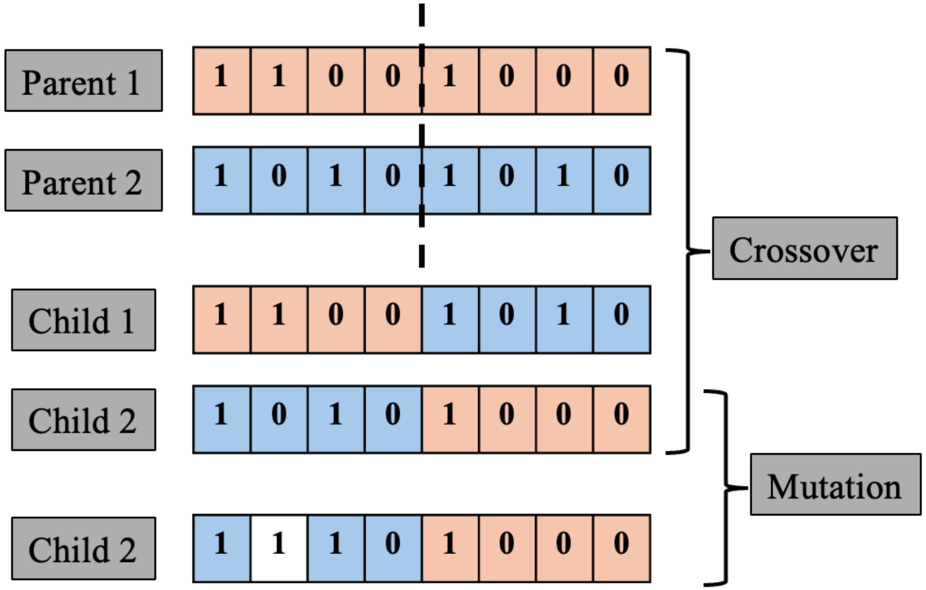
...

XQuartz



Genetic Algorithm Background



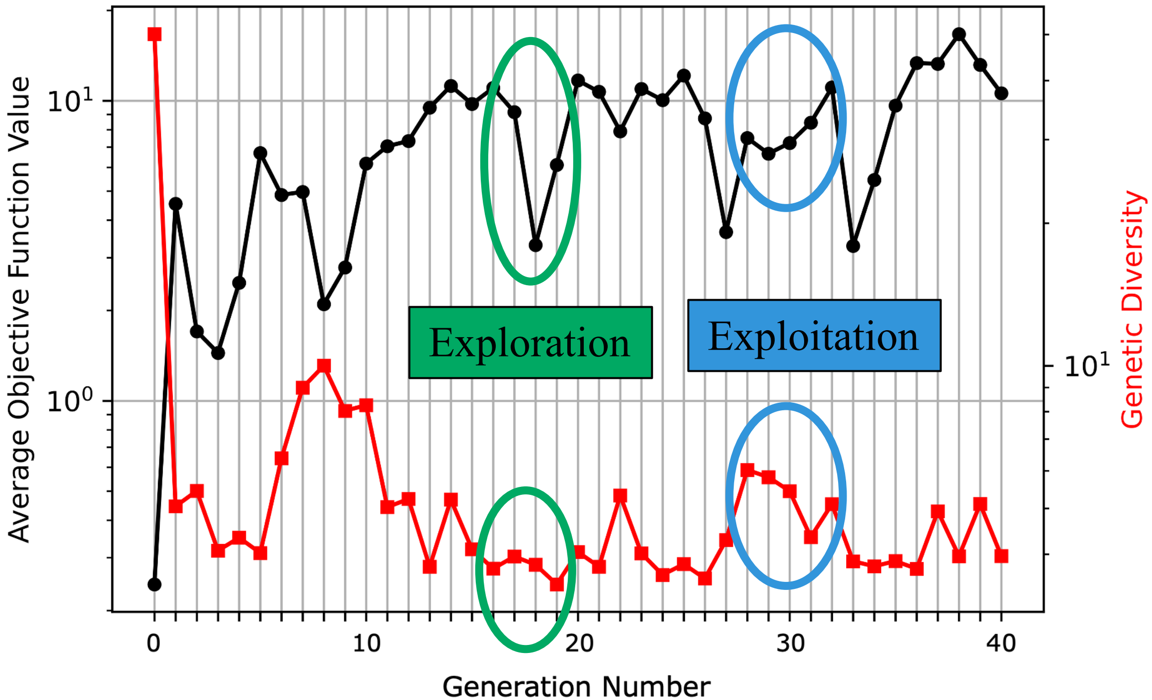


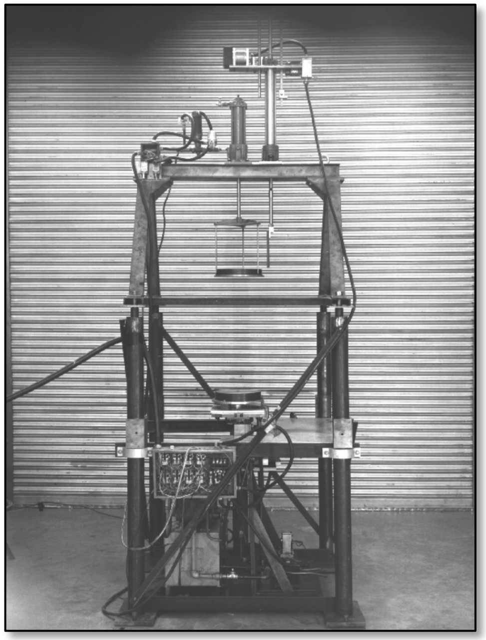
- Crossover between parents (i.e., experiment designs) is probabilistic – the Wheel of Fortune is an easy way to think about this - larger slices of the Wheel (i.e., higher probability of design getting selected for crossover) based on design "fitness"
- Fitness is determined by an objective function, or figure of merit (FoM)

C. Darwin, L. Kebler, "On the origin of species by means of natural selection, or the preservation of favoured races in the struggle for life," London: J. Murray (1859), https://lccn.loc.gov/06017473

Verification of Genetic Algorithm

- Verification of the genetic algorithm to converge to global solution
- Two things to test: (1) convergence rate and (2) solution comparison to baseline
- Benchmarked cases of the early Jemima experiments (ICSBEP designation of IEU-MET-FAST-001) were used as a baseline
- Verification goal: converge to solution that shows similar performance to or outperforms baseline set based on calculated FoM

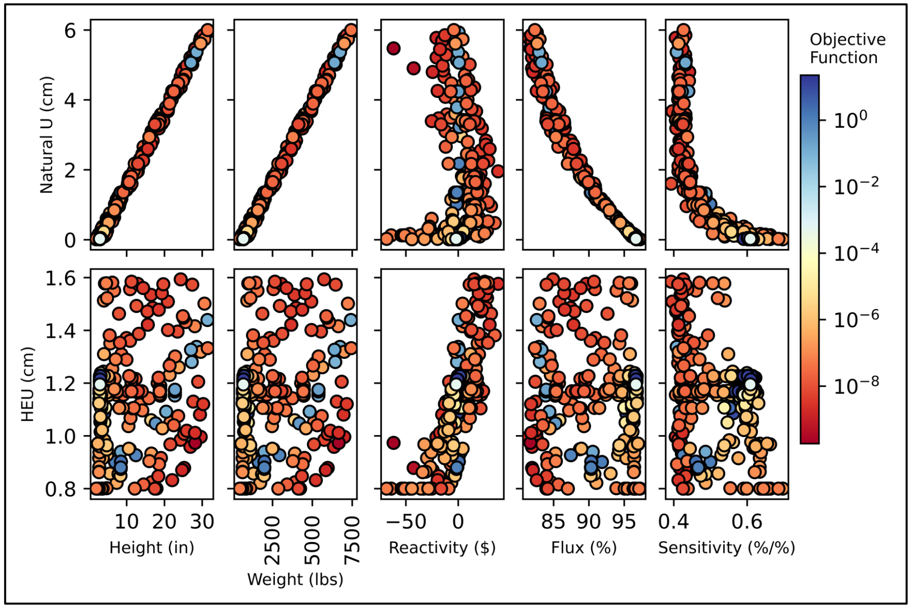


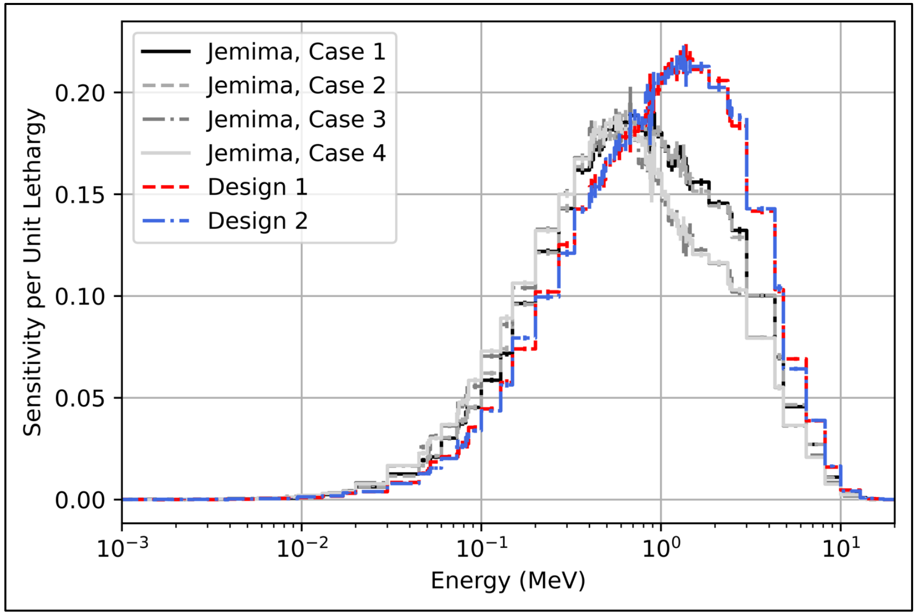


The Jemima experiment (1953)

N. Kleedtke et al., "Genetic Algorithm Optimization of Nuclear Criticality Experiment for Reduction of Intermediate-energy ^{239}Pu Nuclear Data Uncertainties," (In Preparation)

Verification of Genetic Algorithm





$$\text{FoM} = \frac{f(\rho) \cdot I \cdot \left| \int_{1keV}^{600keV} S_{k,^{239}Pu(n,f)} dE \right|}{H/39.3701 \cdot W/\ 2000}$$

$$f(\rho) = \begin{cases} -0.2\,(\rho - 0.4)^2 + 1, & -1.836 < \rho < 2.636 \\ 10^{-6}\left|-0.2\,(\rho - 0.4)^2 + 1\right|^{-1}, & \text{otherwise.} \end{cases}$$

I = intermediate-energy neutron flux fraction
H = total assembly height
W = total assembly weight
ρ = reactivity
$S_{k,\sigma}$ = sensitivity of the neutron multiplication factor k to nuclear data σ

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N. Kleedtke et al., "Genetic Algorithm Optimization of Nuclear Criticality Experiment for Reduction of Intermediate-energy ^{239}Pu Nuclear Data Uncertainties," (In Preparation)

PARADIGM Optimized Experiment Design

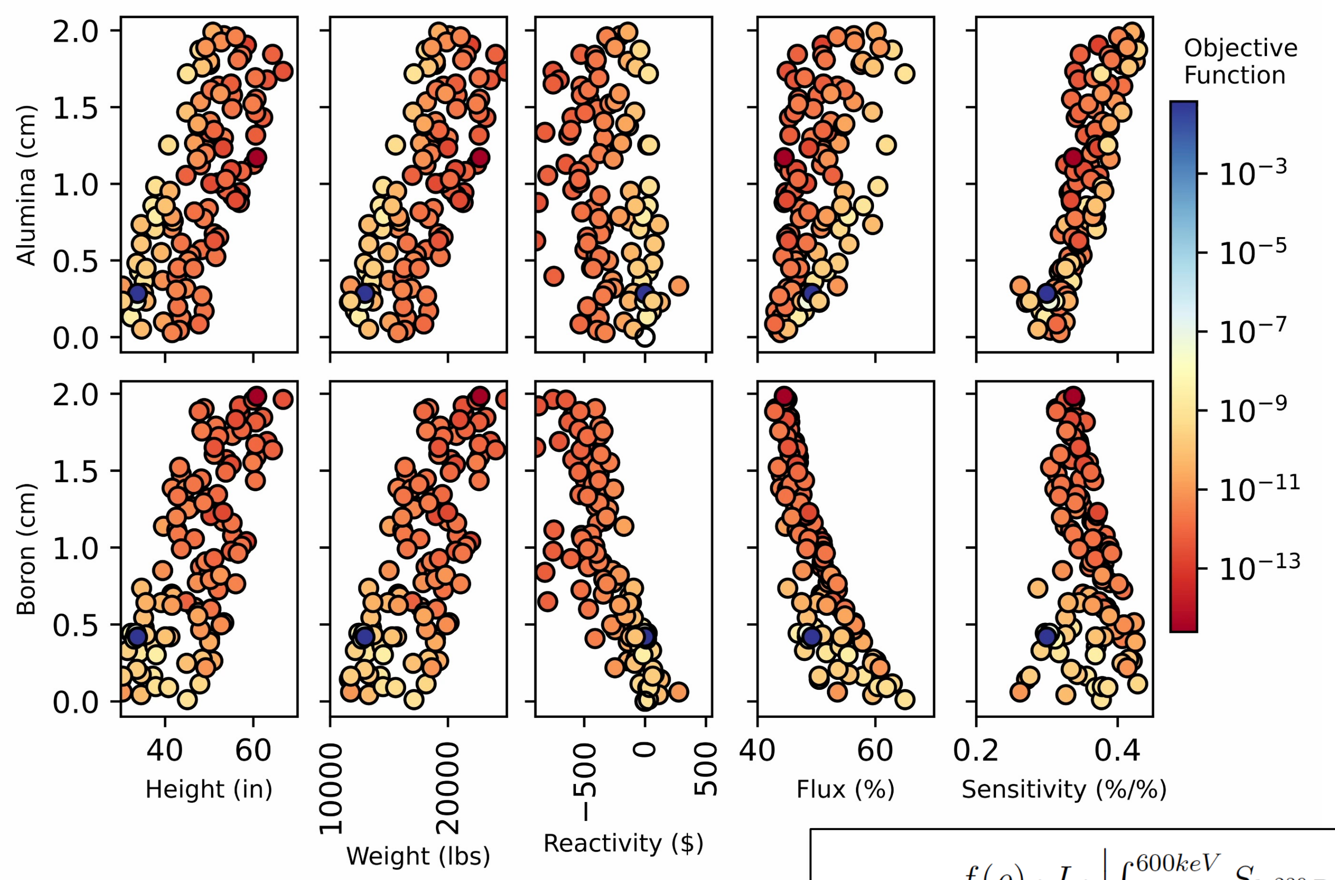
- Optimized experiment design for designs with and without a reflector
- Results shown for 1 of the 3 final optimized experiment designs with copper reflector:

(1) Alumina, Graphite, Boron, Zero Power Physics Reactor (ZPPR) Plutonium Aluminum No-Nickel (PANN) plates, Boron, Graphite, Alumina
(2) Alumina, Graphite, ZPPR Plates, Graphite, Alumina
(3) Alumina, Boron, ZPPR Plates, Boron, Alumina

- 14 total units on Comet assembly machine
- ZPPR plates were arranged in 4x5 array (i.e., 25.40 cm by 30.48 cm) – set to the same dimensions of the Chlorine Worth Study (CWS) experiment fuel configuration
- 30 cm uniform copper reflector, which is similar to outer dimensions of ZEUS copper reflector

N. Kleedtke et al., "Genetic Algorithm Optimization of Nuclear Criticality Experiment for Reduction of Intermediate-energy ^{239}Pu Nuclear Data Uncertainties," (In Preparation)

PARADIGM Optimized Experiment Design



$$\mathrm{FoM} = \frac{f(\rho)\cdot I \cdot \left| \int_{1keV}^{600keV} S_{k,{}^{239}Pu(n,f)} dE \right|}{H/39.3701 \cdot W/10^4}$$

$$f(\rho) = \begin{cases} -0.2\,(\rho-0.4)^2+1, & -1.836<\rho<2.636 \\ 10^{-6}\left|-0.2\,(\rho-0.4)^2+1\right|^{-1}, & \text{otherwise.} \end{cases}$$

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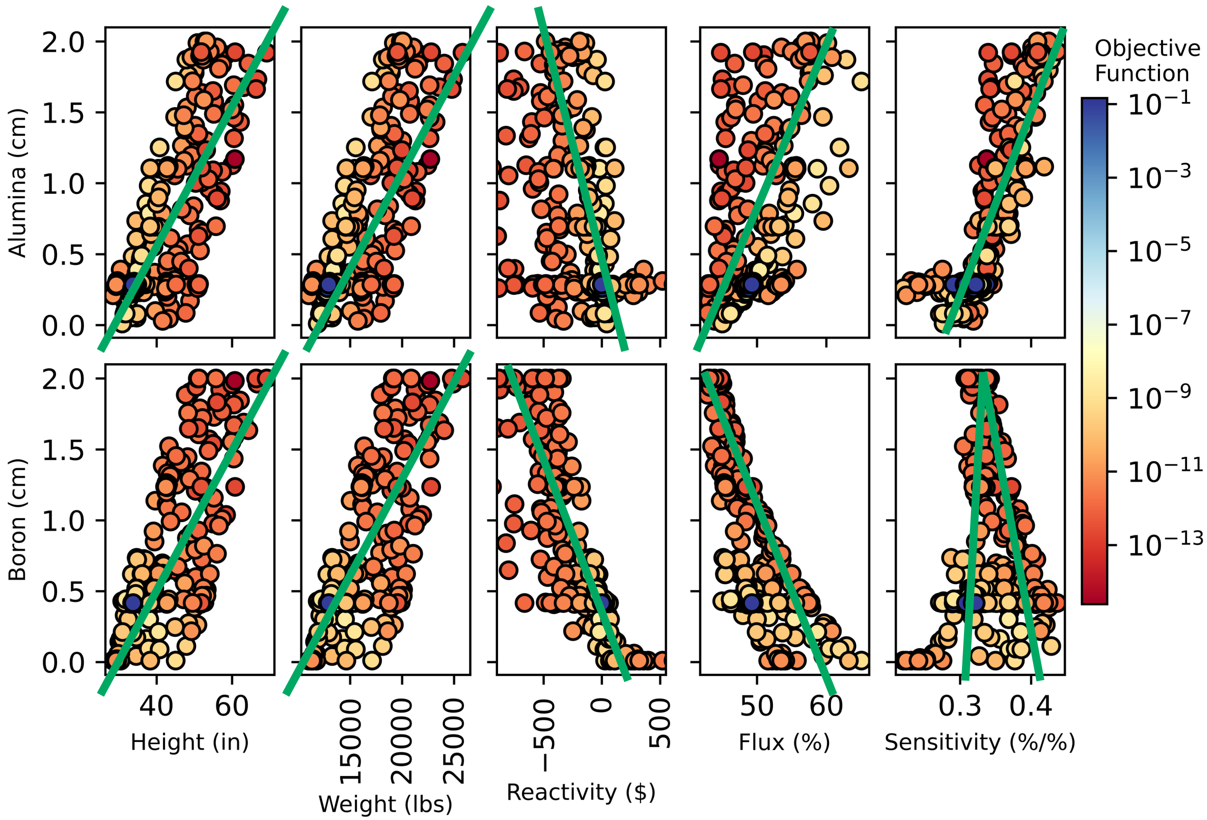
N. Kleedtke et al., "Genetic Algorithm Optimization of Nuclear Criticality Experiment for Reduction of Intermediate-energy ^{239}Pu Nuclear Data Uncertainties," (In Preparation)

PARADIGM Optimized Experiment Design

- Obvious trendlines – trendline for Boron with respect to sensitivity shows inflection
- Designs with highest objective function values are too heavy – need expert-in-the-loop for final design considerations



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N. Kleedtke et al., "Genetic Algorithm Optimization of Nuclear Criticality Experiment for Reduction of Intermediate-energy ^{239}Pu Nuclear Data Uncertainties," (In Preparation)

Conclusions

- Optimized 3 experiment designs (14 units) with copper reflector:

(1) Alumina, Graphite, Boron, Zero Power Physics Reactor (ZPPR) Plutonium Aluminum No-Nickel (PANN) plates, Boron, Graphite, Alumina
(2) Alumina, Graphite, ZPPR Plates, Graphite, Alumina
(3) Alumina, Boron, ZPPR Plates, Boron, Alumina (**shown in this presentation**)

- Optimized experiment designs for all 3 configurations have heights and weights that exceed the Comet assembly machine operational safety limitations; therefore, **final experiment design analysis is needed** before procurement of parts
- Additional detail is needed for high fidelity design – see P. Brain et al., "Impact of Higher Fidelity Design Iterations on Critical System Criteria" 2024 MCNP User Symposium presentation
- **Optimization algorithms**, such as the genetic algorithm used in this work, Gaussian process, or particle swarm optimization (PSO) **should be used in place of traditional iterative methods to save both time and effort**
- Objective function could be revisited to include similarity (e.g., correlation coefficient) and/or nuclear data-induced uncertainty for more targeted design
- Genetic algorithm could include material ordering and material selection in future optimization runs

Acknowledgments

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