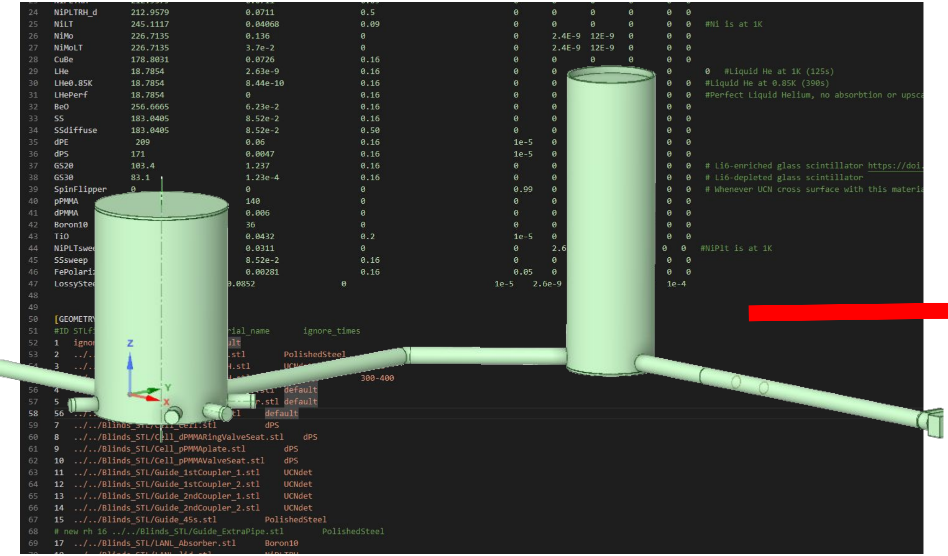
NC STATE UNIVERSITY

nEDM @SNS

How we use PENTrack, a Monte-Carlo UCN Simulation Tool

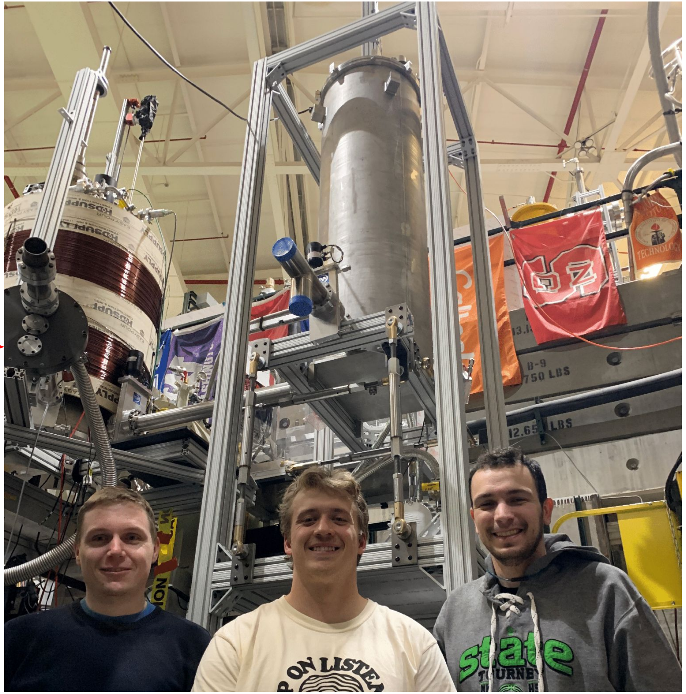
Cole Teander
Almaty, Kazakhstan, April 2024

From this:



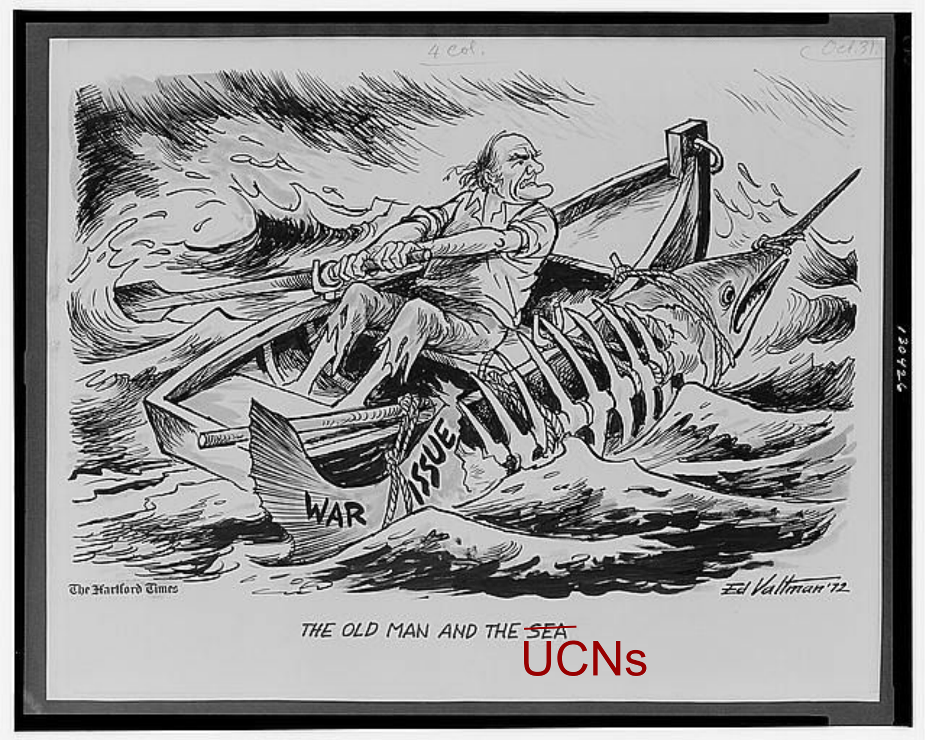
```
NiPLTRH_d      212.9579         0.0711          0.5           0      0      0      0      0   0
NiLT           245.1117         0.04068         0.09          0      0      0      0      0   0   #Ni is at 1K
NiMo           226.7135         0.136           0             0      2.4E-9 12E-9  0      0   0
NiMoLT         226.7135         3.7e-2          0             0      2.4E-9 12E-9  0      0   0
CuBe           178.8031         0.0726          0.16          0      0      0      0      0   0
LHe            18.7854          2.63e-9         0.16          0      0                    0       0   #Liquid He at 1K (125s)
LHe0.85K       18.7854          8.44e-10        0.16          0      0                    0   0   #Liquid He at 0.85K (390s)
LHePerf        18.7854          0               0.16          0      0                    0   0   #Perfect Liquid Helium, no absorbtion or upsca
BeO            256.6665         6.23e-2         0.16          0      0                    0   0
SS             183.0405         8.52e-2         0.16          0      0                    0   0
SSdiffuse      183.0405         8.52e-2         0.50          0      0                    0   0
dPE             209             0.06            0.16          1e-5   0                    0   0
dPS            171              0.0047          0.16          1e-5   0                    0   0
GS20           103.4            1.237           0.16          0      0                    0   0   # Li6-enriched glass scintillator https://doi.
GS30           83.1             1.23e-4         0.16          0      0                    0   0   # Li6-depleted glass scintillator
SpinFlipper    0                0               0             0.99   0                    0   0   # Whenever UCN cross surface with this materia
pPMMA                           140             0             0      0                    0   0
dPMMA                           0.006           0             0      0                    0   0
Boron10                         36              0             0      0                    0   0
TiO                             0.0432          0.2           1e-5   0                    0   0
NiPLTswe                        0.0311          0             0      2.6                0   0   #NiPlt is at 1K
SSsweep                         8.52e-2         0.16          0      0                    0   0
FePolari                        0.00281         0.16          0.05   0                    0   0
LossySte                       0.0852                  0             1e-5   2.6e-9              1e-4


[GEOMETRY
#ID STLf                       rial_name       ignore_times
1   ignor                      ult
2   ../..                      .stl        PolishedSteel
3   ../..                      H.stl       UCN
                                                   300-400
4                                   default
5                              r.stl default
56  ../..                      tl      default
7   ../../Blinds_STL/Cell_Cell.stl          dPS
8   ../../Blinds_STL/Cell_dPMMARingValveSeat.stl    dPS
9   ../../Blinds_STL/Cell_pPMMAplate.stl        dPS
10  ../../Blinds_STL/Cell_pPMMAValveSeat.stl    dPS
11  ../../Blinds_STL/Guide_1stCoupler_1.stl     UCNdet
12  ../../Blinds_STL/Guide_1stCoupler_2.stl     UCNdet
13  ../../Blinds_STL/Guide_2ndCoupler_1.stl     UCNdet
14  ../../Blinds_STL/Guide_2ndCoupler_2.stl     UCNdet
15  ../../Blinds_STL/Guide_45s.stl          PolishedSteel
# new rh 16 ../../Blinds_STL/Guide_ExtraPipe.stl        PolishedSteel
17  ../../Blinds_STL/LANL_Absorber.stl      Boron10
```

To this:



People from left to right:
Wolfgang Schreyer (ORNL), *Cole Teander* (NCSU), *Clark Hickman* (NCSU)

UCN Transport is Difficult!



THE OLD MAN AND THE ~~SEA~~ UCNs

(but simulations can help us understand it)

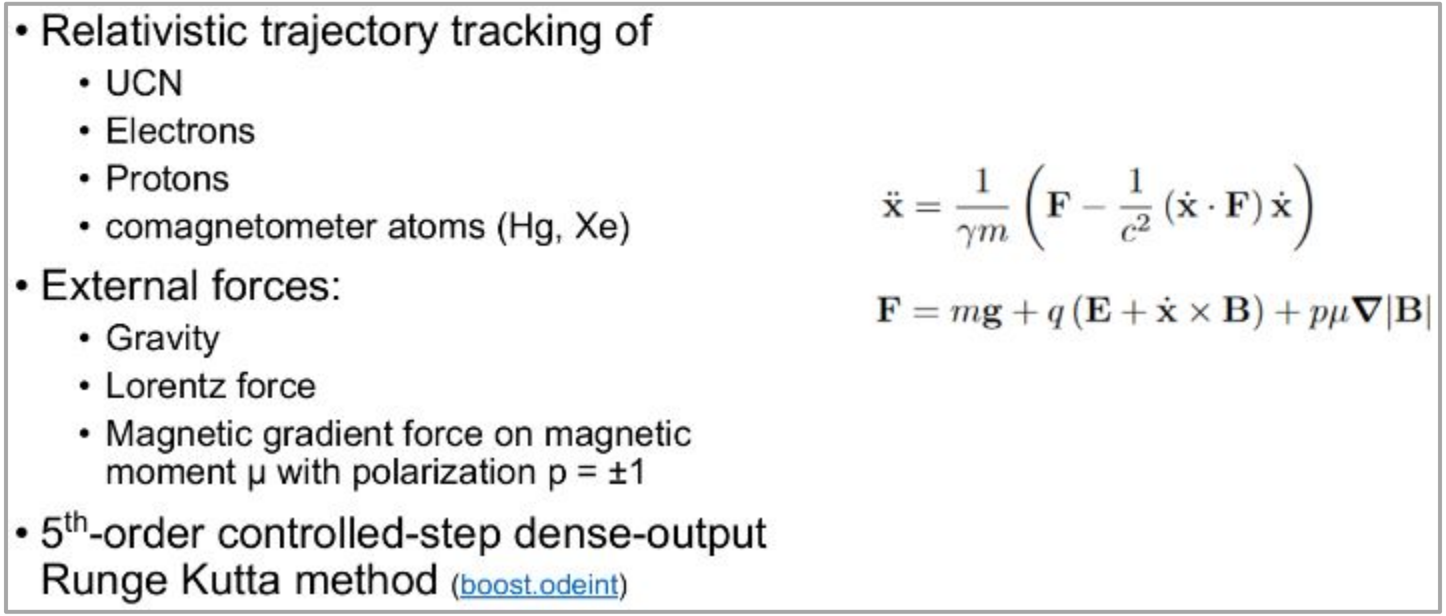
Monte-Carlo Simulation Tools for UCN

Name:	Learn More Here:	Get Access Here:
PENTrack	[1610.06358] (arxiv.org) (W. Schreyer et al., 2017)	GitHub - wschreyer/PENTrack:
MCUCN	[1709.05974] (arxiv.org) (G. Zsigmond, 2018)	MCUCN Code | UCN Physics | Paul Scherrer Institut (PSI) (Email Dr. Geza Zsigmond for access)
Kassiopeia	[1811.05972](arxiv.org) (Z. Bogorad et al., 2022)	GitHub - KATRIN-Experiment/Kassiopeia:
STARucn	Their site (link on the right) or from review paper: [1806.10778] (arxiv.org)	STARucn / Wiki / Home (sourceforge.net)
Geant4UCN	The simulation of ultracold neutron experiments using GEANT4 - ScienceDirect (not on arxiv, I think) (F. Atchison et al., 2005)	Start here Geant4 (cern.ch) Then find UCN specific extensions

What is PENTrack?

- PENTrack, developed by Wolfgang Schreyer, is a Monte-Carlo trajectory tracking simulation tool optimized for UCNs.

(*boxed sections on upcoming slides copied with permission from Wolfgang Schreyer*)



- Relativistic trajectory tracking of
  - UCN
  - Electrons
  - Protons
  - comagnetometer atoms (Hg, Xe)
- External forces:
  - Gravity
  - Lorentz force
  - Magnetic gradient force on magnetic moment μ with polarization p = ±1
- 5^{th}-order controlled-step dense-output Runge Kutta method (boost.odeint)

$$\ddot{\mathbf{x}} = \frac{1}{\gamma m}\left(\mathbf{F} - \frac{1}{c^2}\left(\dot{\mathbf{x}}\cdot\mathbf{F}\right)\dot{\mathbf{x}}\right)$$

$$\mathbf{F} = m\mathbf{g} + q\left(\mathbf{E} + \dot{\mathbf{x}}\times\mathbf{B}\right) + p\mu\nabla|\mathbf{B}|$$

Link from image: (boost.odeint)

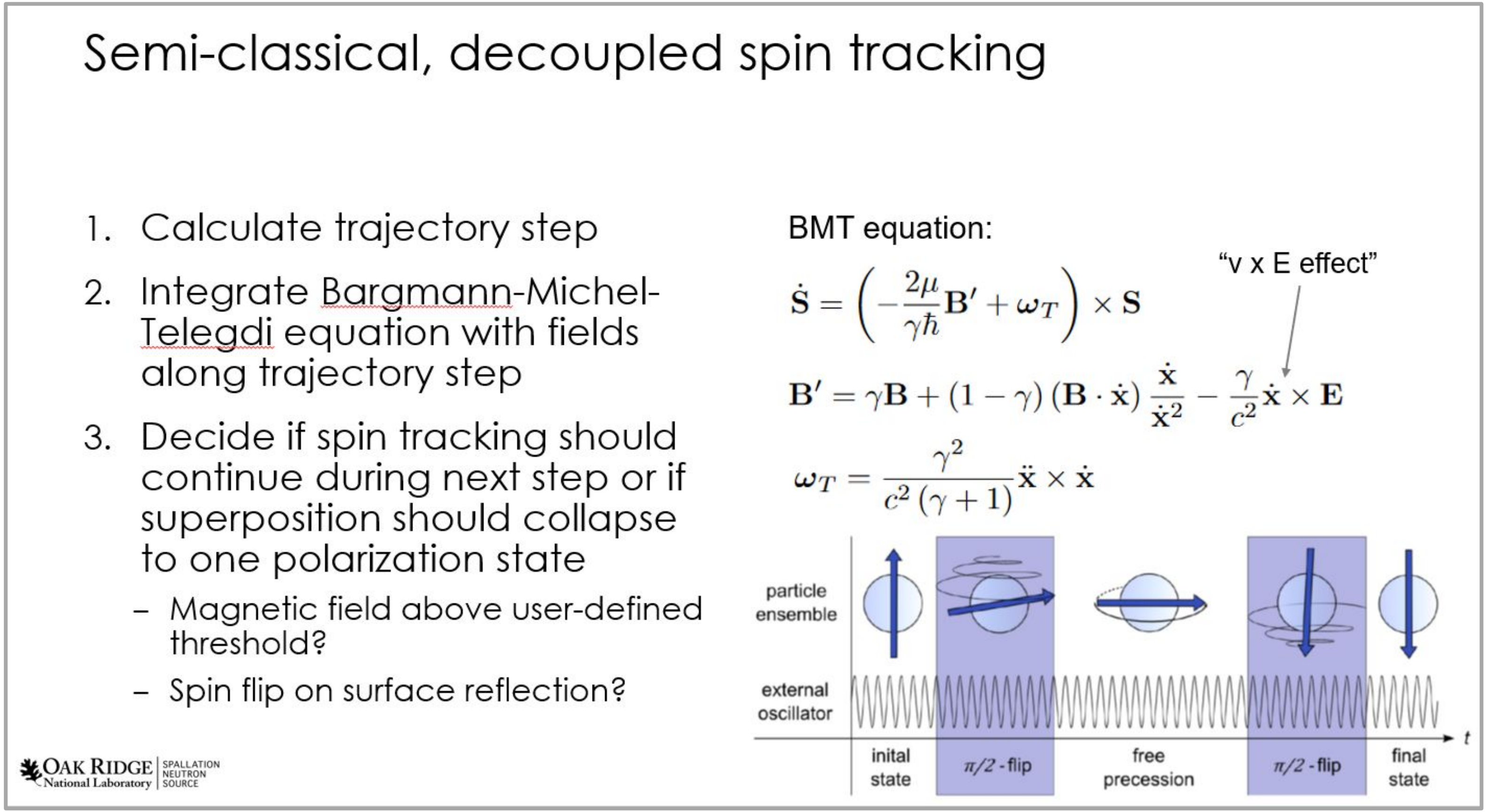
Key Abilities of PENTrack

Specific design goals of PENTrack

- Import any arbitrary geometry designed in CAD software as an STL file
- Simulate UCNs in all conditions/strengths of magnetic fields
    - Import (or define) arbitrary 2D & 3D magnetic & electric field maps (from, ie: OPERA, ANSYS)

All while being (mostly) easy to use without (too much) coding

Spin-Tracking for UCN with PENTrack



Semi-classical, decoupled spin tracking

1. Calculate trajectory step
2. Integrate Bargmann-Michel-Telegdi equation with fields along trajectory step
3. Decide if spin tracking should continue during next step or if superposition should collapse to one polarization state
   - Magnetic field above user-defined threshold?
   - Spin flip on surface reflection?

BMT equation:

$$\dot{\mathbf{S}} = \left(-\frac{2\mu}{\gamma\hbar}\mathbf{B}' + \omega_T\right) \times \mathbf{S}$$

"v x E effect"

$$\mathbf{B}' = \gamma\mathbf{B} + (1-\gamma)\left(\mathbf{B}\cdot\dot{\mathbf{x}}\right)\frac{\dot{\mathbf{x}}}{\dot{\mathbf{x}}^2} - \frac{\gamma}{c^2}\dot{\mathbf{x}}\times\mathbf{E}$$

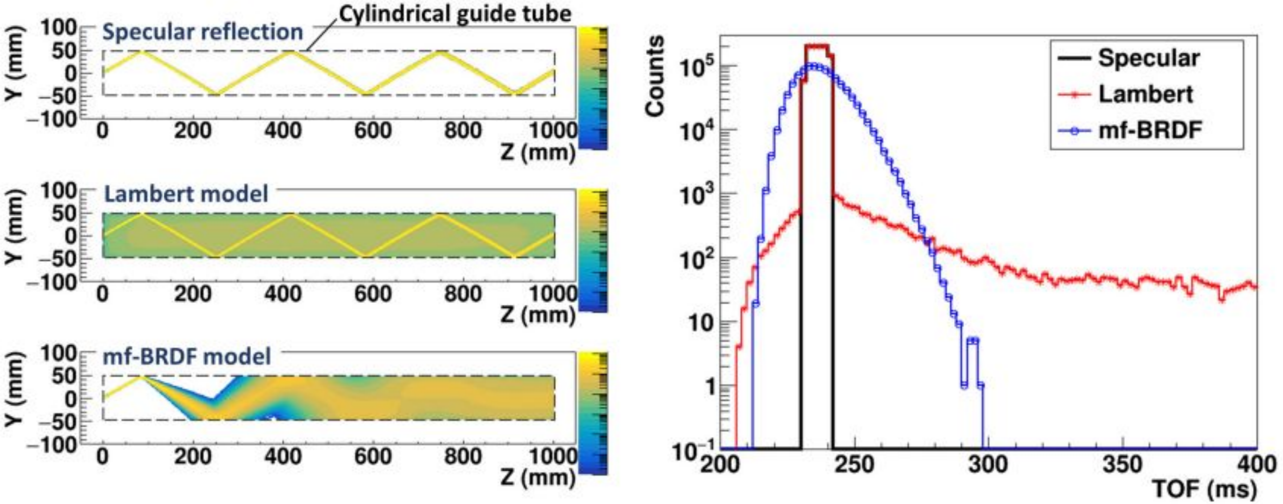
$$\omega_T = \frac{\gamma^2}{c^2\left(\gamma+1\right)}\ddot{\mathbf{x}}\times\dot{\mathbf{x}}$$

Oak Ridge National Laboratory | Spallation Neutron Source

slide taken with permission from W. Schreyer

Diffuse Scattering Models & Transport

- UCN transport is strongly dependent on surface properties of the guides
- PENTrack currently handles:
  - Lambert
  - “Modified Lambert”
  - Microroughness
- A new model, mf-BRDF (Imajo et al. 2022) or “macro-roughness”, is in the process of being added to PENTrack
  - supposed to most accurately represent coated metal guides



Monte-Carlo Trajectory density map and TOF spectrum for 10^6 mono-energetic UCN, down a 1 meter guide. (This was not simulated in PENTrack)

Some Examples of PENTrack Usage

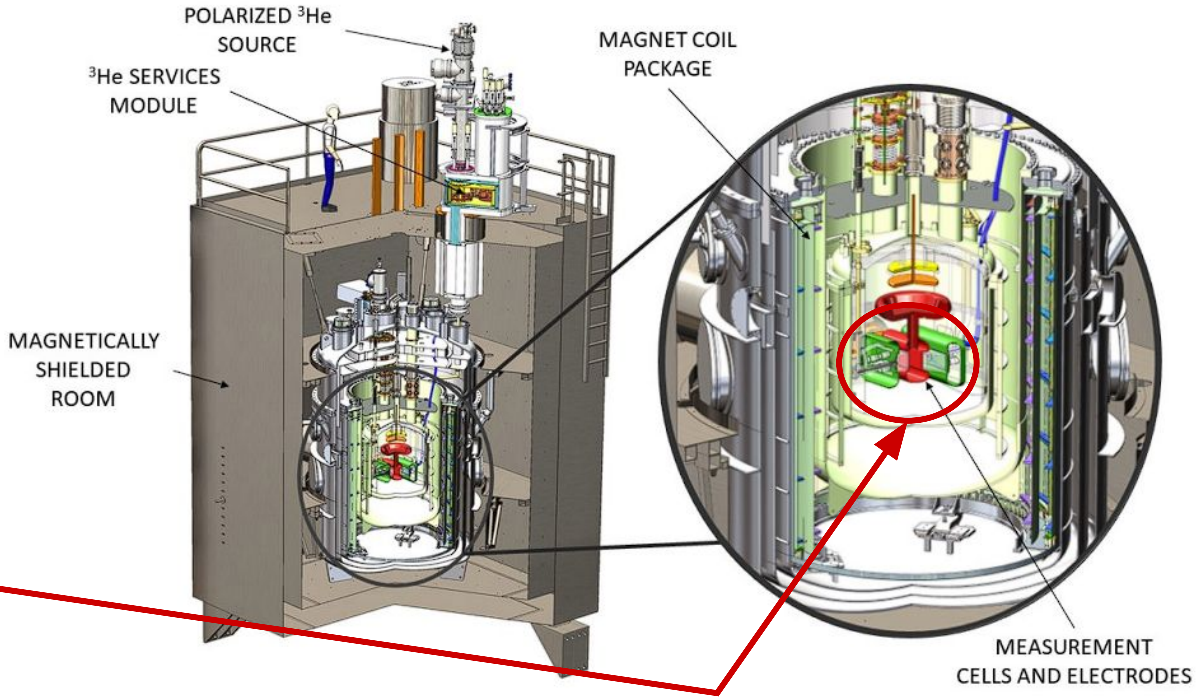
- PENeLOPE
  - Operational optimization - time varying strong magnetic fields (W. Schreyer et al., 2017) [1610.06358] (arxiv.org)
- Extensive use at TRIUMF
  - Optimizing TUCAN EDM performance - (S. Sidhu et al., 2023) [2212.04958] (arxiv.org)
  - First testing new UCN source at TRIUMF (S. Ahmed et al., 2019) [1809.04071](arxiv.org)
- LANL nEDM -
  - Studying transport of Polarized UCN (Douglas Wong Ph.D. Thesis, 2023)
- And everything else you'll see in this slideshow!

Our Experiment and Simulations

The Experiment Formerly Known as nEDM@SNS

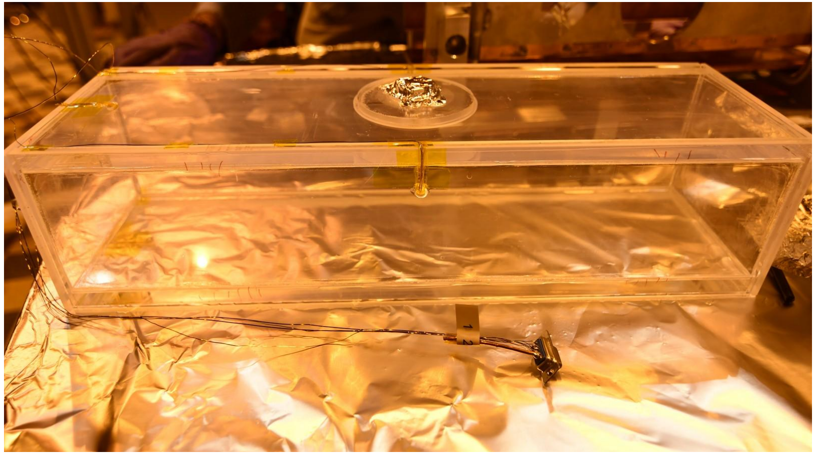
- A unique nEDM experiment designed to produce and then measure **UCN in-situ** via interactions with Helium.

My focus: characterizing the measurement cells



(M. W. Ahmed et al., 2019) [1908.09937] (arxiv.org)

The Measurement Cell



A prototype measurement cell for the nEDM@SNS experiment which underwent UCN storage tests at Los Alamos during this work. The internal cell walls are coated with a dPS and dTPB mixture .

For optimal experimental operation and statistics, this cell must:

- Transmit 8.9 Å cold neutrons to produce UCN in superfluid Helium
- Lengthen 80 nm LHe scintillation light to pass through to external photo-detectors
- Retain ^{3}He polarization
- No magnetic components, and stable in E-field,

-&-

- Have a cell specific UCN storage lifetime of 1000-2000s (ideally for a wide spectrum of energies)

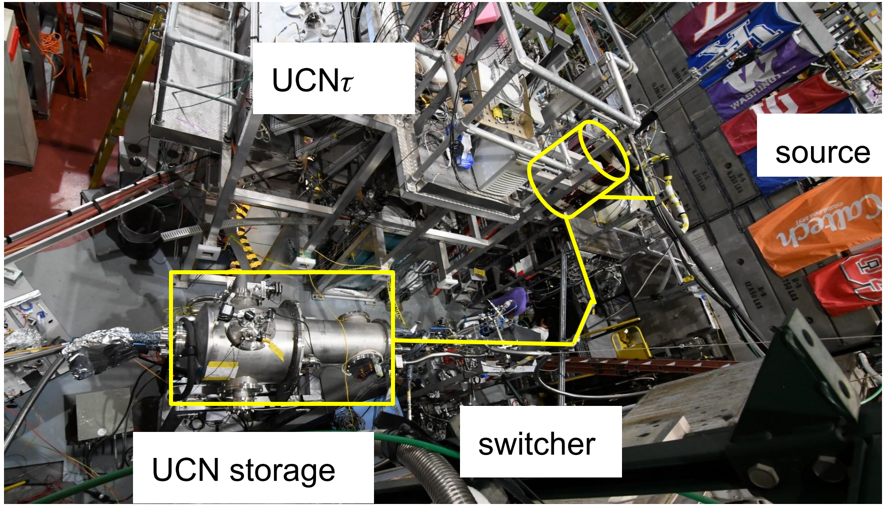
Paper forthcoming (this Summer?)

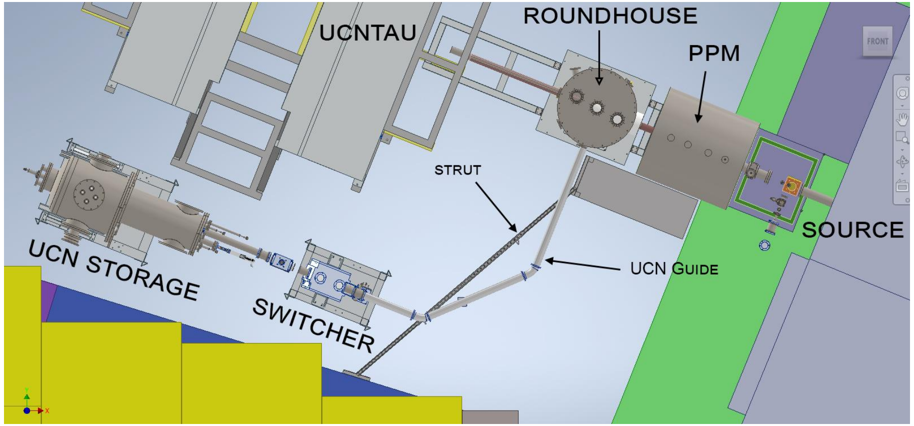
Initial Storage Tests

At LANL, we fill, hold, then count remaining UCN in our cells. The most recent one had:

- A total τ_{storage} (β-decay included) = 570±22 s @ 36K
- or, $\tau_{\text{cell}} \cong$ 1600s @ 36K

However: *we had no knowledge of the E-dependence of this storage time*!

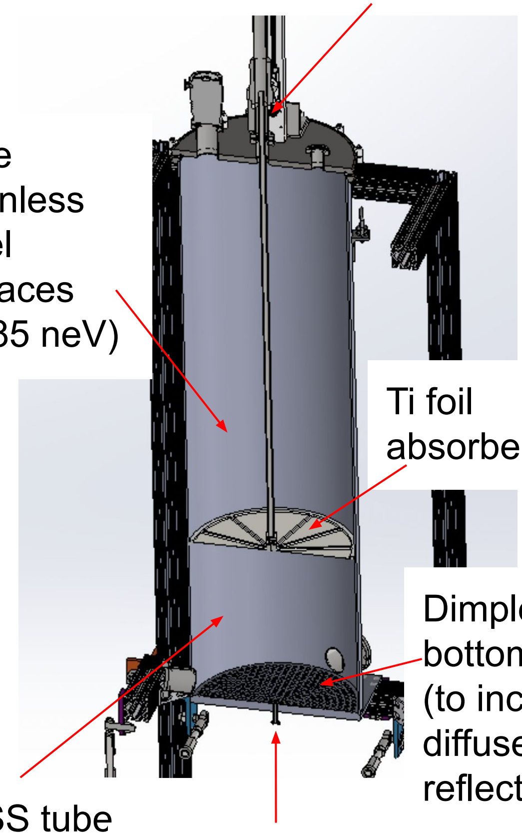




New “Low-Pass” Filter

- Installed in February 2024, to be tested next beam cycle
- Can actuate absorber from a height of 50 to 170 cm without breaking vacuum

(PE_{UCN} goes 1 neV ≈ 1 cm height)



Magnetically-coupled motion feedthrough.

Bare Stainless steel surfaces (~185 neV)

Ti foil absorber

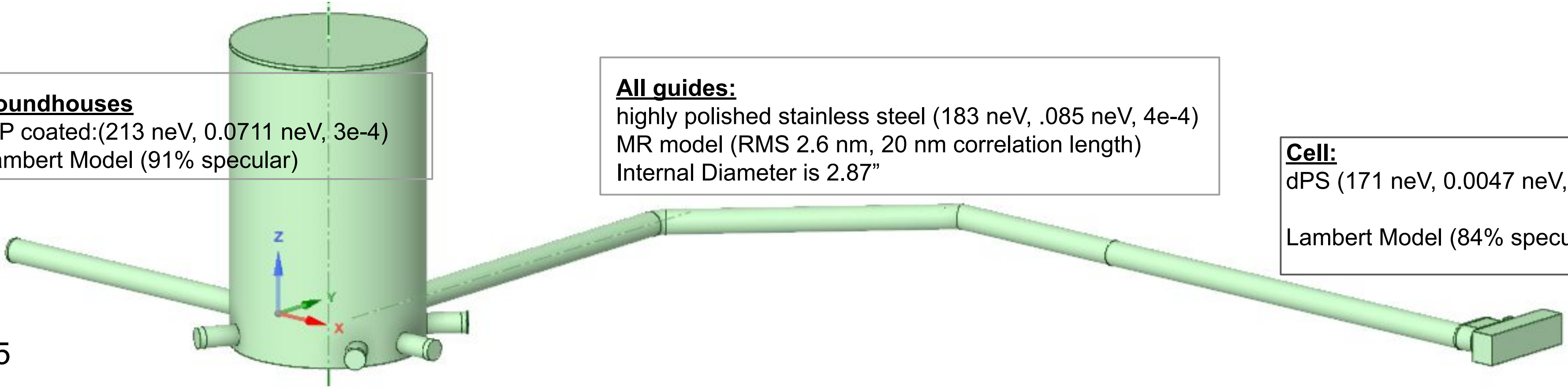
Dimpled SS bottom plate (to increase diffuse reflection)

20”∅ SS tube

1”∅ detector port

How We Used PENTrack

1.) Built model of system in CAD
2.) Assigned material properties, initial UCN source geometry/spectrum, desired output information
3.) Benchmarked simulations against experimental results
    a.) Updated model (added “gaps”, adjusted loss coefficients & specularity constants)
4.) Created results



Roundhouses
NiP coated:(213 neV, 0.0711 neV, 3e-4)
Lambert Model (91% specular)

All guides:
highly polished stainless steel (183 neV, .085 neV, 4e-4)
MR model (RMS 2.6 nm, 20 nm correlation length)
Internal Diameter is 2.87”

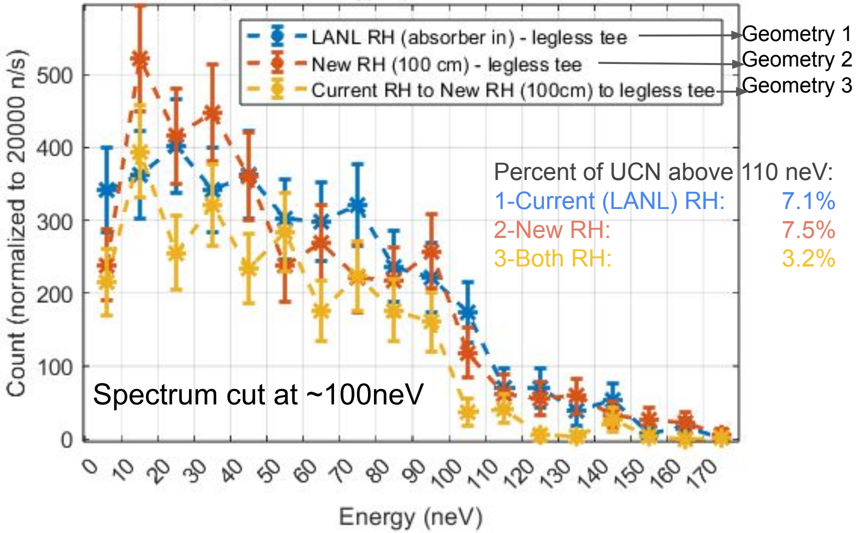
Cell:
dPS (171 neV, 0.0047 neV, 2.7e-5)

Lambert Model (84% specular)

PENTrack Results

- In a direct comparison simulation, we showed our new design was ~twice as effective at cleaning the UCN spectrum than LANL's current roundhouse's absorber

Energy Spectrum For Different Roundhouse Conditions at End of Fill



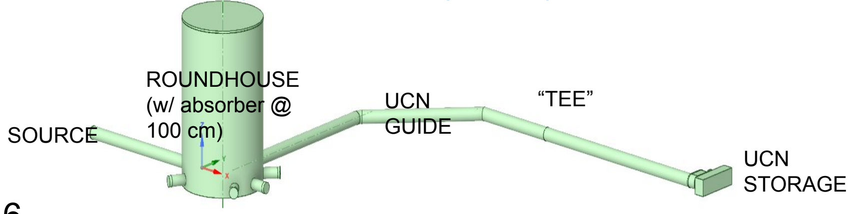
Geometry 1
Geometry 2
Geometry 3

Percent of UCN above 110 neV:

1-Current (LANL) RH: 7.1%
2-New RH: 7.5%
3-Both RH: 3.2%

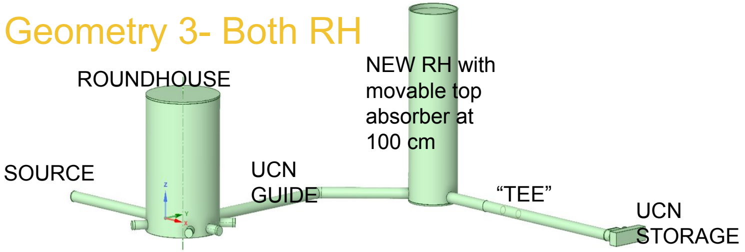
Spectrum cut at ~100neV

Geometry 1- current (LANL) RH



SOURCE
ROUNDHOUSE (w/ absorber @ 100 cm)
UCN GUIDE
"TEE"
UCN STORAGE

Geometry 3- Both RH



ROUNDHOUSE
NEW RH with movable top absorber at 100 cm
SOURCE
UCN GUIDE
"TEE"
UCN STORAGE

Conclusions & Acknowledgements

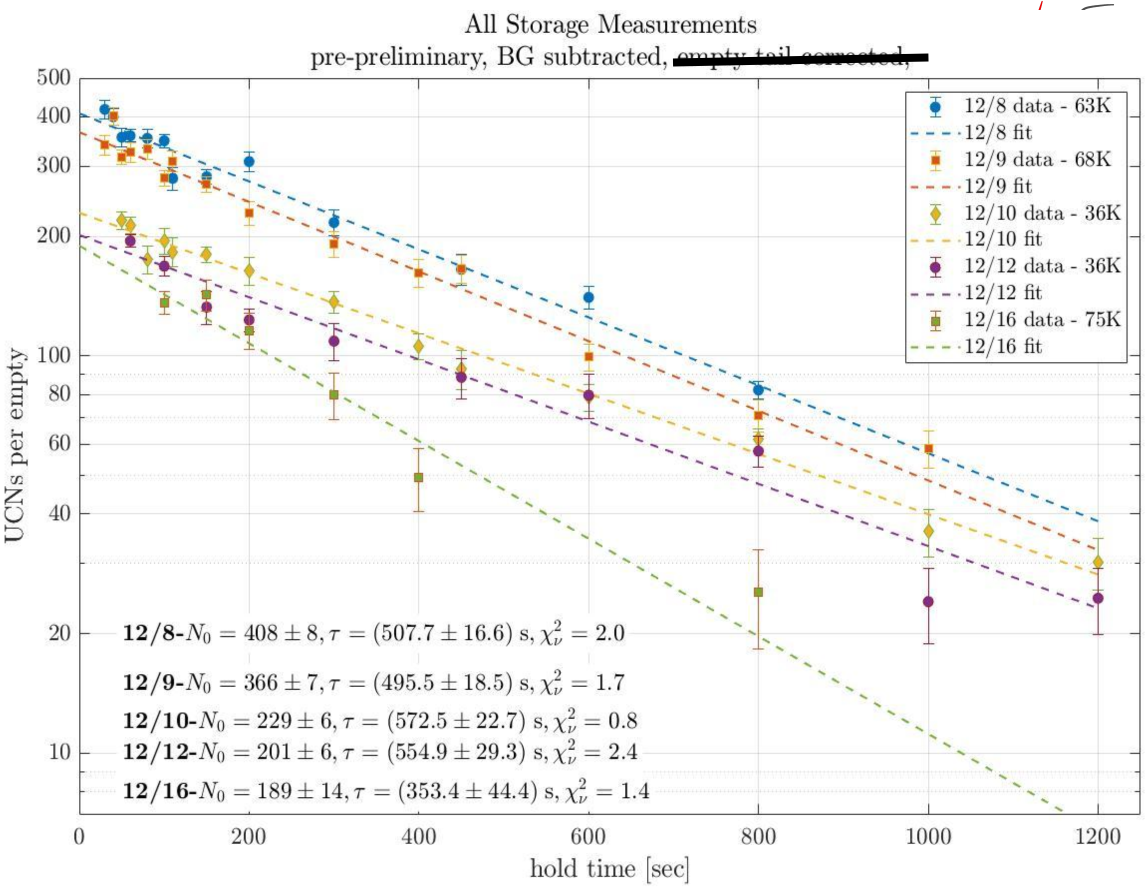
- UCN simulations are necessary for understanding transport
- Today’s Monte-Carlo simulation tools (such as PENTrack) are remarkably versatile, and easy(ish) to use!

People:

NCSU: Clark Hickman, Ekaterina Korobkina, Bob Golub, Paul Huffman, Albert Young, Matt Morano, Adam Dipert, Christian White
LANL: Martin Cooper, Tito Takeyasu, Mark Makela, Chris O'Shaughnessy, Wade Ulrich, Chris Morris, Steven Clayton, Scott Currie, TJ Schaub
Bartoszek Engineering: Larry Bartoszek
Montclair State University: Kent Leung, Bill Klos
ORNL: Wolfgang Schreyer, Andy Saunders

Backup Slides

2021 Results

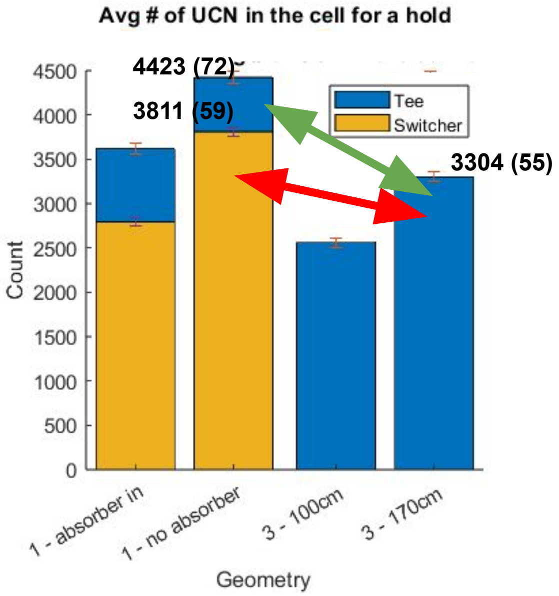


Data from 2021. We now assume the significant decrease in lifetime from the 12/16 data to be from accidentally venting dirt into the system.

Simulation Results

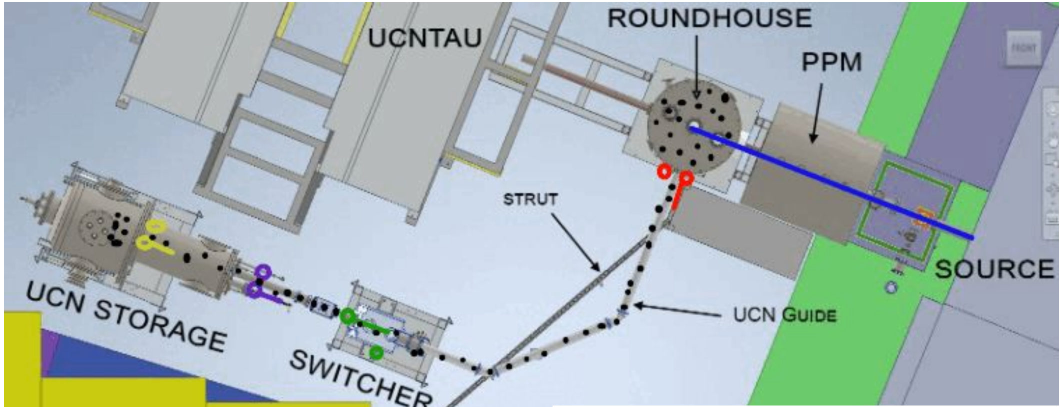
- Adding our new roundhouse decreases the number of neutrons we can obtain in our measurement cell
    - Green arrow represents a direct comparison - showing ~25% loss
- **But,** by replacing the lossy switcher with a tee, we expect to recuperate some loss
    - The red arrow represents this - showing a ~9% decrease

The decrease is well within our acceptable tolerances for the functionality gain of the new RH

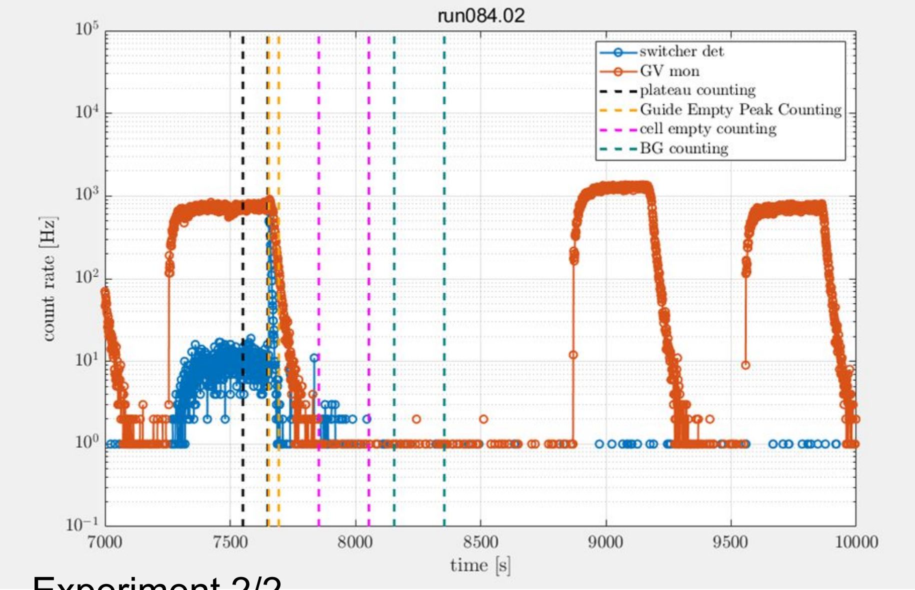


<u>Geometry</u>
1 - Current RH
3 - Current RH to New RH

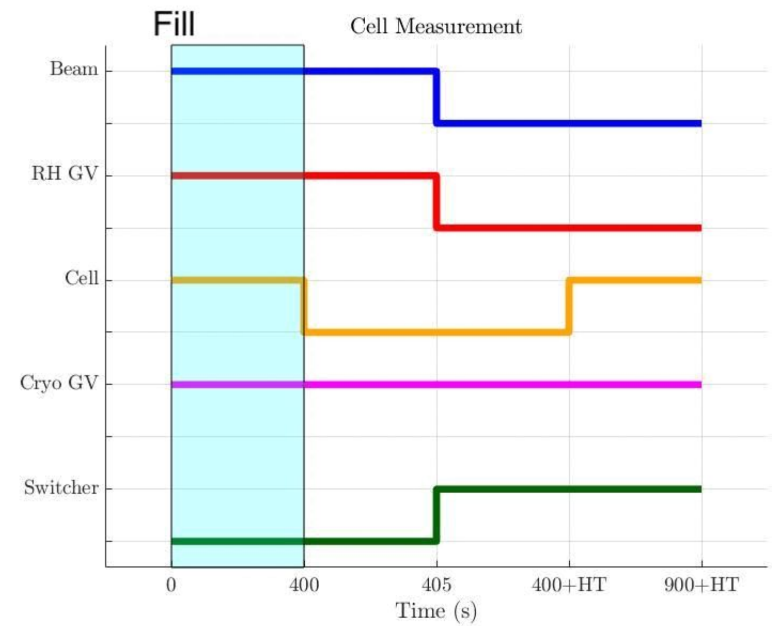
Overview of Measurement



200 sec hold



Experiment 2/2

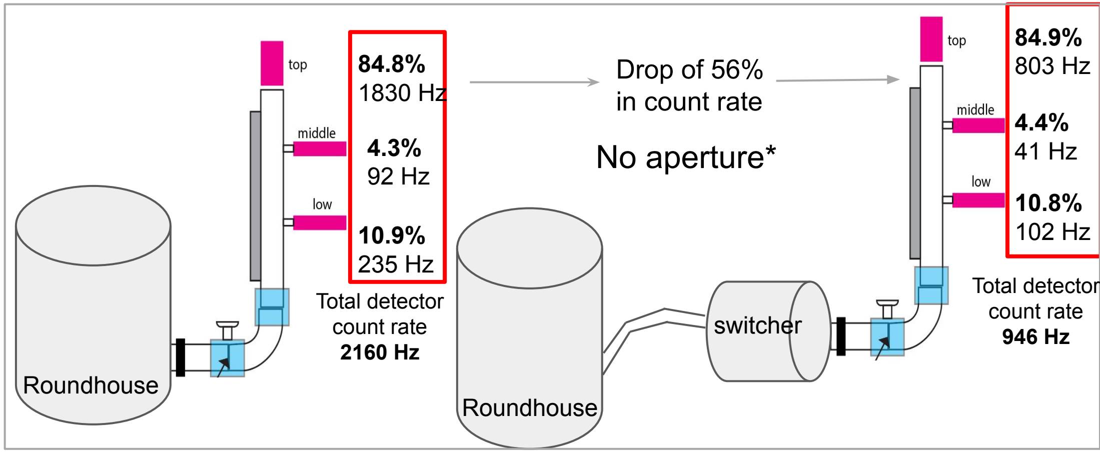


Benchmarking my simulations

Setting Loss Parameters in Guide

- Reproducing the experimental absolute count rates in simulation is *very* difficult
- However, I simulated our comparative TES experiment to try to set guide loss parameters by matching the *relative* count rates
- The main parameter I varied was the gap length at the switcher
- Note - This experiment gives us no further insight into the loss rate of the cold section of guide. Further work is being carried out on that.

Experiment



84.8%
1830 Hz

4.3%
92 Hz

10.9%
235 Hz

Total detector
count rate
2160 Hz

Drop of 56%
in count rate

No aperture*

84.9%
803 Hz

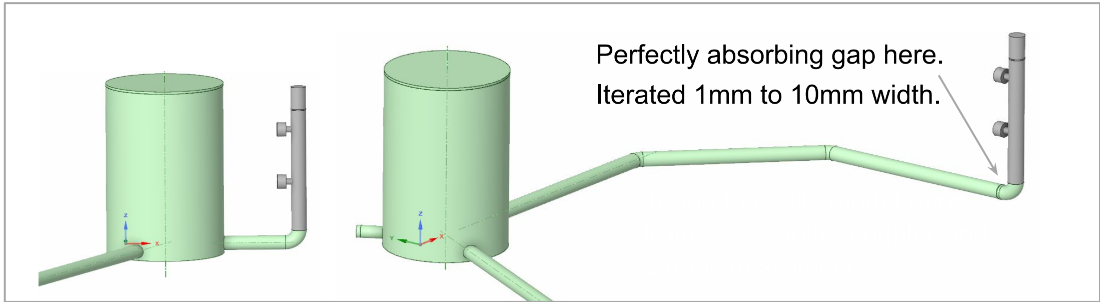
4.4%
41 Hz

10.8%
102 Hz

Total detector
count rate
946 Hz

*for aperture results, see slideshow notes or Feb 2023 collaboration meeting slides

Simulation Geometry



Perfectly absorbing gap here.
Iterated 1mm to 10mm width.

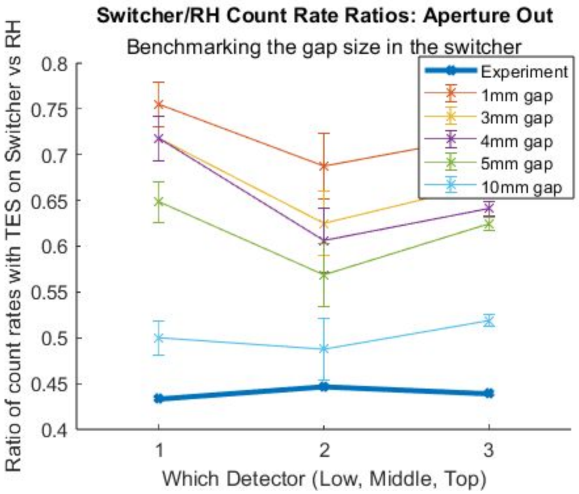
Loss Parameters Continued

- We plotted the ratio of the count rate on each TES detector as simulated after the switcher compared to on the roundhouse. The thick blue line is the experimental results.
    - ○ Top graph is the case with the 1cm Ni foil aperture out, bottom graph is with the 1cm Ni foil aperture in
- The non-aperture simulations suggest that our simulated guide needs more than 10 mm of gaps in it to reproduce the relative count rates down guide.
- The aperture simulations suggest that the relative count rates are roughly similar to the experiment with anywhere between 4-10 mm gaps to reproduce experimental results

Our Conclusion: Rather than have a single 1cm gap in the switcher, we opted to have 0.5mm gaps at each coupler and a 5mm gap in the switcher. (totaling 7mm of gaps)

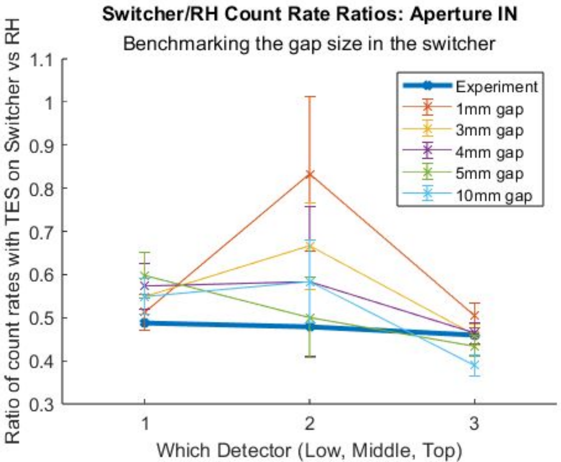
More neutrons make it down guide

Less neutrons make it down guide



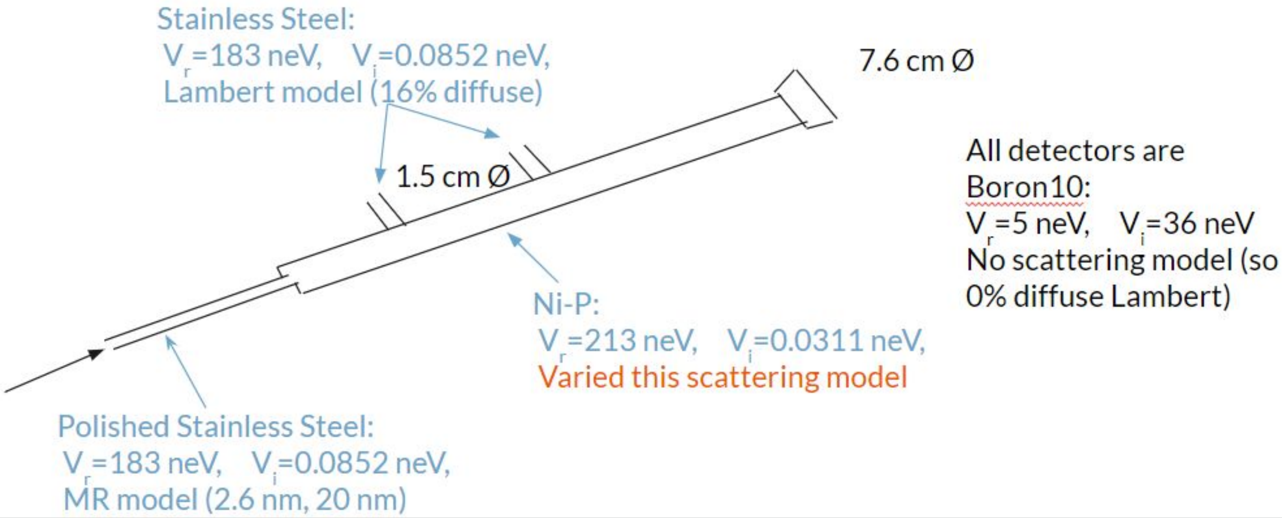
More neutrons make it down guide

Less neutrons make it down guide



Benchmarking Roughness Model

Filling directly into a horizontal TES from a 1” diameter beam guide



Stainless Steel:
V_r=183 neV, V_i=0.0852 neV,
Lambert model (16% diffuse)

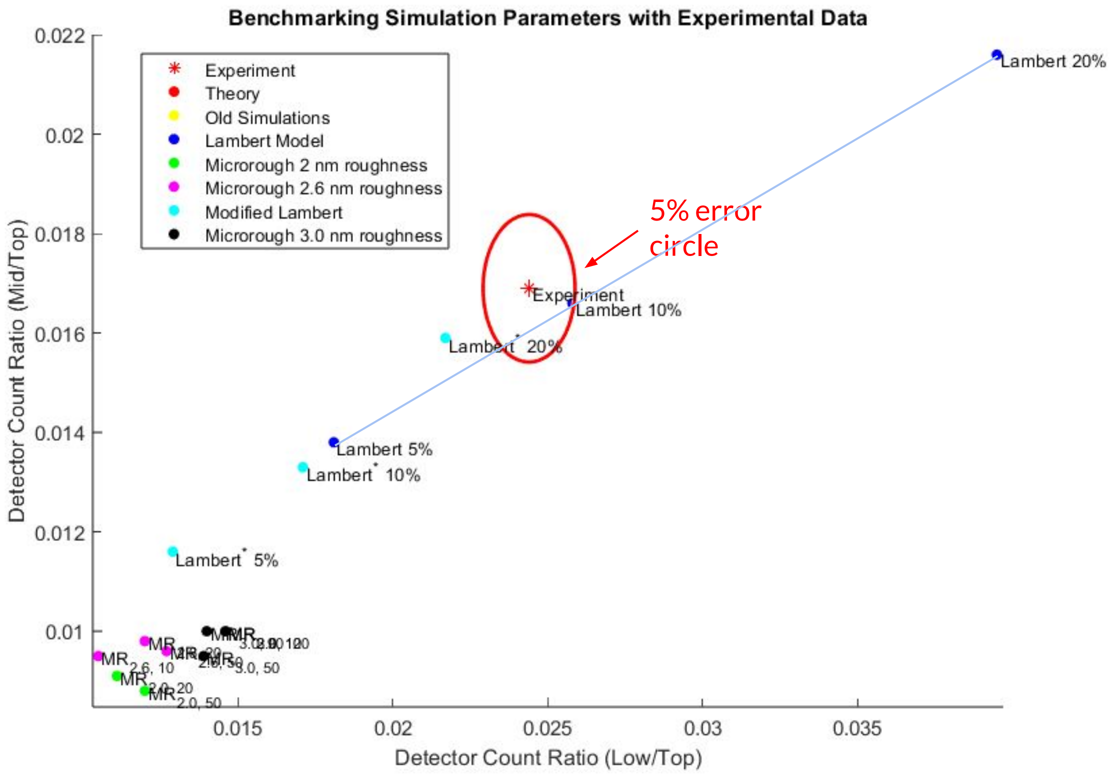
All detectors are Boron10:
V_r=5 neV, V_i=36 neV
No scattering model (so 0% diffuse Lambert)

Ni-P:
V_r=213 neV, V_i=0.0311 neV,
Varied this scattering model

Polished Stainless Steel:
V_r=183 neV, V_i=0.0852 neV,
MR model (2.6 nm, 20 nm)

Benchmarking Roughness Model

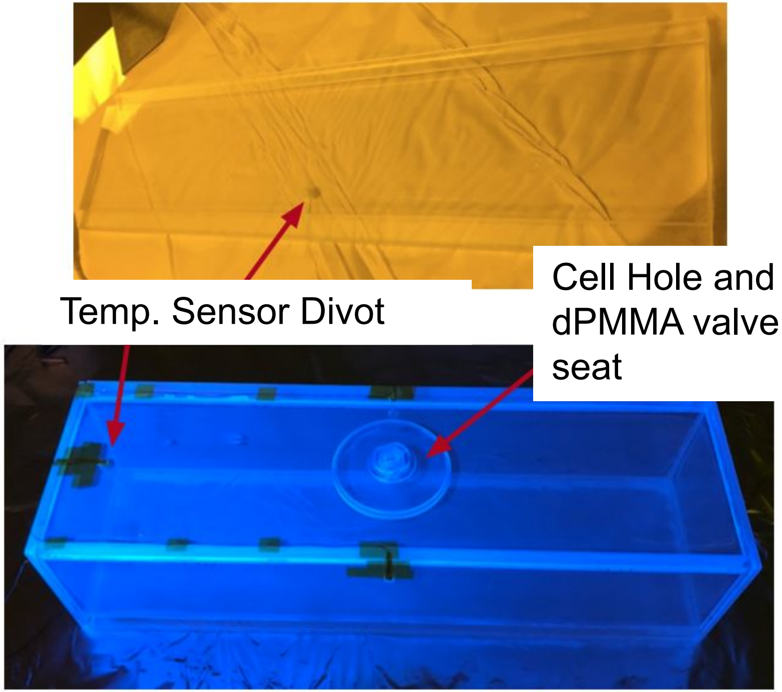
More
Neutrons in
middle
detector



More Neutrons in lowest detector

UCN Storage – Cell Requirements

- Highly non-magnetic
- Stable in high- electric fields and across pressure gradients
- Non-electrically conductive (pPMMA) walls held together by deuterated “cement”
- Do not spin depolarize UCNs and co-magnetometers (dPS coating)
- Coating that wavelength shifts light (dTPB coating)



Credit: Kent Leung