Geant4 Simulations Framework for nEDM@SNS

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Contributions From nEDM@SNS Simulations Team

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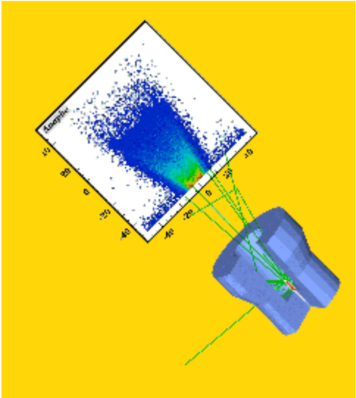
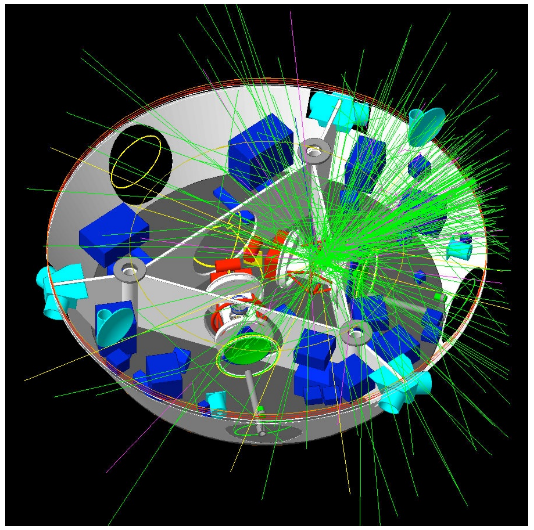
Outline

- Overview of Geant4
- Geant4 simulations written by nEDM@SNS simulations team.
- Integrating nEDM Geant4 simulations into a unified framework.
- SNS Moderator Simulations.
- Running Geant4 in an HPC Environment.

Overview of Geant4

- Geant4 (for GEometry ANd Tracking) is a platform for "the simulation of the passage of particles through matter," using Monte Carlo methods.
- It is the successor of the GEANT series of software toolkits developed by CERN, and the first to use object oriented programming (in C++).
- Development, maintenance, and user support are taken of care by the international Geant4 Collaboration.
- Application areas include high energy physics and nuclear experiments, medical, accelerator and space physics studies.





*Graphics from Geant4 Collaboration.

Geant4 for nEDM

Pros

- Extensive physics processes (no need to re-invent the wheel).
- Robust geometry package.
- Large community support.
- Open source - (Not owned by any country)
- Object Oriented design allows for extensibility.
- Currently being rewritten to include large levels of parallelism for many core architectures (Intel MIC, GPUs, etc.) -> Geant5.

Cons

- Learning curve.
- Large code base (>1M LOC) & class templating make Geant4 a "black box" to most.
- Lack of validation for low energy neutron scattering (although this is improving).

Simulations for nEDM@SNS

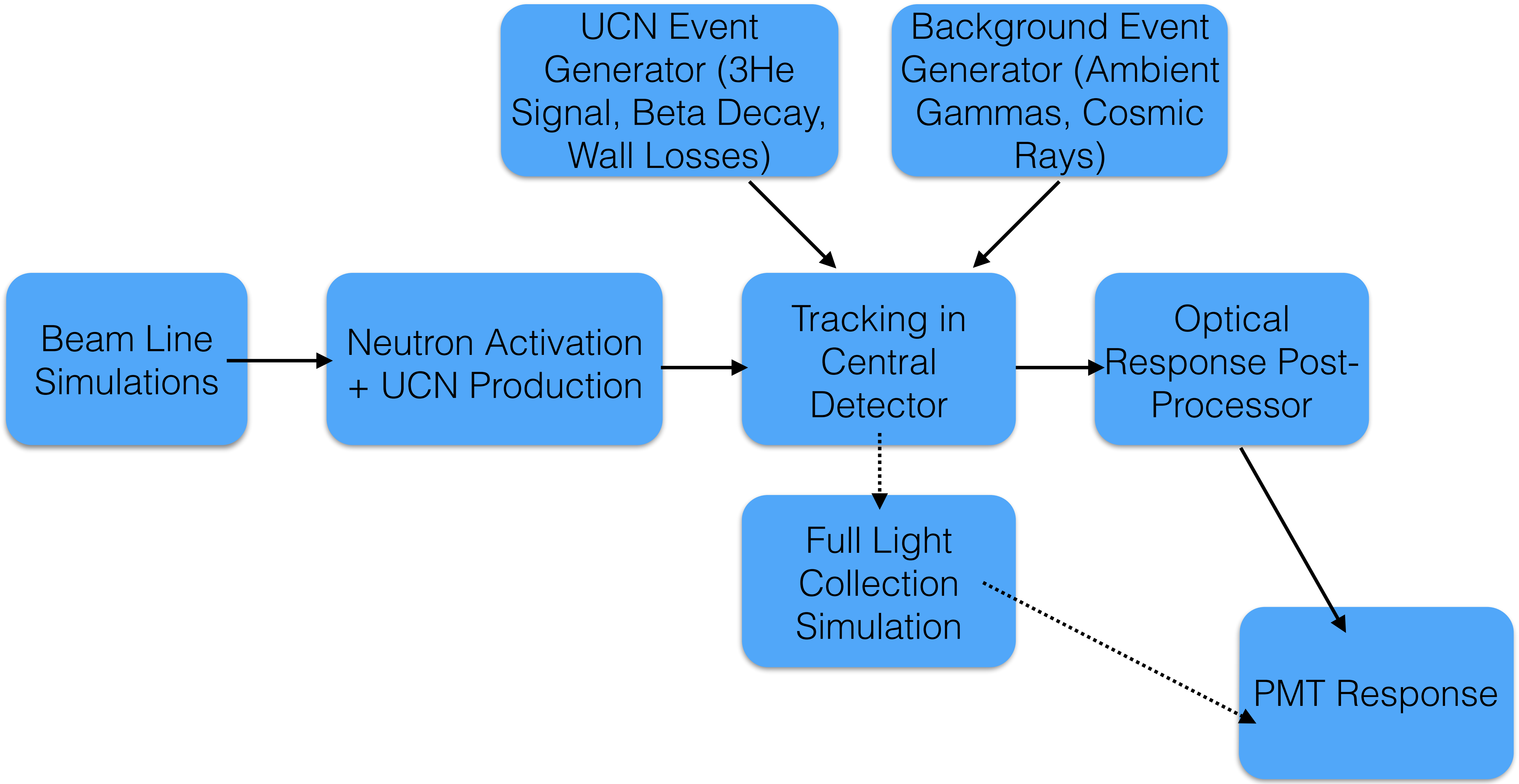
In this talk (all Geant4 based)

- SNS Cold Neutron Beam Transport - *Wolfgang Korsch*
- Neutron Activation + UCN Production - *Vanya Logashenko, Jed Leggett, Vince Cianciolo, Dipangkar Dutta*
- Central Detector Response - *Brad Plaster, Takeyasu Ito*
- Light Collection - *Zach Raines, Ameya Kolakar, Jed Leggett*

Not In this talk

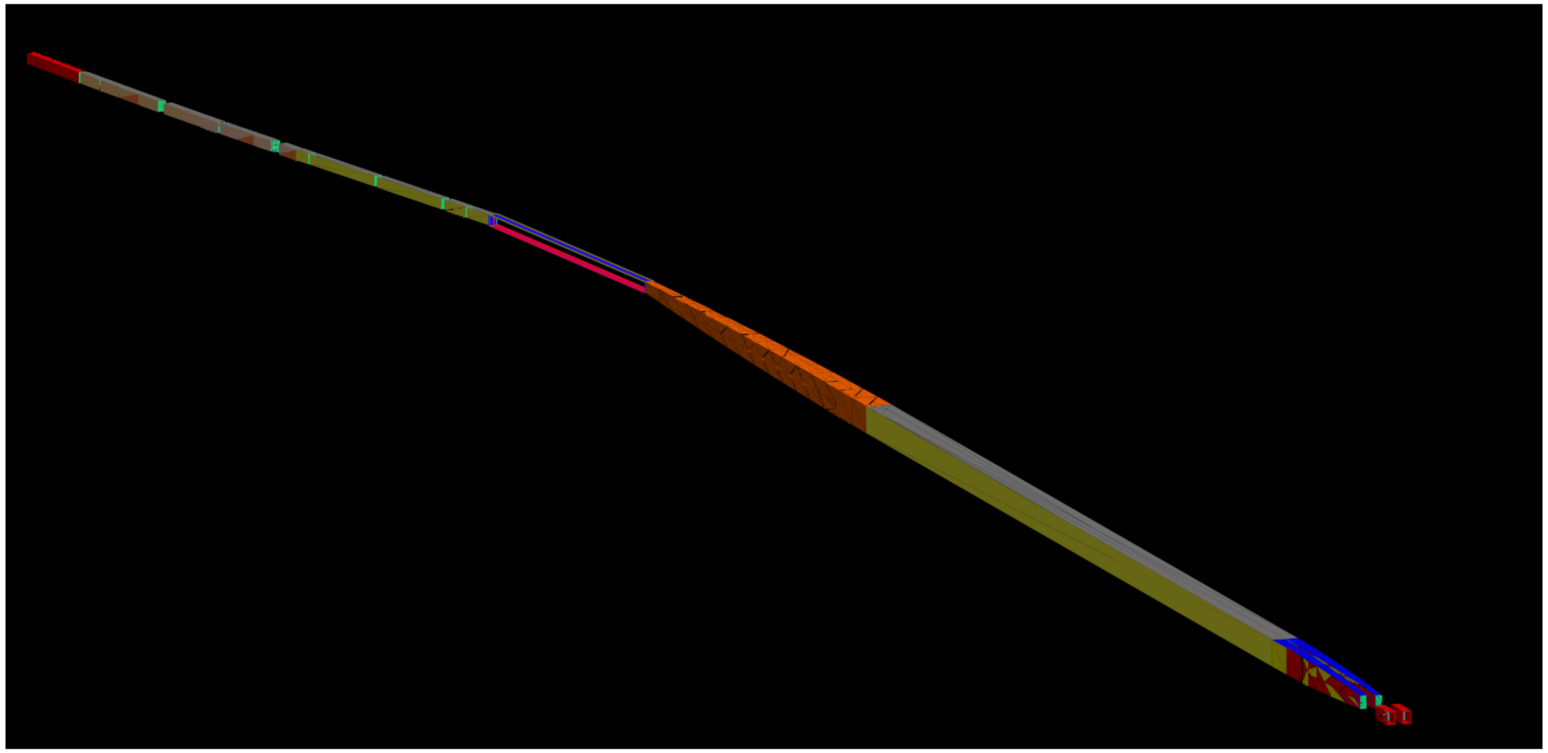
- Geant4 3He Dressed Spin - *Steve Clayton*
- Geometric Phase - *Ricardo Schmidt*
- Multiple Stand-Alone MC - *Takeyasu Ito*
- Others That I'm Forgetting

Sample of Simulations for nEDM@SNS



Cold Neutron Beam Transport

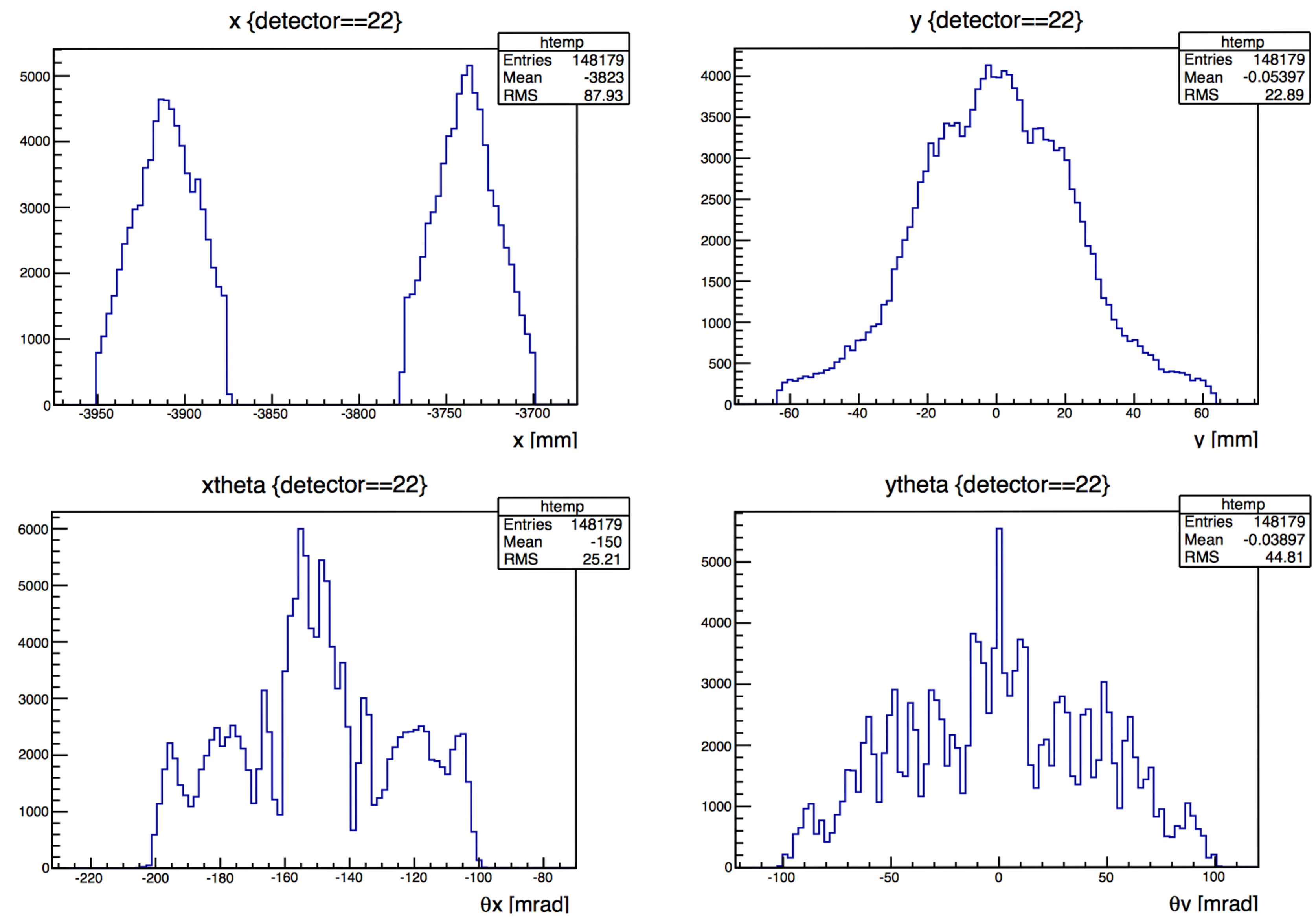
- Simulations start at entrance of neutron guide.
  - Uses positions (x, y) and velocities v = (vx, vy, vz) → θx, θy from MCNP/McStas file (started at moderator).
- Transport neutrons (8.9 Å) to EDM targets.
  - Use measured non-magnetic and magnetic guide reflectivities (fits to data)



*Wolfgang Korsch - University of Kentucky

Cold Neutron Beam Transport

x, y, θ_x, θ_y at EDM targets



Phase Space of outgoing neutrons is passed to other simulations.

*Wolfgang Korsch - University of Kentucky

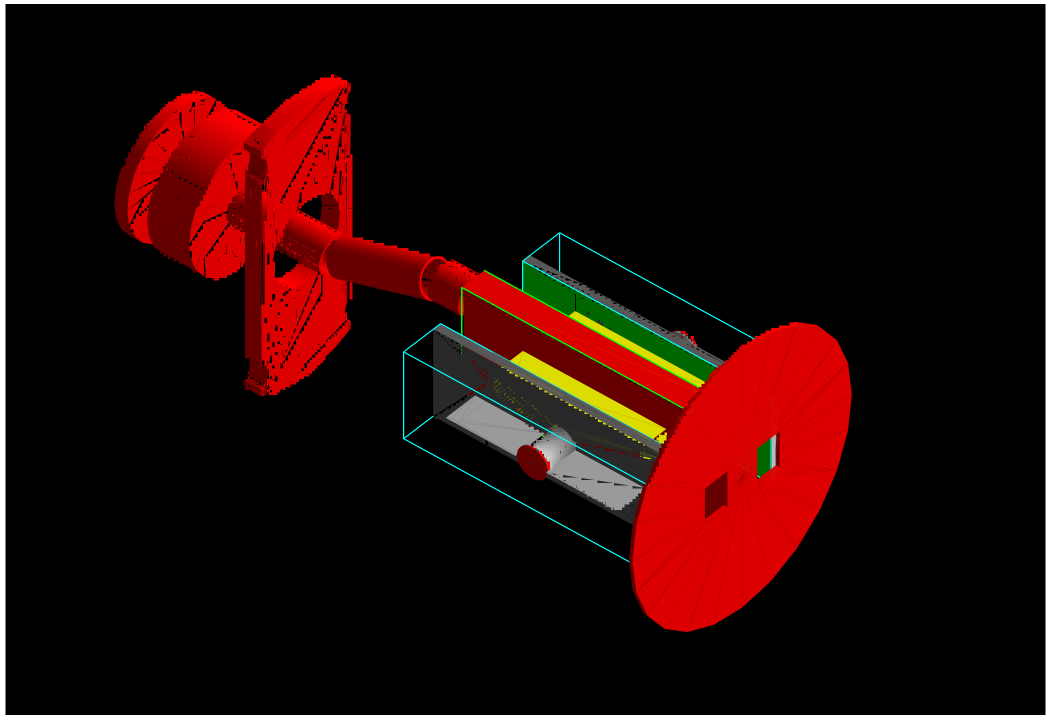
Neutron Activation

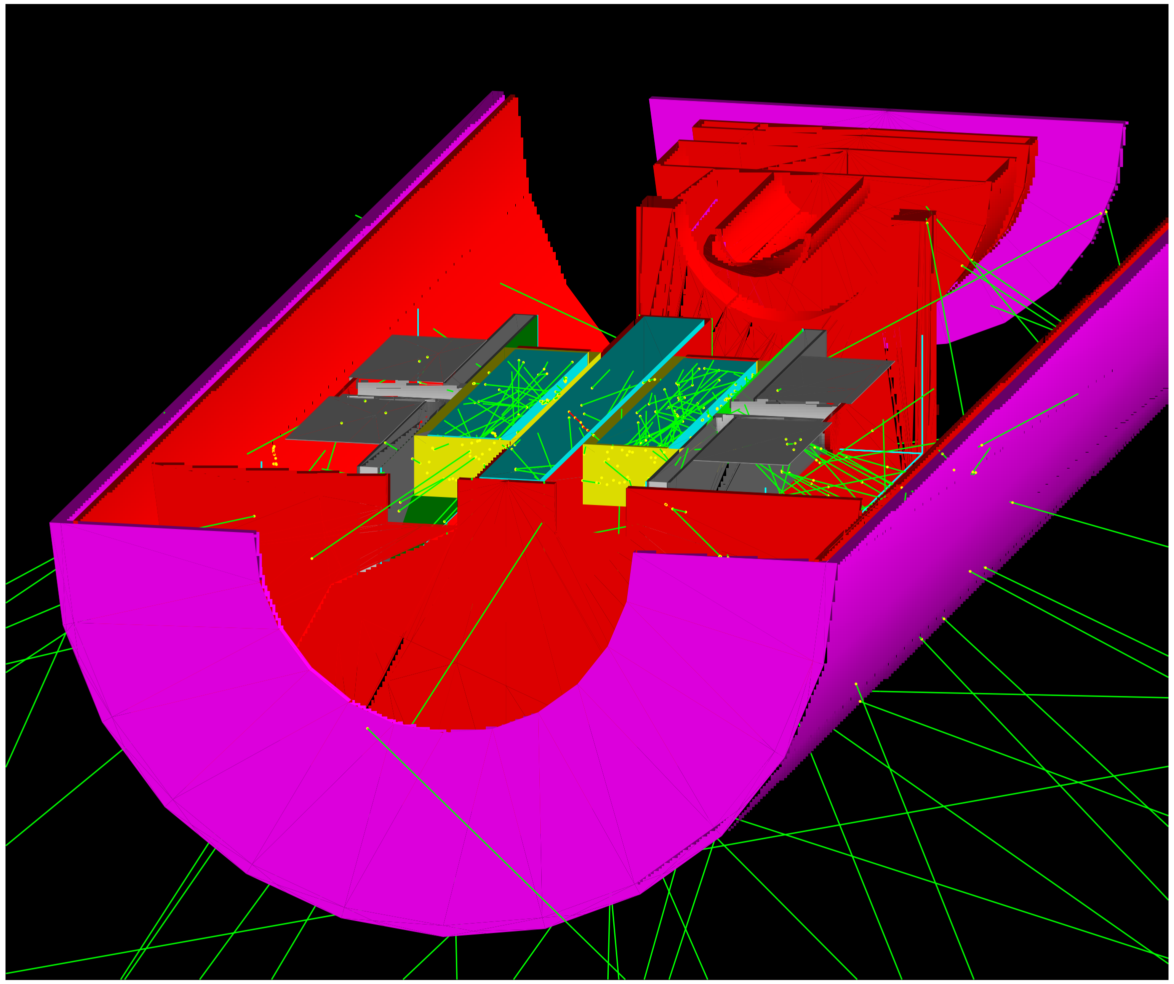
<u>Vanya</u>

- Detailed model of the nEDM central detector geometry.
- Neutron activation from Al & Mn was demonstrated to be small (~20 Hz)

<u>Jed</u>

- Phase space from neutron guide simulations used with geometry model to simulate neutron activation of electrode coating materials.





UCN Production

- In order to correctly simulate neutron scattering for background calculations, a custom Geant4 process was created for neutron scattering from single phonons in 4He.

Analytical

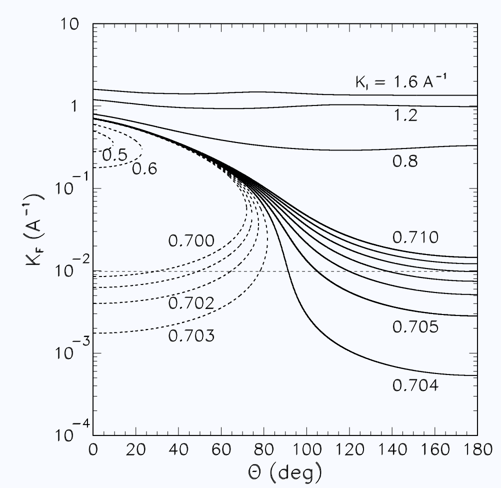
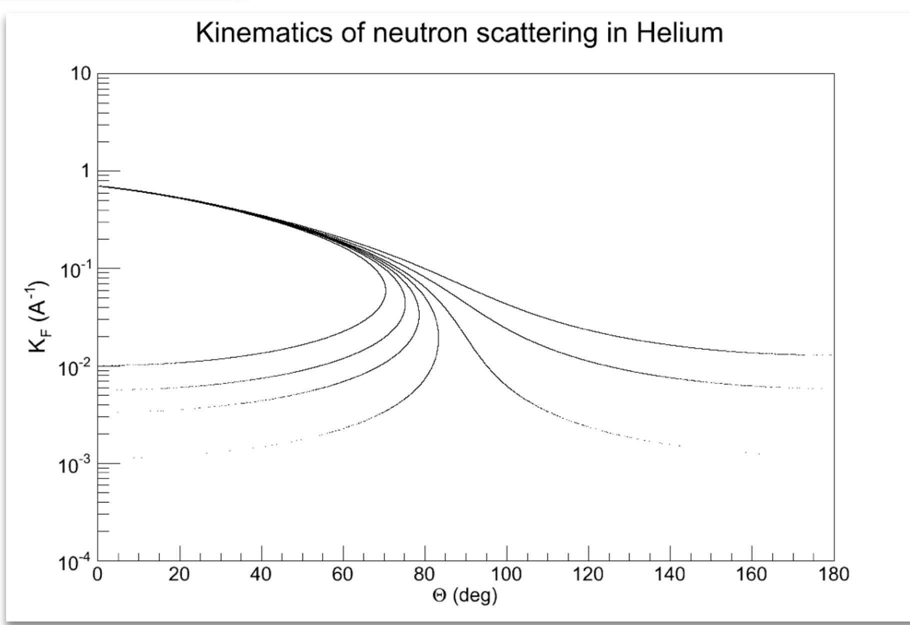


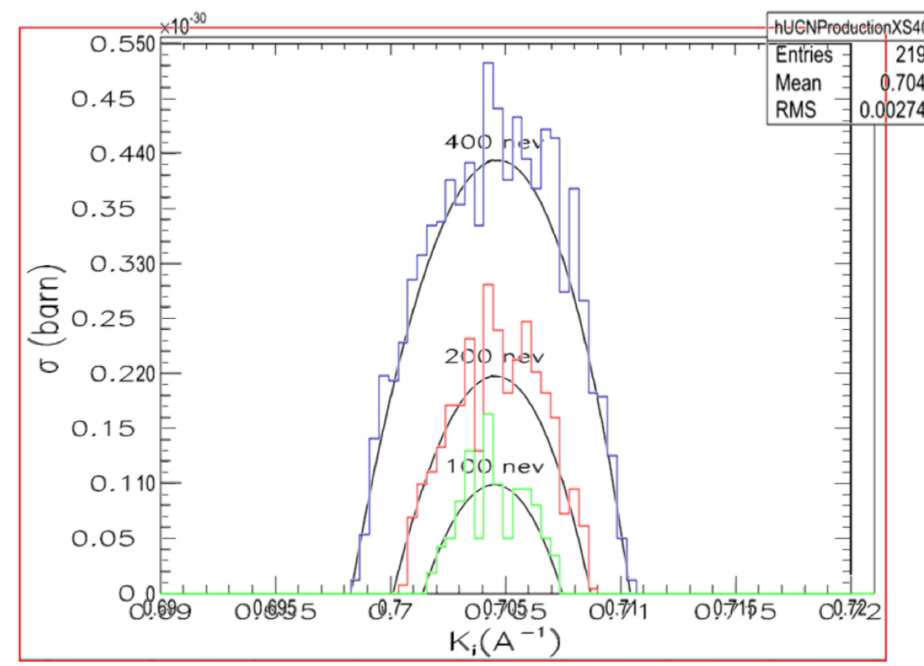
Figure 2: Kinematics of the neutron scattering off a superfluid ^4He target. Momenta of the scattered neutrons (k_F) are plotted as a function of the neutron laboratory scattering angle (θ) for several incident neutron momenta (k_i). The horizontal dashed curve corresponds to a UCN wall potential of 200 nev.

69

Simulation



- As a by product, UCN production rates could be estimated.



Neutron Activation

- In order to validate the simulation as well as possible, we extracted several parameters from the simulation and checked them against stand-alone MC simulations.

- The number of activated nuclei for a mono-isotopic material exposed to a instantaneous, monoenergetic field of neutrons can be calculated using the following formula.

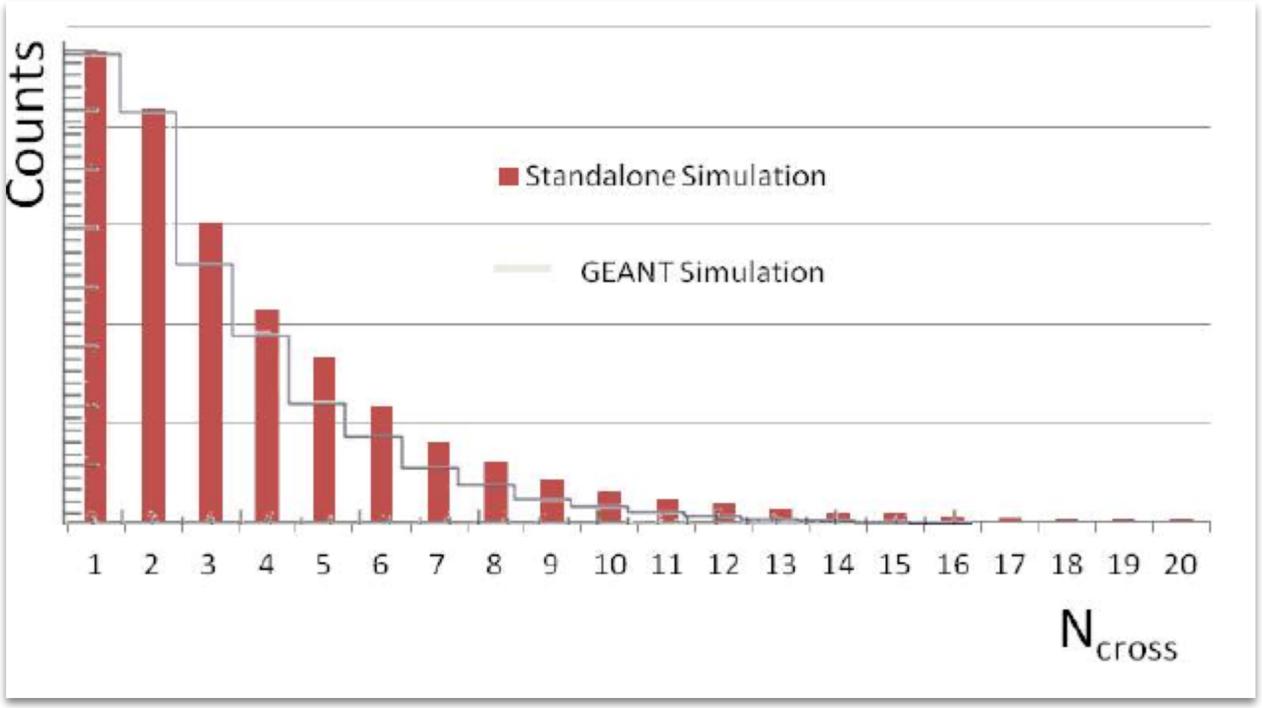
$$N_{act} = N_{in} \frac{f_{scat} N_{cross}}{f_{shield}} \frac{\sigma_{th}}{v/v_{th}} \frac{\rho N_A}{A} \frac{t}{< \cos(\theta) >}$$

Exposure-specific	• N_{in} is the number of incident neutrons.
Geometry-specific	• f_{scat} is the fraction that scatter.
Geometry-specific	• N_{cross} is the average number of times a neutron crosses the material.
Geometry-specific	• f_{shield} is the fraction of neutrons shielded from the material.
Material-specific	• σ_{th} is the material's capture cross section at thermal energies.
Known	• v/v_{th} is the ratio of the neutron velocity to thermal velocity.
Material-specific	• ρ is the material density.
Known	• N_A is Avagadro's number.
Material-specific	• A is the material's atomic number.
Geometry-specific	• $t/ < \cos(\theta) >$ is the average pathlength through the material (the thickness corrected for the average angle of incidence).

Parameters were extracted from the Geant4 simulation and verified with a Stand-Alone MC

Parameter		GEANT	SMC
f_{scat}	Front Cell Wall	6.7%	7%
	Cell Helium	2.5%	2%
	Back Cell Wall	6.1%	6.4%
	Total	15.3%	15.4%
N_{cross}		3.3	3.7
f_{shield}		2.7	$2.7 * (1.8/2.1) = 2.3$
$1/ < \cos(\theta) >$		2.5	2.1
$\mathcal{F} = \frac{f_{scat} N_{cross}}{f_{shield} < \cos(\theta) >}$		0.47	0.52

Increases to 1.33 w/ realistic phase space.

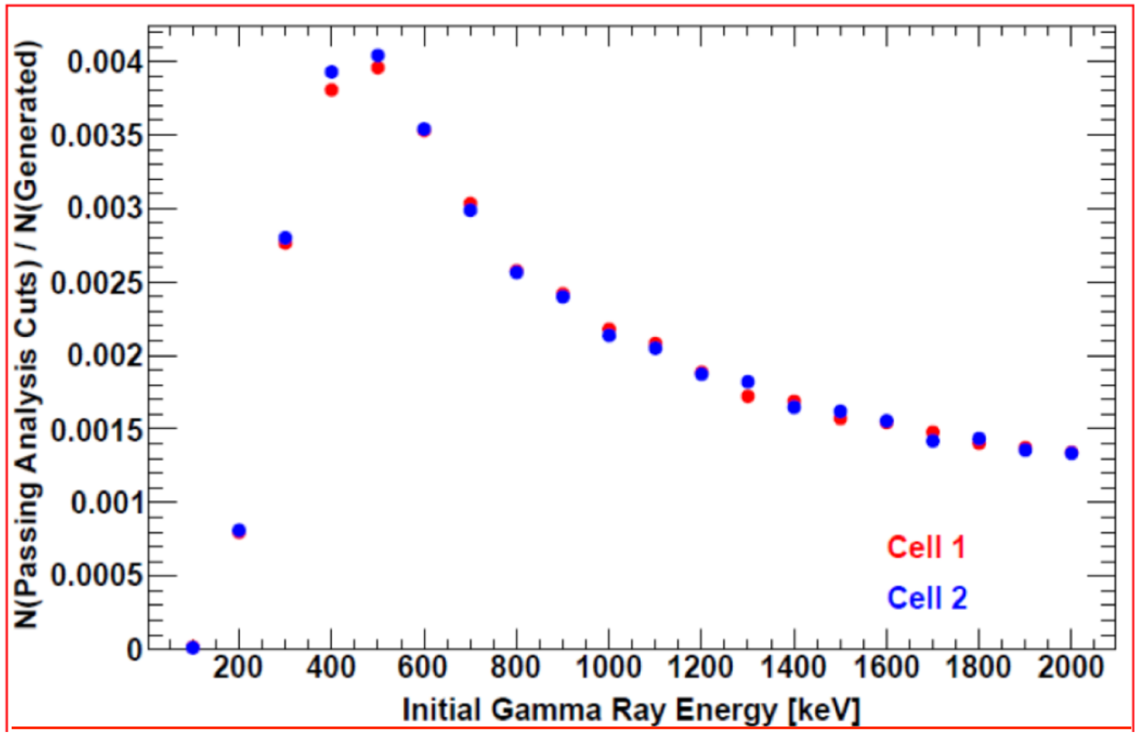


Neutron Activation

To get the number of background counts we need to know the probability for produced γ's to pass background cuts.

$$N_{bkd} = N_{act} N_{\gamma} \otimes \mathcal{P}(E_{\gamma})$$

This can be obtained by randomly generating gammas on the surface of the electrodes in the central detector simulation and varying the energy.



P(Eγ = 412 keV) = 0.76%, absolute normalization is somewhat position-dependent, shape not so much.

Neutron Activation

- Initial formula was for mono-isotopic samples and instantaneous exposures.
- More general formula:

$$\mathcal{R}_{bkd}(0) = \frac{1}{2}\frac{\Phi\mathcal{F}N_A t}{v/v_{th}}\sum_i \frac{\sigma_{th,i}\rho_i}{A_i} N_{\gamma,i} \otimes \mathcal{P}(E_\gamma)\left[(1-\exp(-t_f/\tau_i))\frac{1-\exp(-t_c/\tau_i)^{N_c+1}}{1-\exp(-t_c/\tau_i)}\exp(-t_w/\tau_i)\right]$$

Sum over isotopes

Saturation of build-up for short-lived isotopes

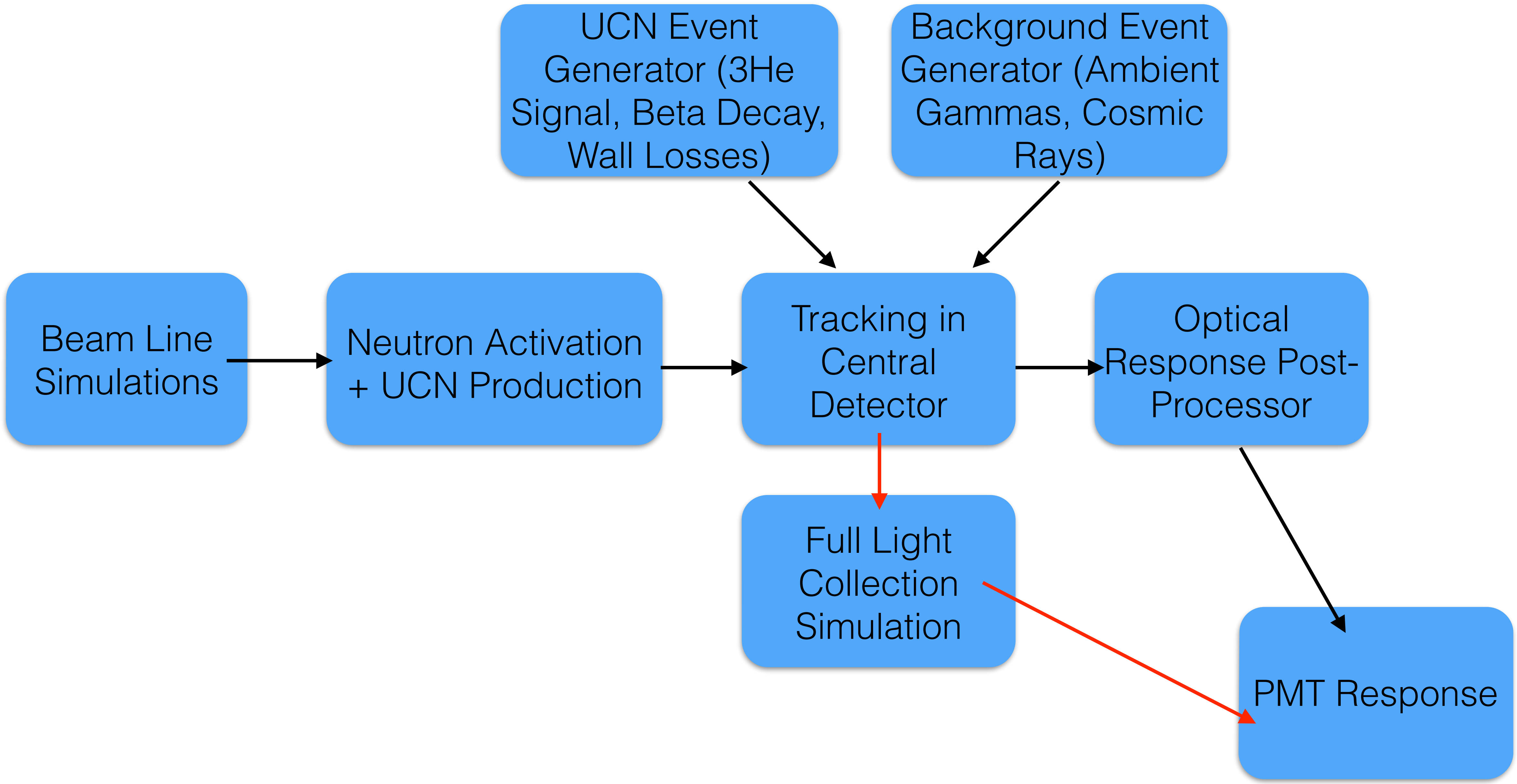
Build-up of long-lived isotopes over multiple run-cycles

Decay of short-lived isotopes between shutter closing and start of run

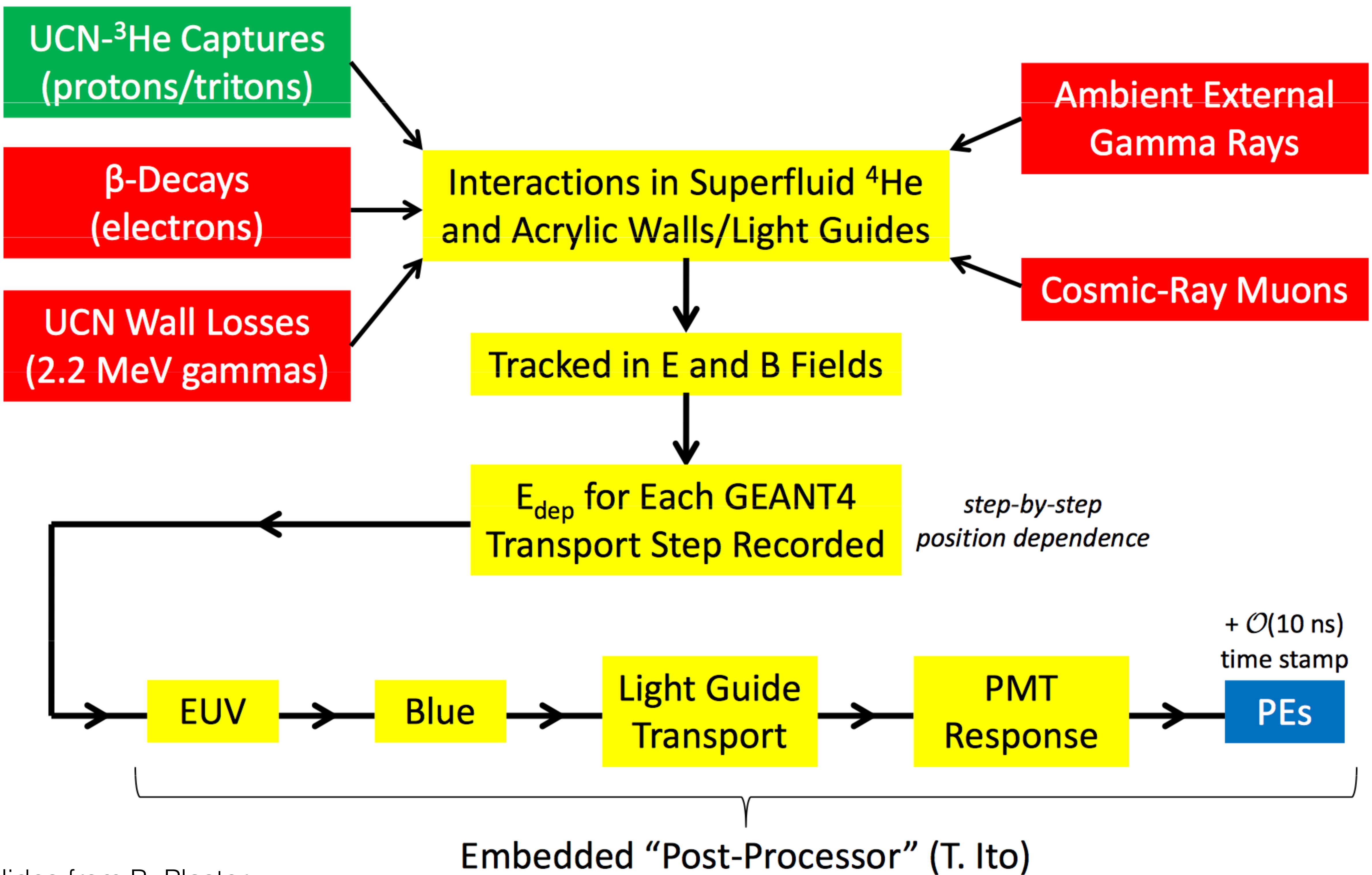
Coating	$\mathcal{R}(0)$ (Hz/cell) (Perfect Masking)	$\mathcal{R}(0)$ (Hz/cell) (No Masking)
Gold	130	273
ITO (nat.)	117	242
ITO (In-113)	13	28
Cu	1.2	2.6

Table 5: Final results for 50 nm coatings, as described in the text.

Sample of Simulations for nEDM@SNS



Measurement Cell Simulation



*Slides from B. Plaster

Measurement Cell Simulation

Rate Function

Events generated according to rate function :

$$\Phi(t) = \left[\Gamma_{n,3}\left(1 + P_{n,0}P_{3,0}e^{-\Gamma_P t}\cos(\omega t + \phi)\right) + \Gamma_\beta + \Gamma_{\text{wall}}\right]N(t) + B + A(t)$$

activation (time-dependent)

capture, β-decay, UCN wall loss

ambient gamma, cosmic-ray (time-independent)

$$\Gamma = \Gamma_{n,3} + \Gamma_\beta + \Gamma_{\text{wall}}$$
$$\Gamma_{n,3} = 1/\tau_{n,3}$$
$$\Gamma_\beta = 1/\tau_\beta$$
$$\Gamma_{\text{wall}} = 1/\tau_{\text{wall}}$$
$$\Gamma_P = \frac{T_{2,n} + T_{2,3}}{T_{2,n}T_{2,3}}$$

where number of surviving neutrons *N*(*t*) is :

$$N(t) = N_0 \exp\left[-\Gamma t - \Gamma_{n,3}P_{n,0}P_{3,0}e^{-\Gamma_P t}\left(\frac{-\Gamma_P\cos(\omega t + \phi) + \omega\sin(\omega t + \phi)}{\Gamma_P^2 + \omega^2}\right)\right]$$

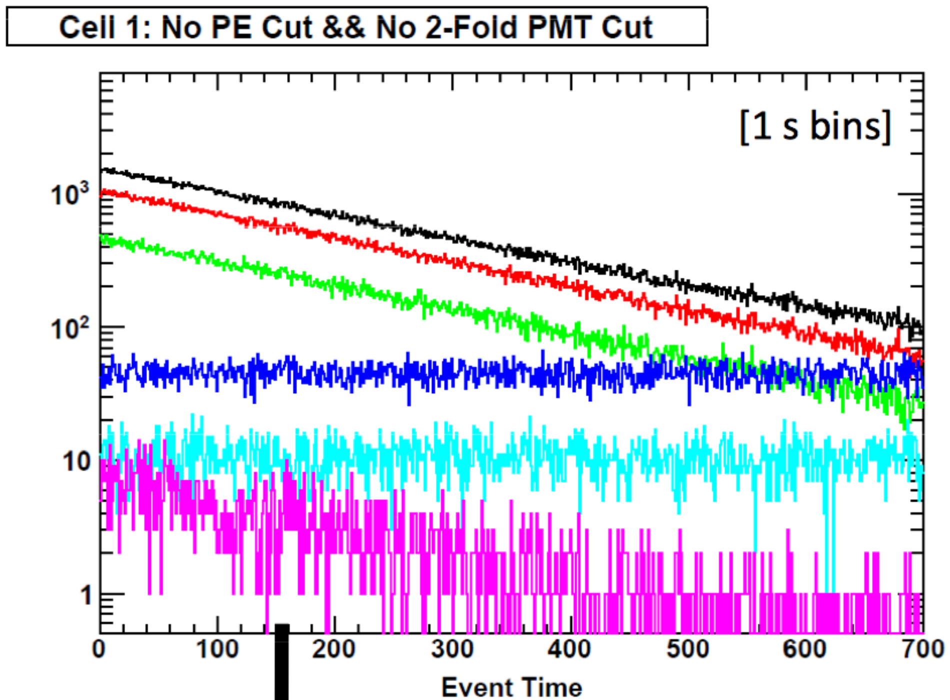
$$\cong N_0 e^{-\Gamma t}\left[1 - \frac{\Gamma_{n,3}}{\omega}P_{n,0}P_{3,0}\sin(\omega t + \phi)\right]$$

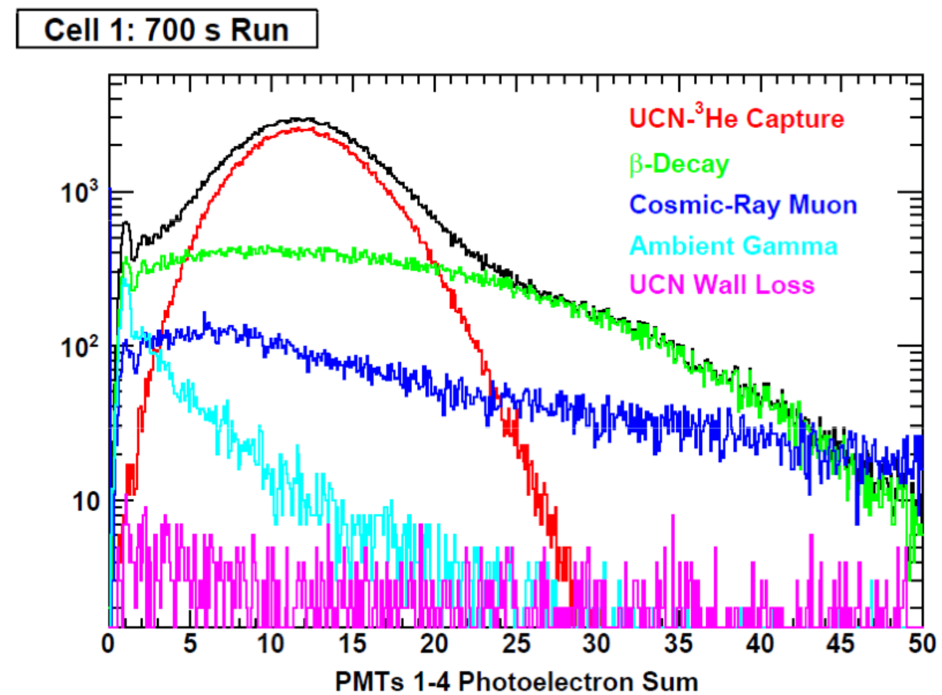
$$\sim \frac{1/400}{2\pi \times 9.8} \sim 4\times10^{-5}$$

*Slides from B. Plaster

Measurement Cell Simulation

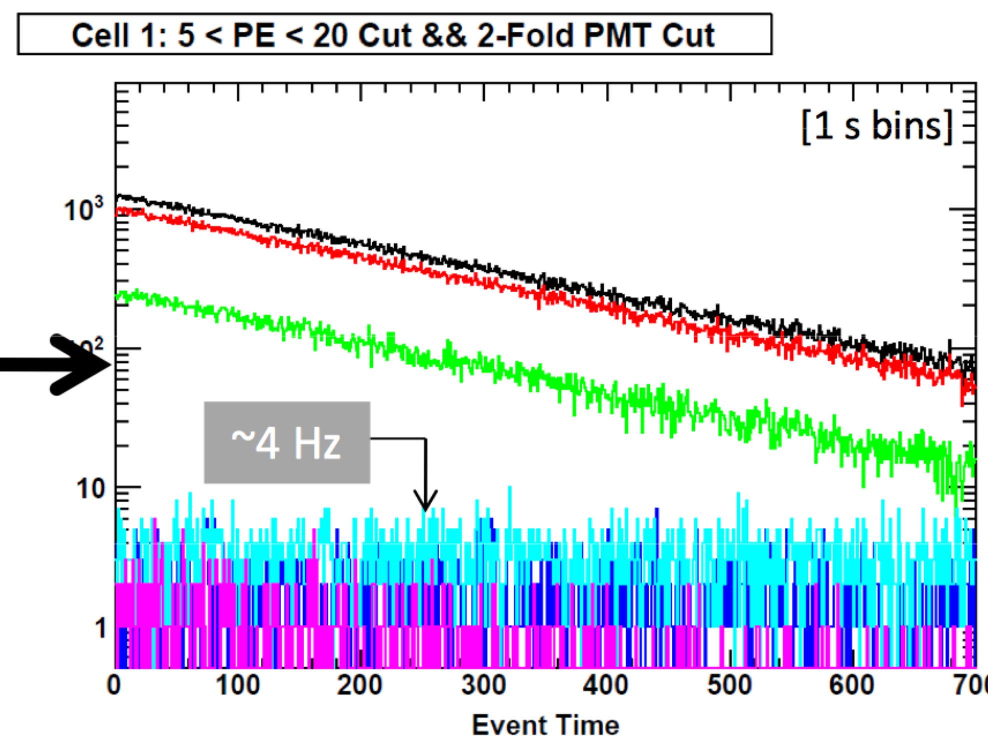
Timing and Photoelectron Spectra

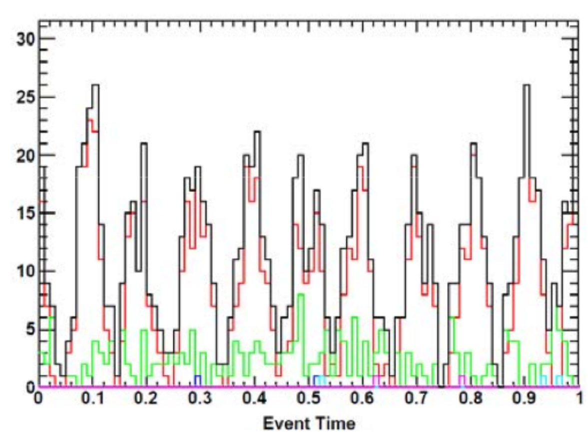




muon MIP
peak at ~150

PE Cut
5 < PE < 20
&&
2-Fold PMT
Coincidence Cut

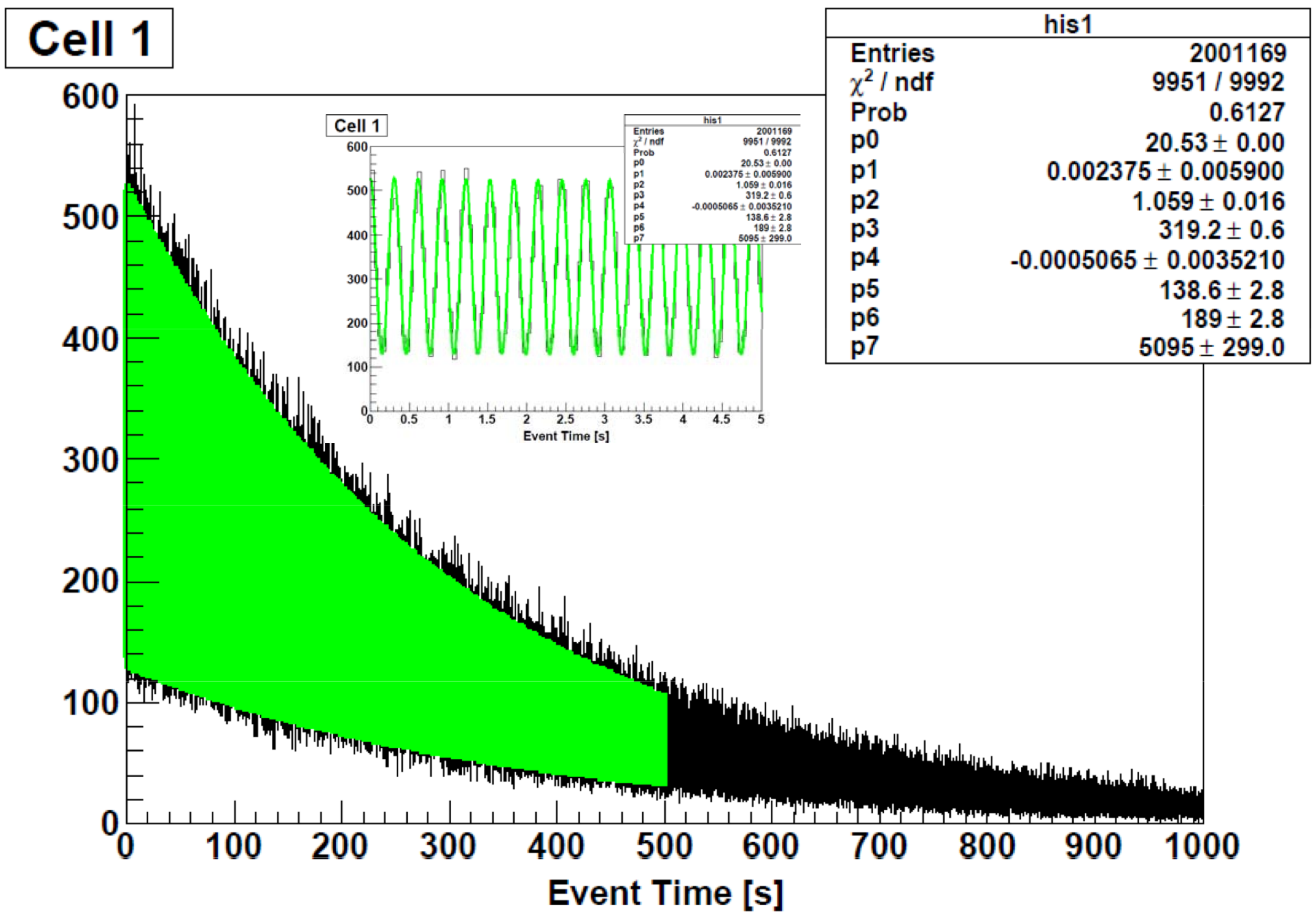




*Slides from B. Plaster

Mock Data Challenge

- A data set containing 10^9 events was generated for a “Mock Data Challenge”.
- Analyzers had to find a hidden nEDM on the 10^{-27} e- cm level.



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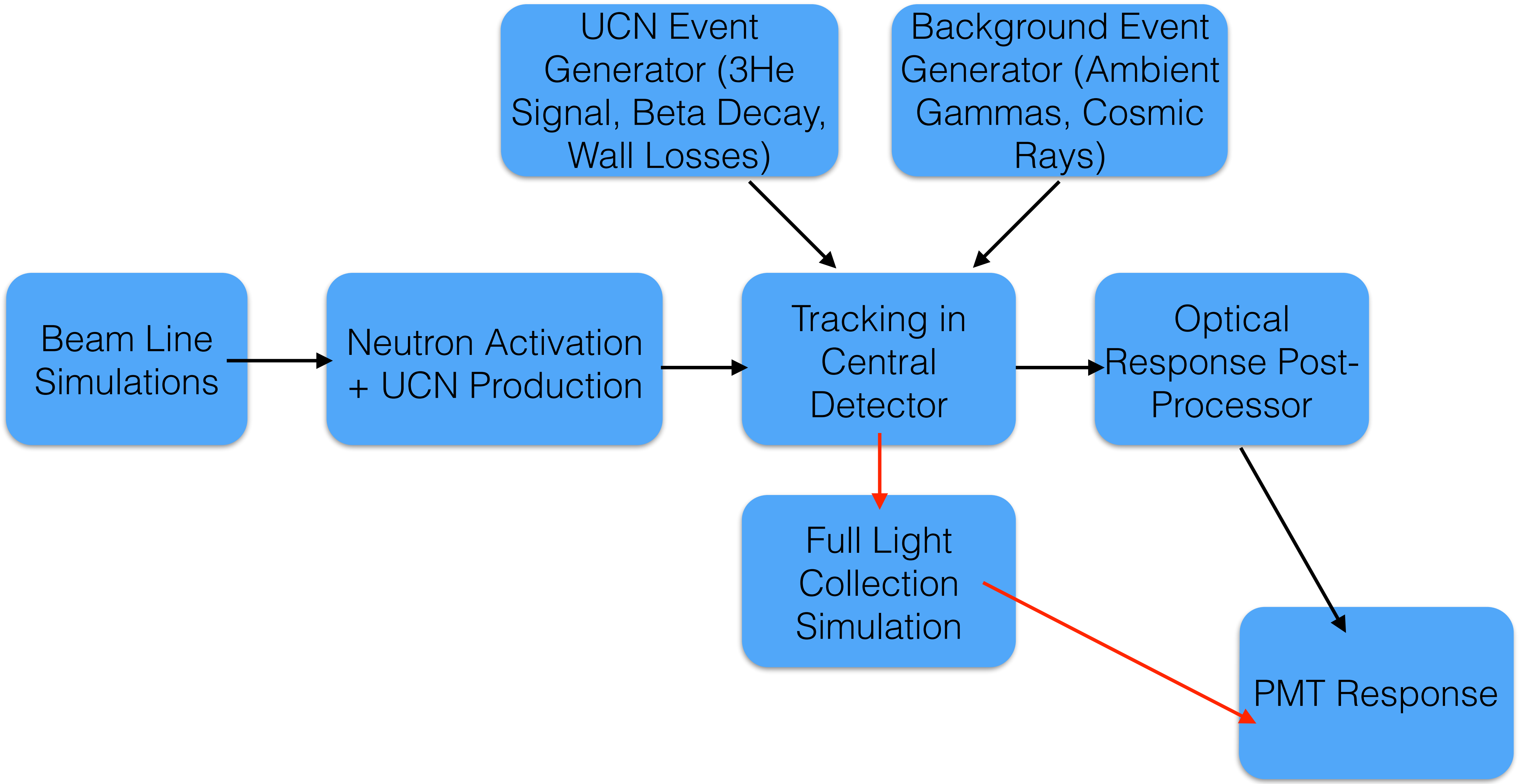
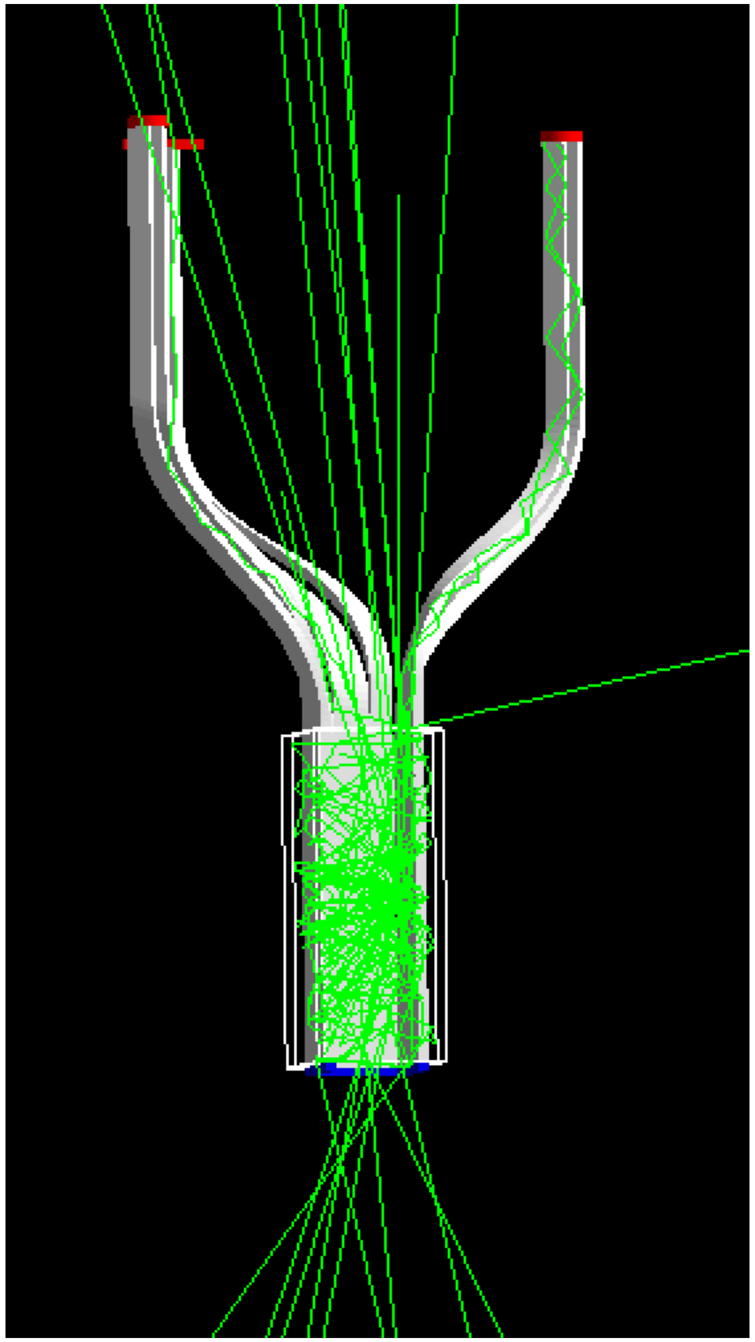
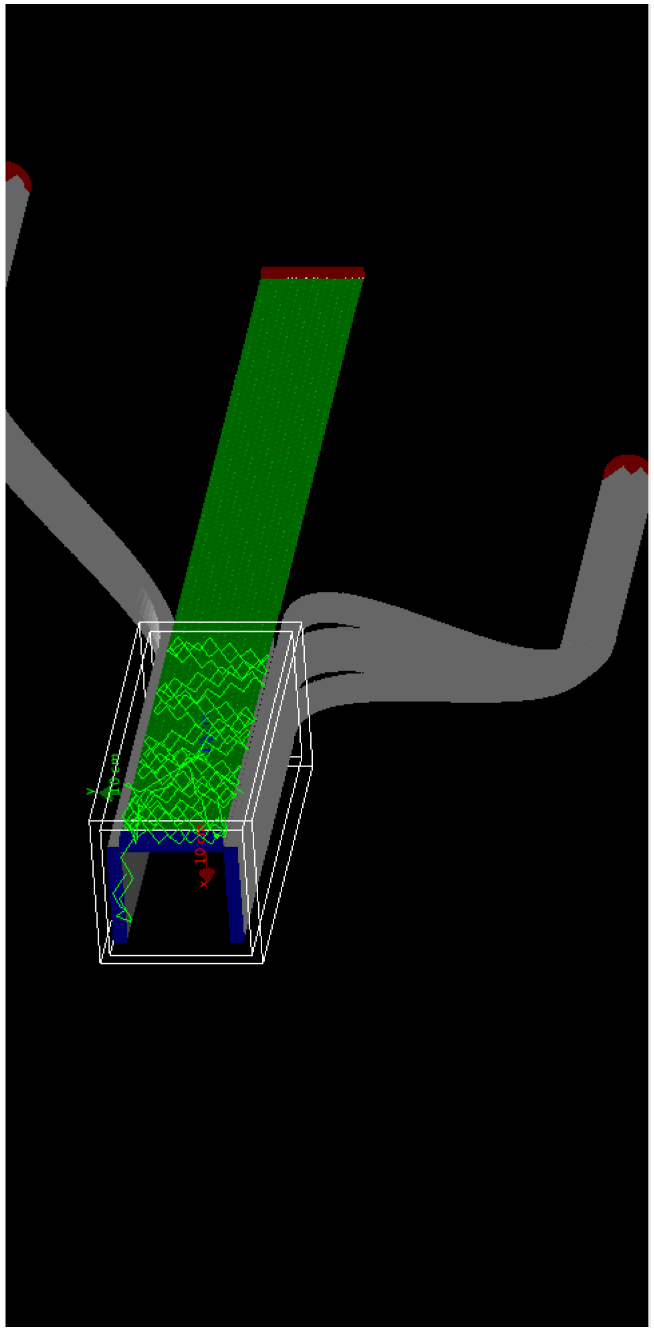


Light Collection Simulation

- Originally developed by Zach Raines @ Boston Univ.
- Includes TPB wavelength shifting of 80 nm scintillation light.
- Implements novel geometry methods developed by Peter Gumplinger of Triumf to realize “bent” light guides.



Light Collection Simulation



- Recently extended to include wavelength shifting fibers and silicon photomultipliers in Light Collection test stand @ ORNL.
- TPB process modified to include production of blue light outside of optical medium.
- Currently being benchmarked against optical response post-processor.

Integrated Simulations Framework

<u>Goals</u>

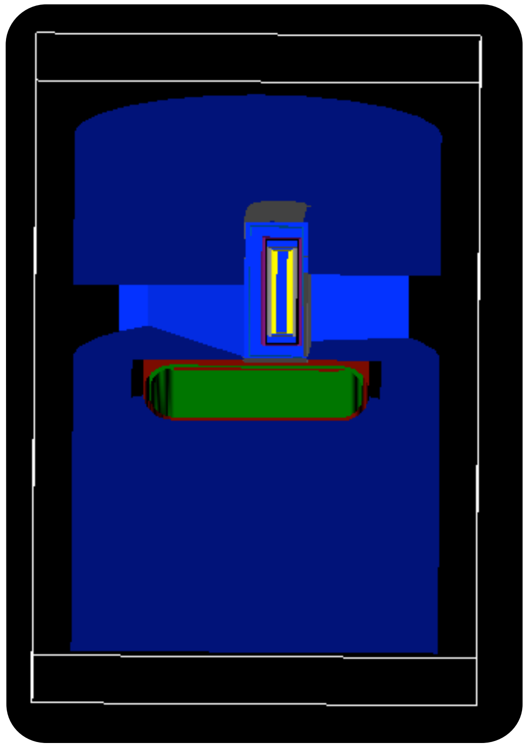
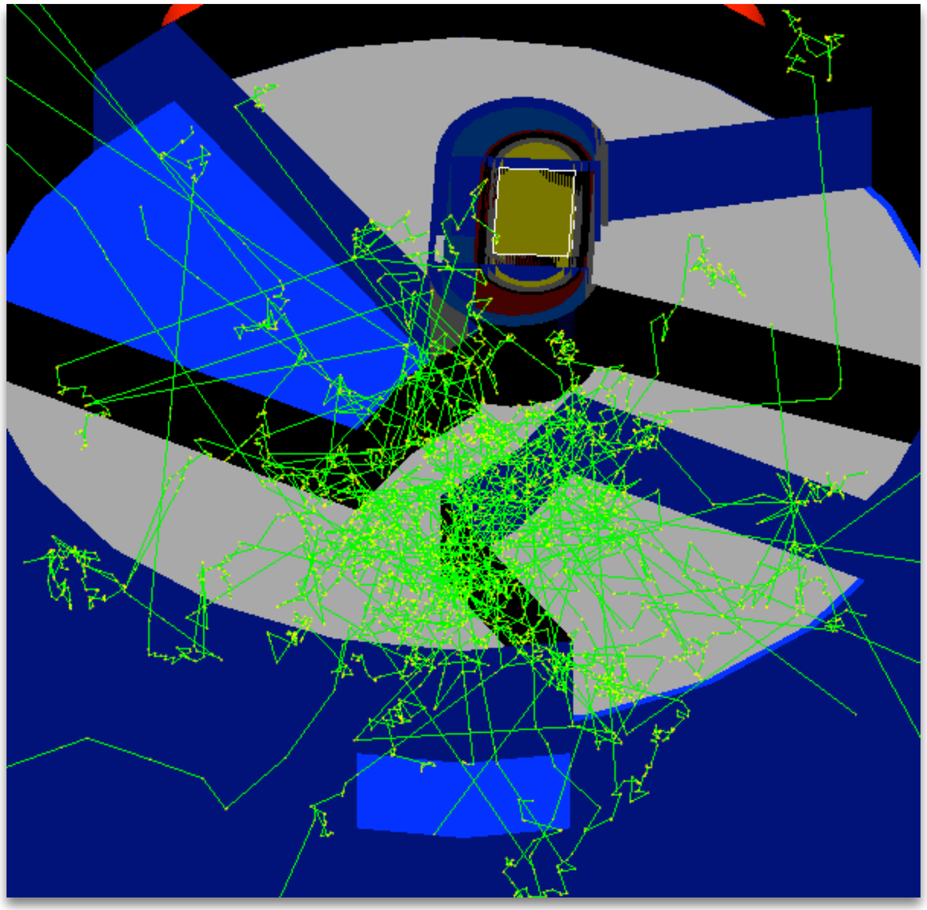
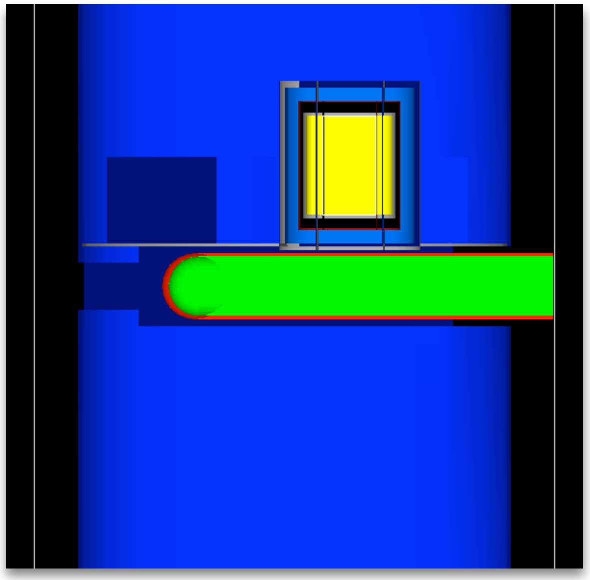
- Curate code developed over the last decade for continued use by the collaboration.
- Create highly modularized geometry to accommodate major design changes.
- Facilitate streamlined workflows.
- Reduce learning curve for new simulations team members.

<u>Strategy</u>

- Migrate to modern version control using git.
- Recode all geometry files using approach of Peter Gumplinger.
- Standardize I/O classes for both online and offline I/O.
- Implement vast array of messenger classes to maximize runtime flexibility.

SNS Moderator Simulations

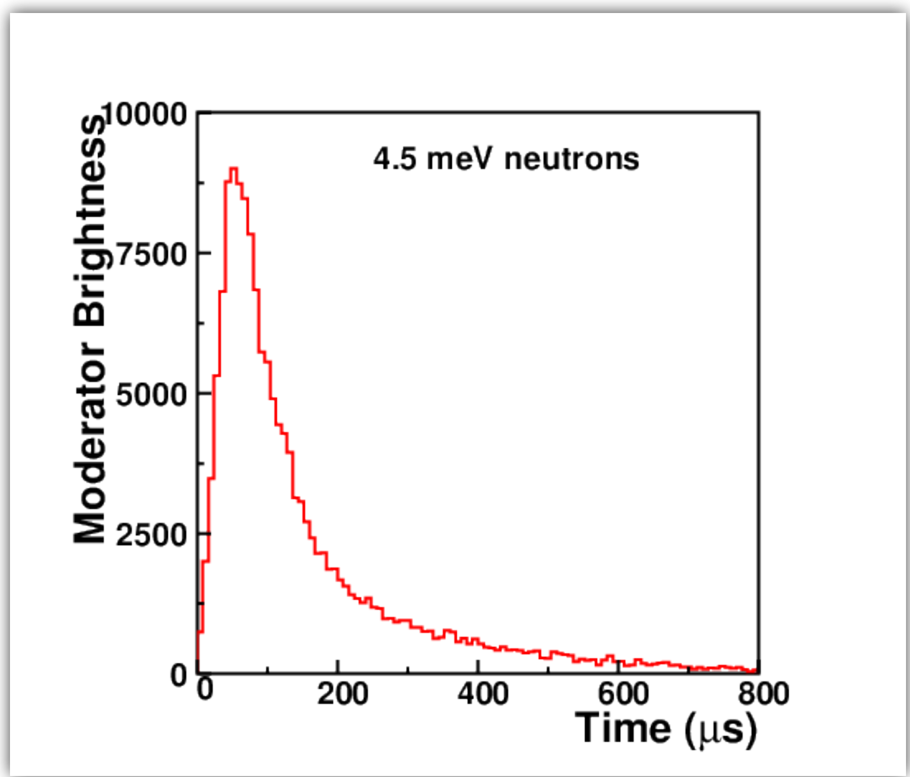
- Due to Export Control concerns with MCNP, we were funded to investigate the feasibility of using Geant4 for neutron moderator simulations.
- We implemented a simplified geometrical model of the SNS target and top downstream moderators.

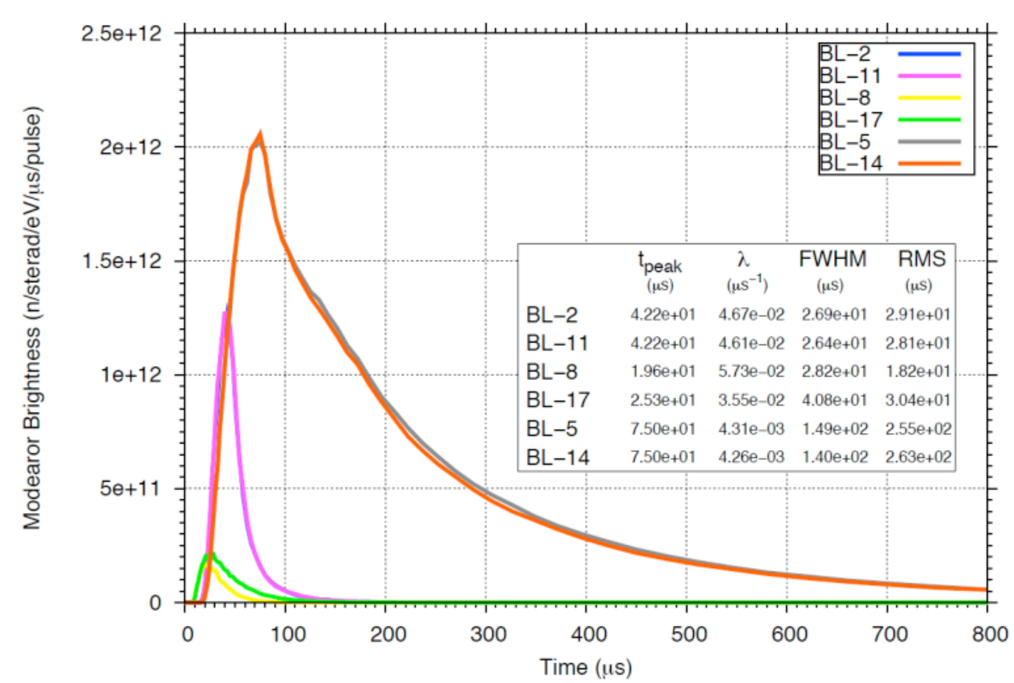
SNS Moderator Simulations

Simulations of BL-14 brightness showed reasonable agreement with MCNPX.

Geant4



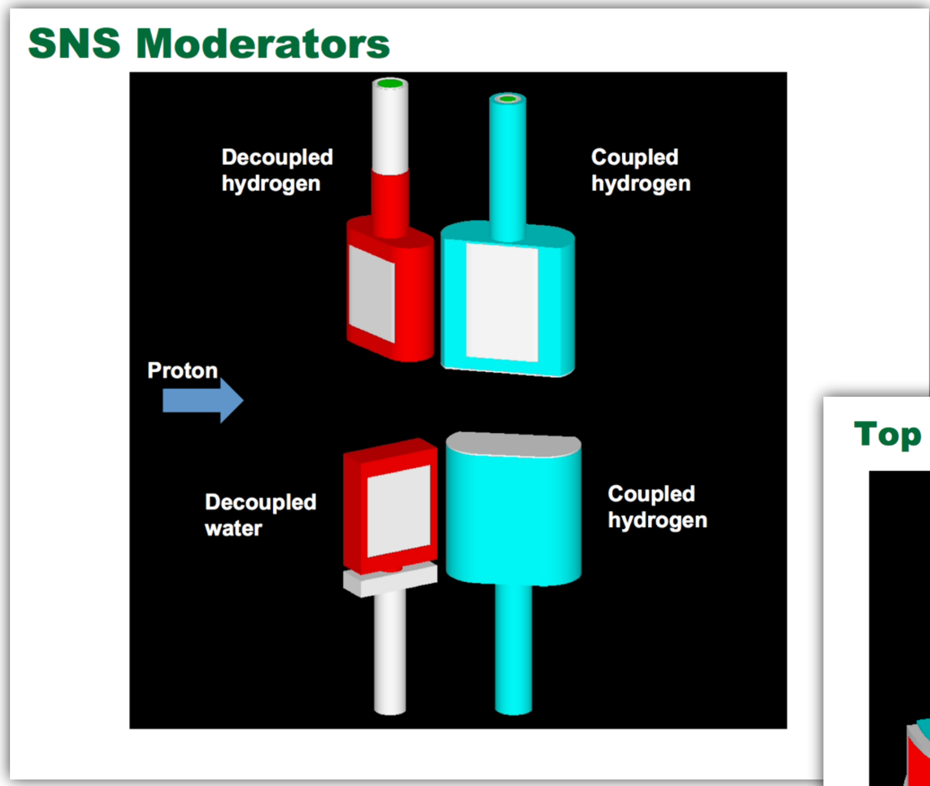
MCNPX

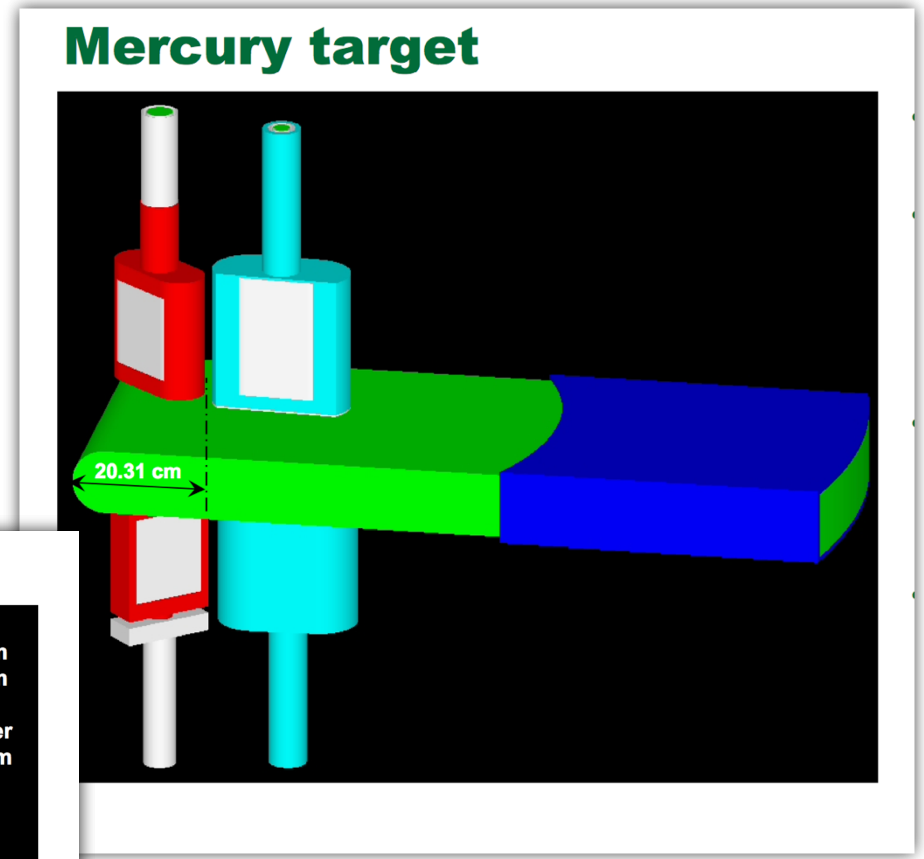


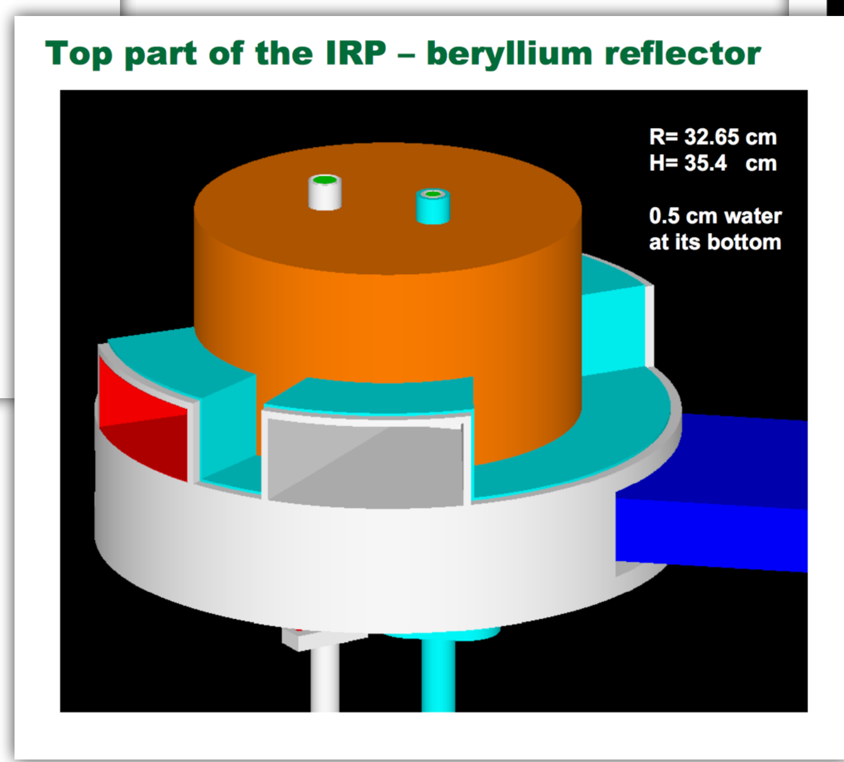
	t_{peak} (μs)	λ (μs^{-1})	FWHM (μs)	RMS (μs)
BL−2	4.22e+01	4.67e−02	2.69e+01	2.91e+01
BL−11	4.22e+01	4.61e−02	2.64e+01	2.81e+01
BL−8	1.96e+01	5.73e−02	2.82e+01	1.82e+01
BL−17	2.53e+01	3.55e−02	4.08e+01	3.04e+01
BL−5	7.50e+01	4.31e−03	1.49e+02	2.55e+02
BL−14	7.50e+01	4.26e−03	1.40e+02	2.63e+02

SNS Moderator Simulations

Success of our simple model led the SNS group to develop a full Geant4 model.



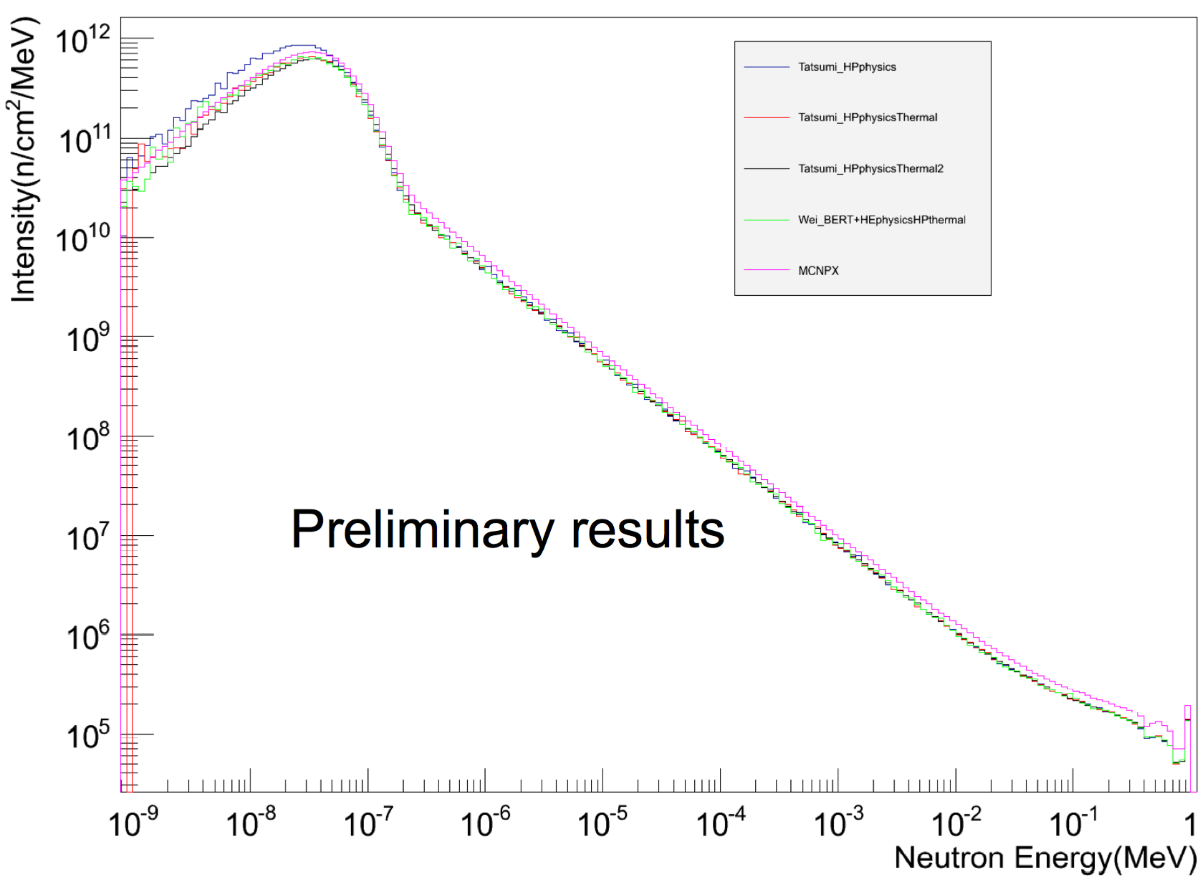




SNS Moderator Simulations

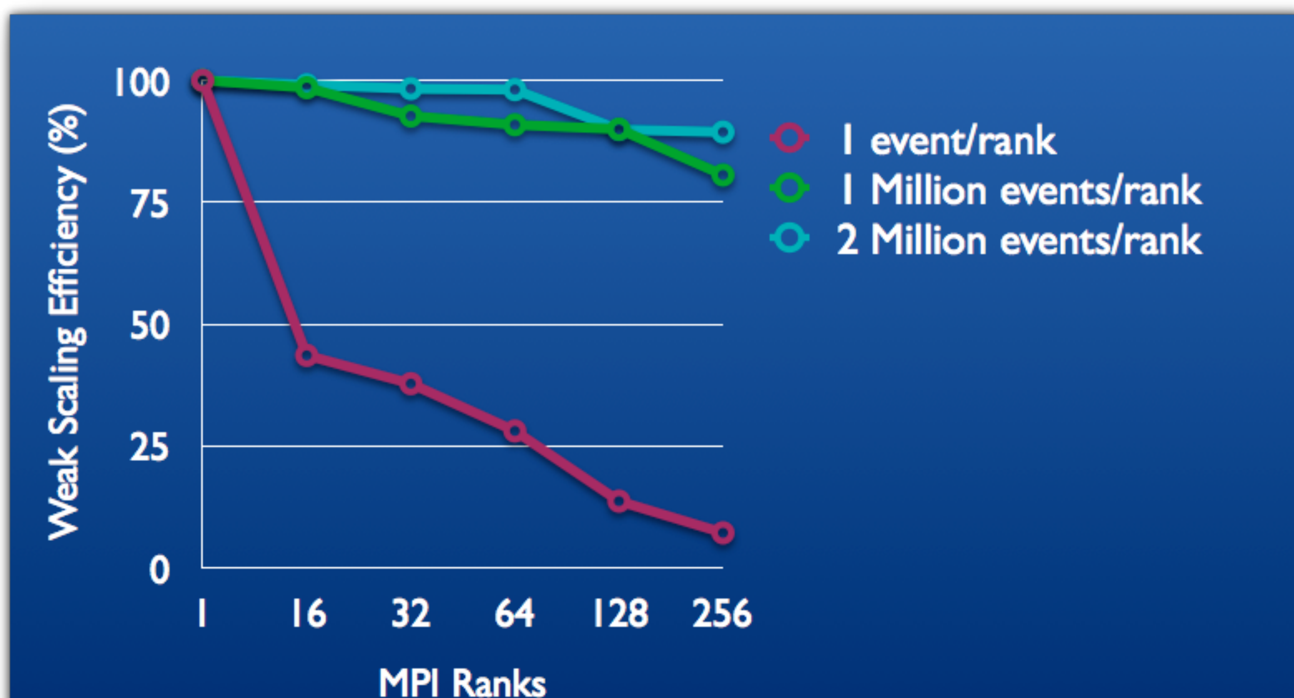
We are currently working with the SNS group and the Geant4 collaboration to perform a detailed comparison of all low energy neutron scattering kernels in Geant4 and MCNPX.

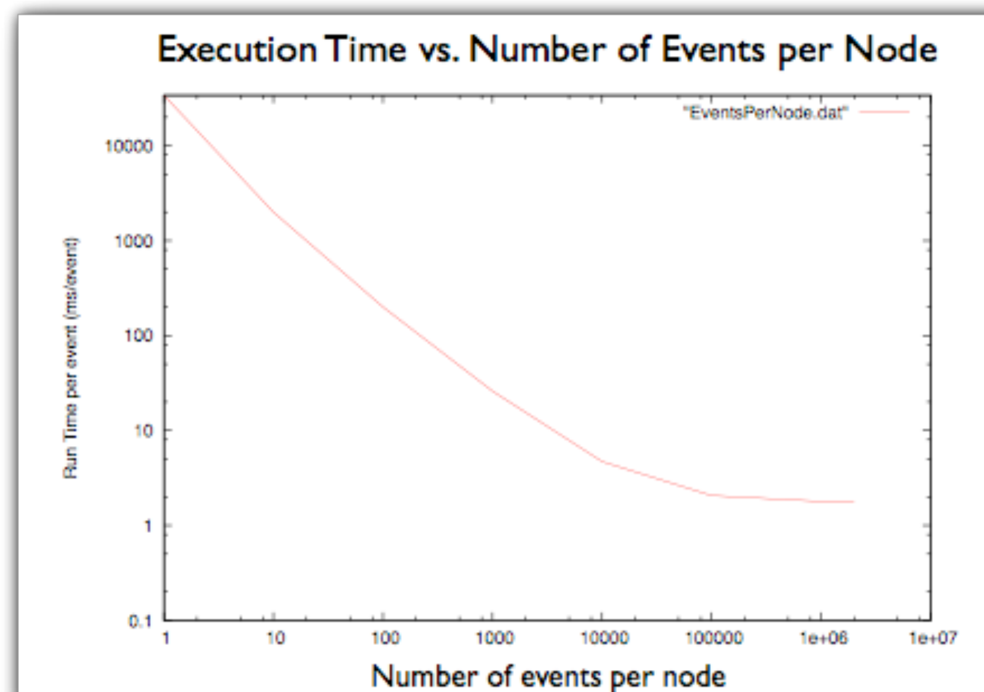
Benchmark of water scattering kernel



Geant4 On Titan

- As part of our SNS work, we were allotted time on the Titan Supercomputer.
- We were able to implement an MPI layer to parallelize across ~10,000 cores.





Conclusion

- Geant4 is a versatile toolkit that has many areas of application for nEDM simulations.
- Once a general simulations framework is built, it can be made extremely user friendly through the creation of customized runtime commands.
- Geant4 will continue to evolve to take advantage of the next generation of computer hardware.