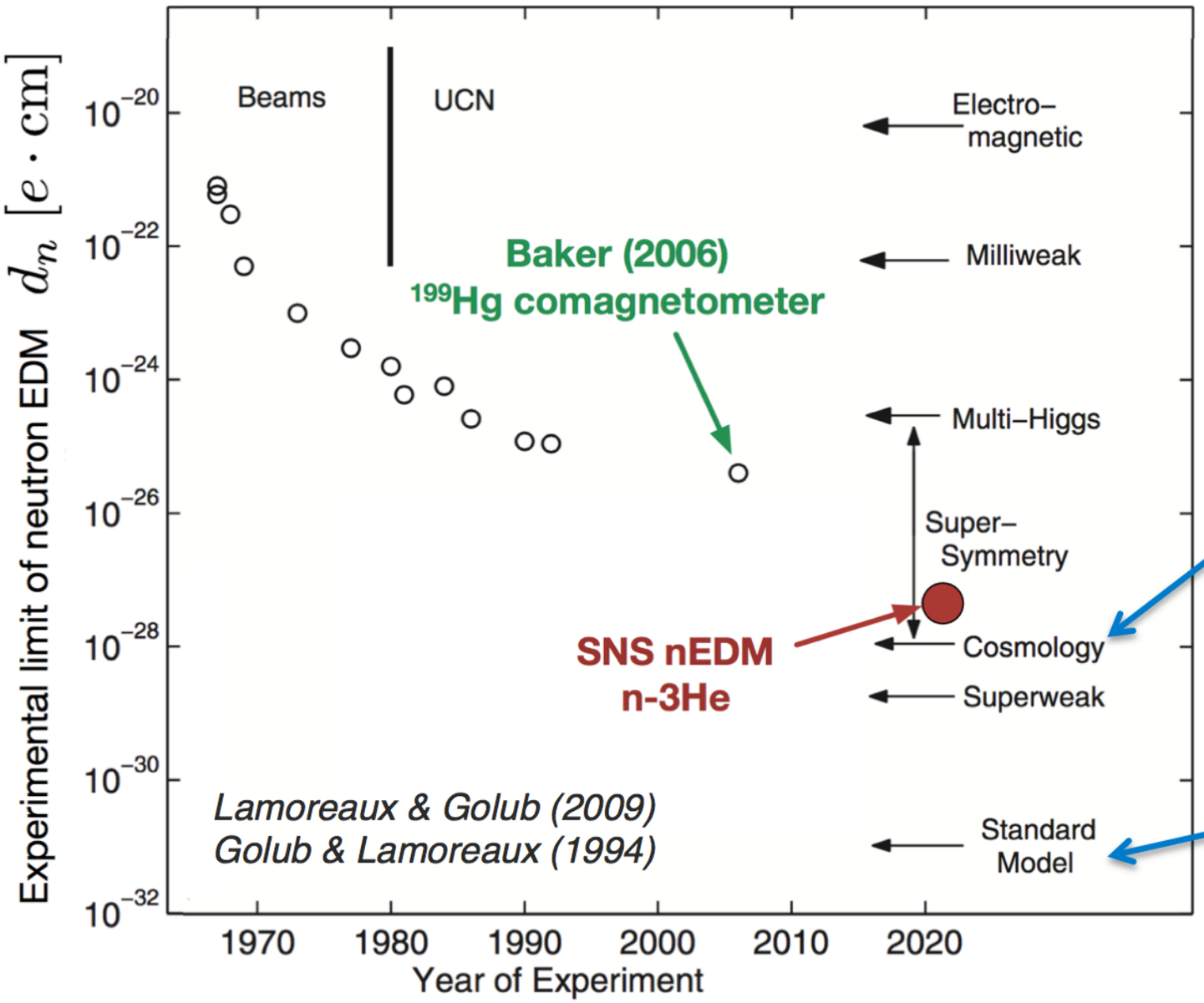
nEDM Panda Payload Development for OLCF

BigPanda Technical Interchange Meeting, UTA
January 17, 2018

Jed Leggett
Contributions From nEDM@SNS Simulations Team

Overview of nEDM@SNS Experiment



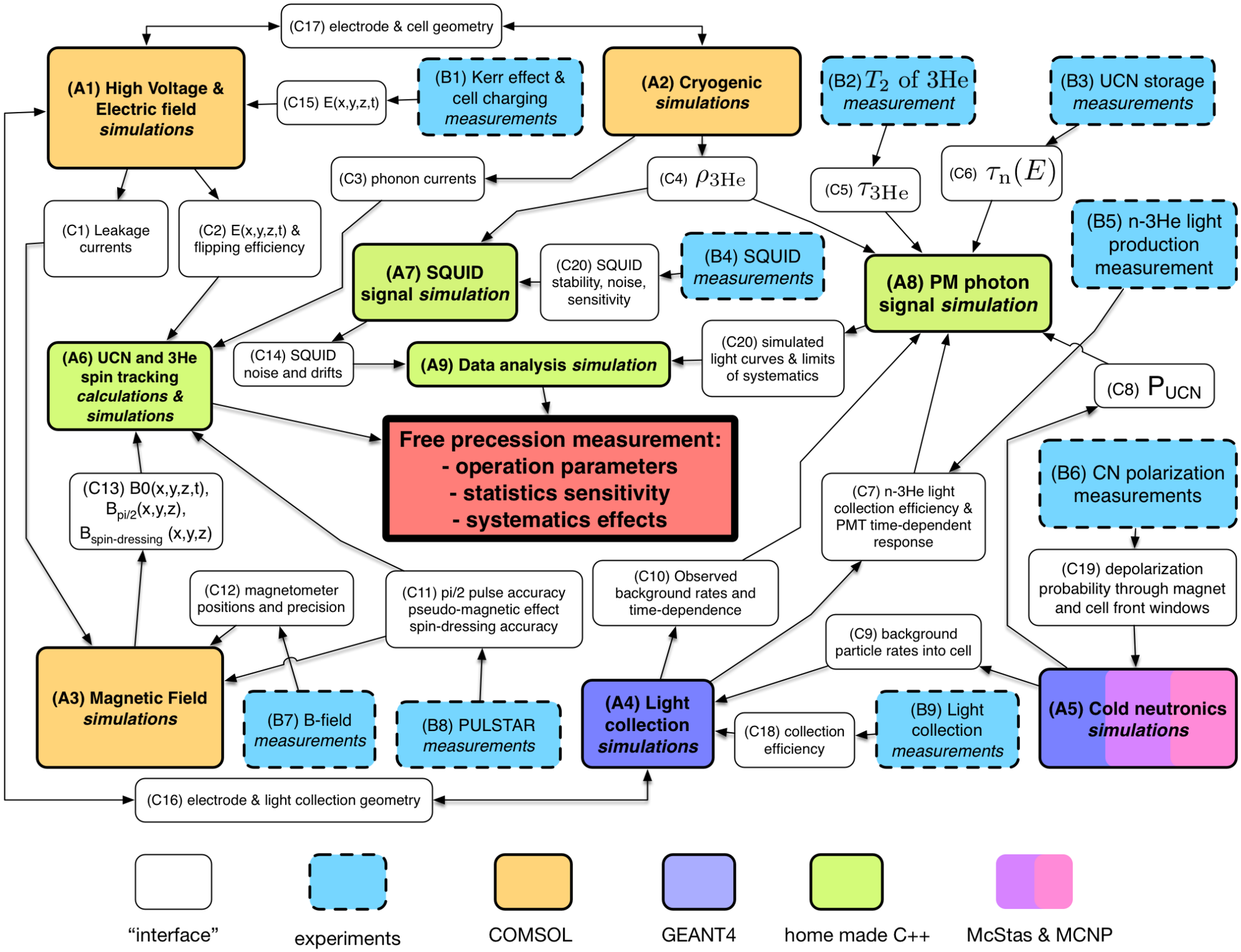
Rich History of nEDM Measurements, Started at ORNL in 1950

minimum neutron EDM that produce observed baryon-asymmetry due to known CP-violation along with baryon nonconservation. *Ellis et al. (1981)*

The size of nEDM predicted from known amounts of *CP*-violation in the standard model.

*Slide from Ken Leung.

nEDM Simulations Framework



K Leung (NCSU), B Plaster (UKy), L Broussard (ORNL)

Largest Computational Needs

Data Challenge 2.0

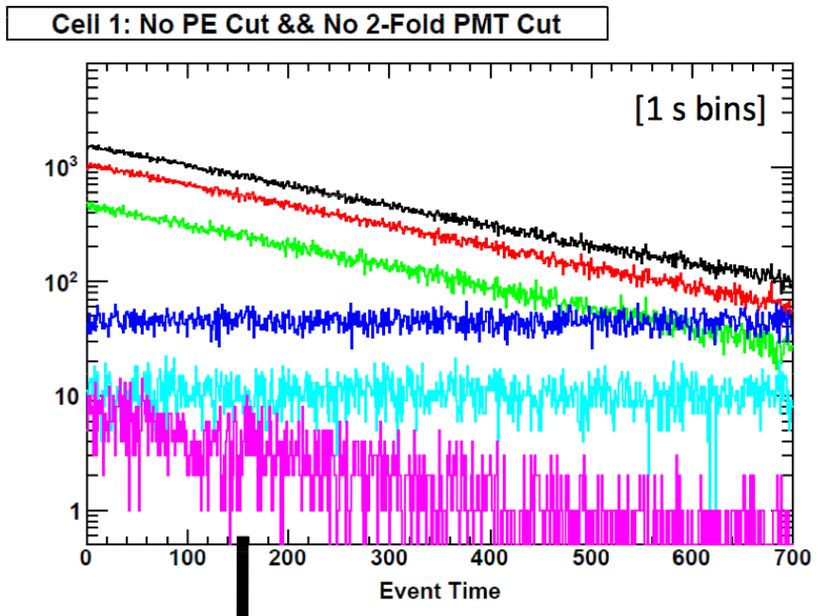
- Experiment runs at Spallation Neutron Source 2020+
- We want to have data analysis workflows in place when data collection begins.
- Previous Data Challenge produced 10^9 simulated events with backgrounds.
- Current iteration will produce >10^{11} events: 100k Titan node-hours, or 1.6M core-hours and 20 TB of data.

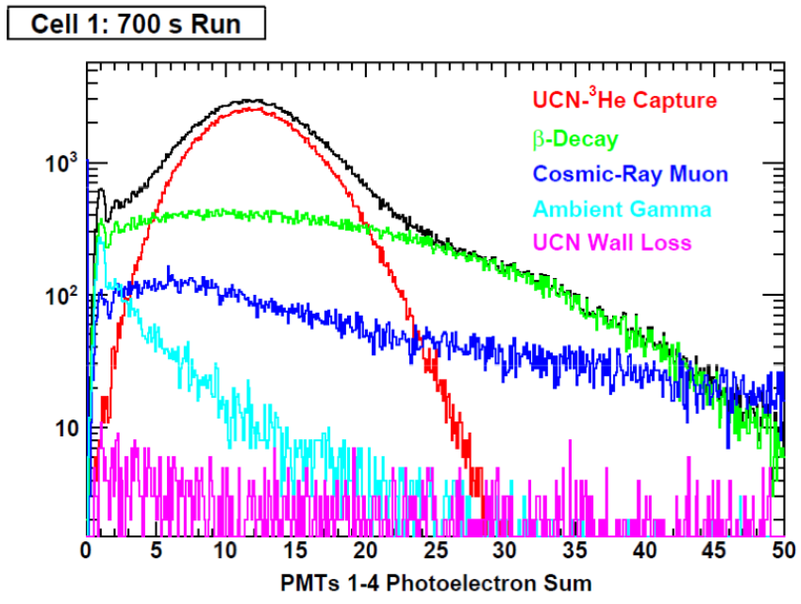
Systematic Studies

- Detailed tracking of spin propagation in magnetic field is needed to understand systematic uncertainties.
- On the order of 10^8 core-hours and 100 TB required for these studies.
- Stand alone C++ application with ROOT dependency (R. Shmid Dissertation)
- Currently being investigated for GPU vectorization.

Expected Science Results for Data Challenge

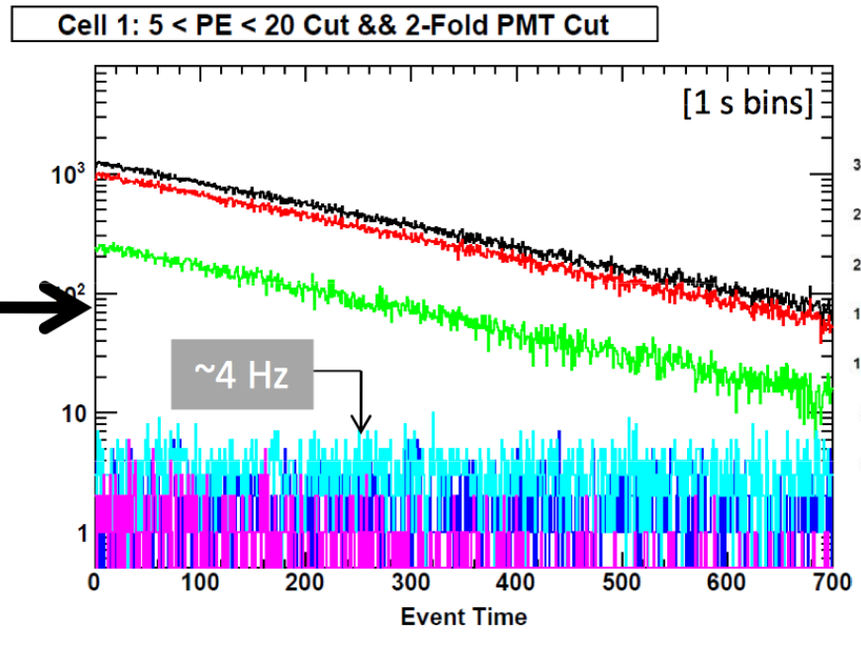
Timing and Photoelectron Spectra

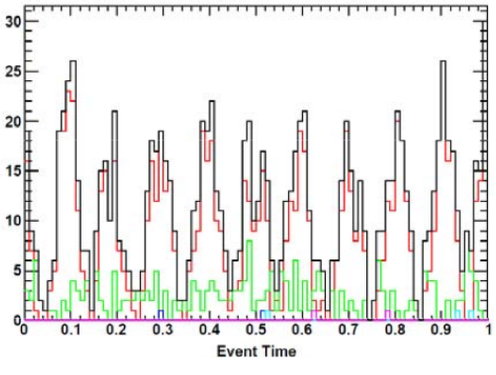




muon MIP peak at ~150

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

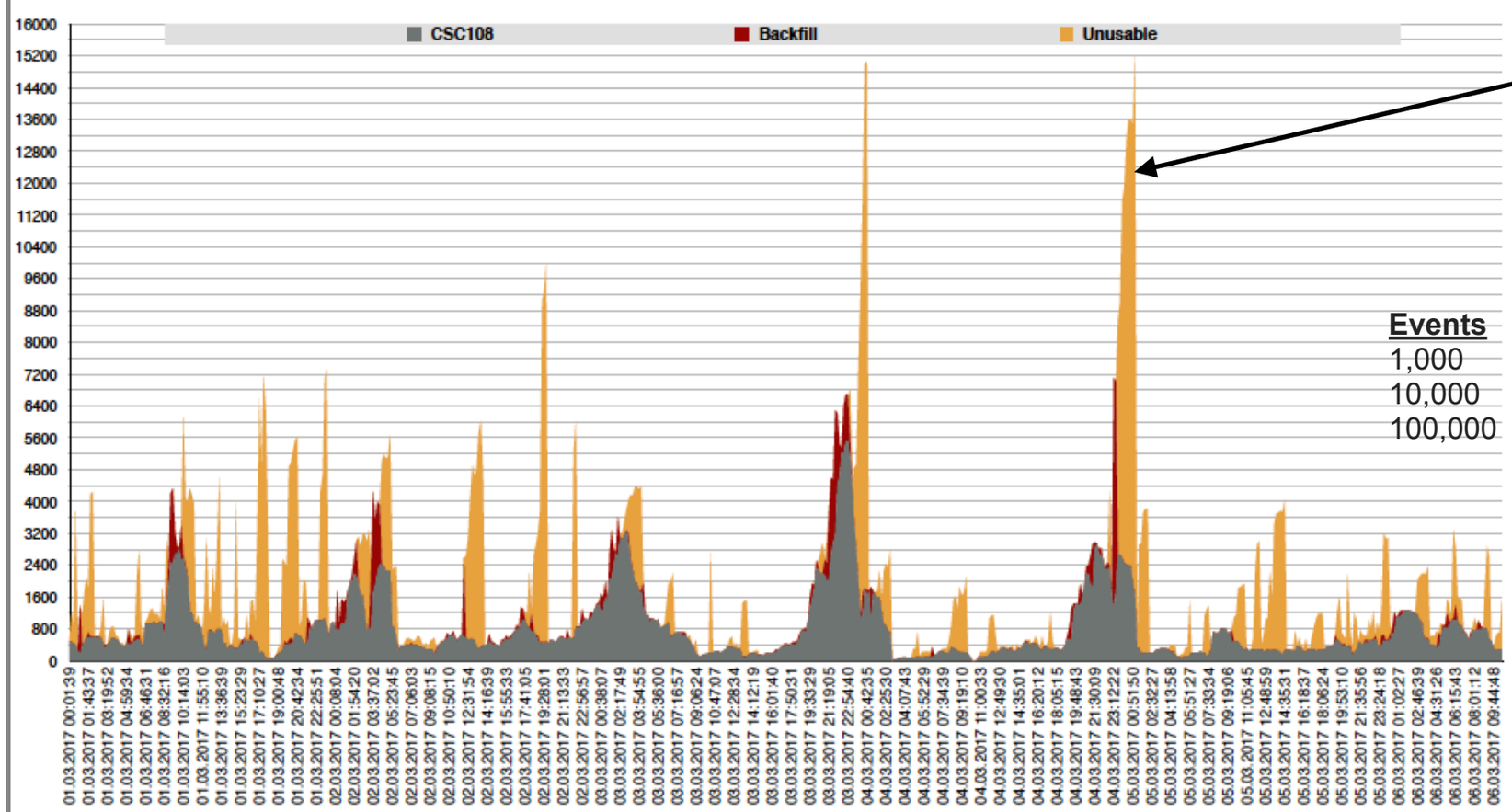




5

Short Job Backfilling on Titan

And Details of Backfill Like This



Events
1,000
10,000
100,000

Kaushik De *Mar 31, 2017* 4

nEDM Central Cell Simulations can efficiently utilize short duration openings.

Geant4 Running Time	Wall Clock Time
~3 s	~13 s
~33 s	~43 s
~330 s	~345 s

nEDM on Panda

Minimize extra workforce requirements needed to utilize available computational resources.

- No nEDM collaborators work full time on simulations, but many make intermittent contributions.

Take advantage of fine grained backfill potential.

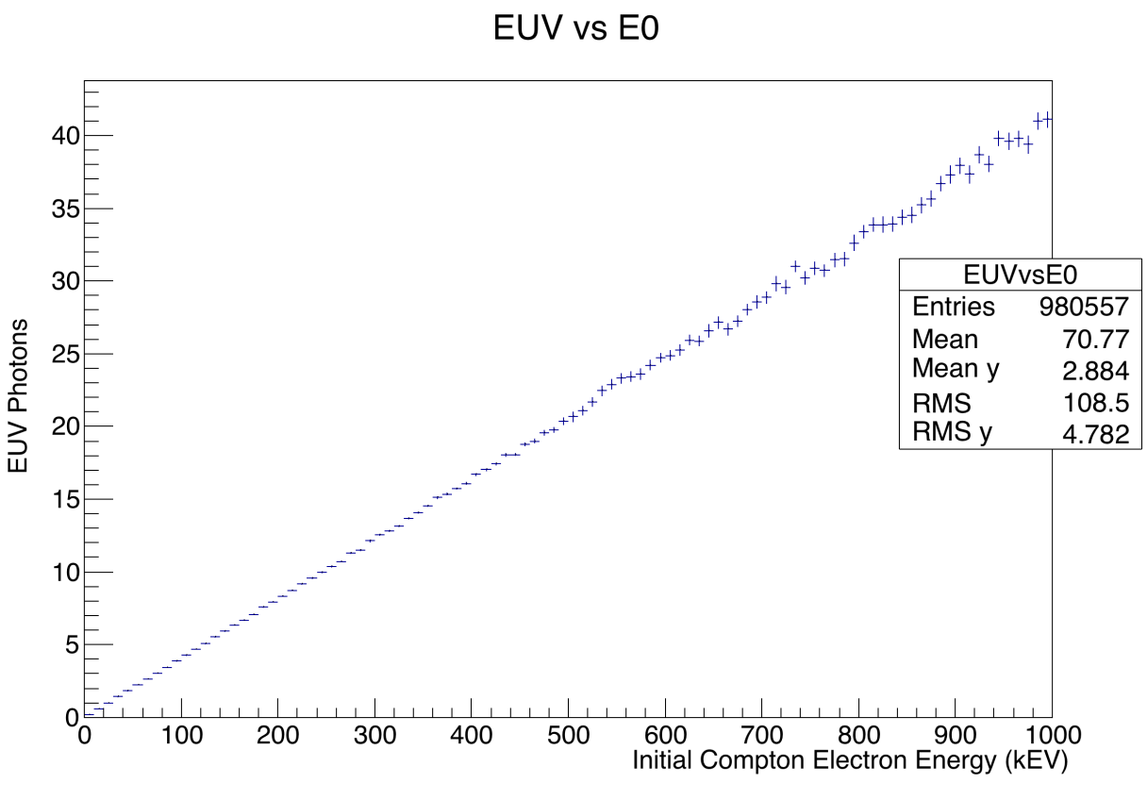
- nEDM Central Cell Simulation can utilize as little as a few node-minutes in an efficient manner.
- Results for Data Challenge can be accumulated over time.

Data Challenge 2.0 production runs tested on Panda

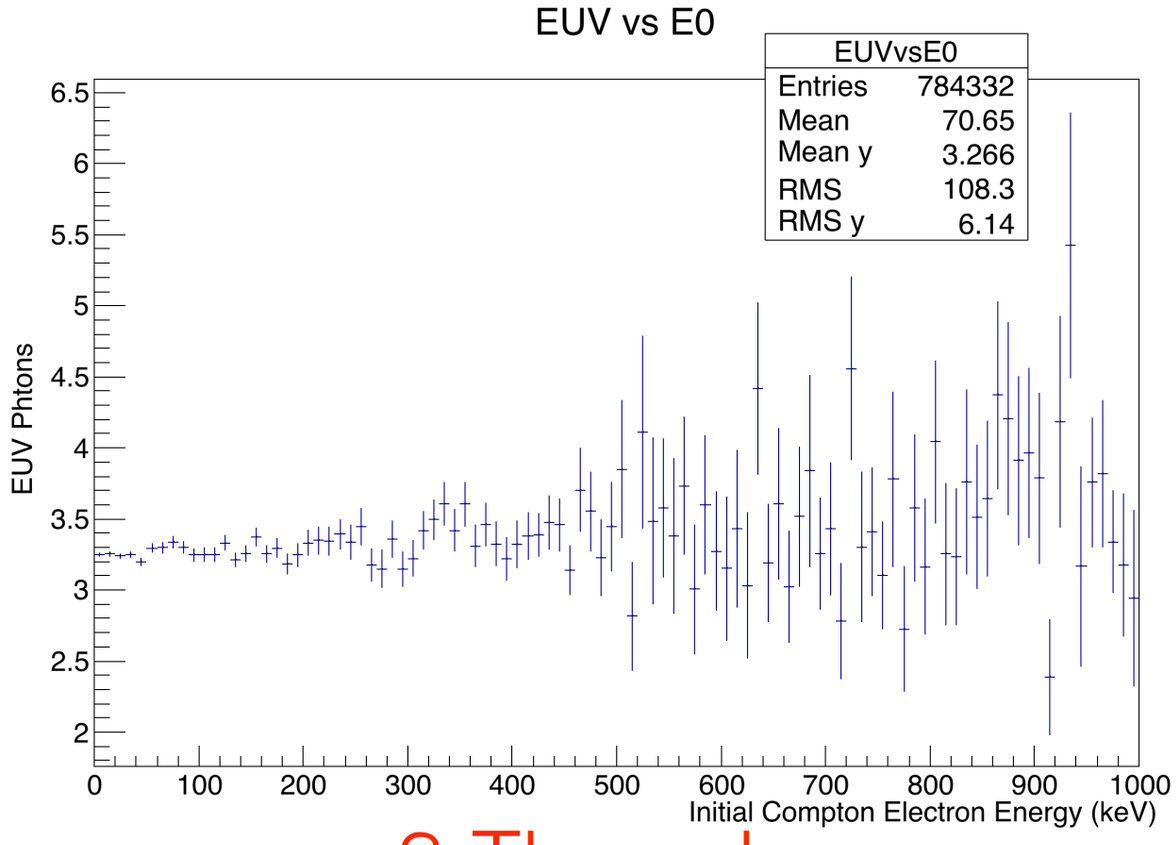
- Significant delays due to software bugs.
- Remaining nph118 hours will be utilized through Panda submission by end of January.

Race Condition in nEDM Simulation

When inspecting simulation data, we noticed several oddities that were eventually traced to a race condition in the analysis output.



One Thread



8 Threads

Race Condition Work Around

The Collaboration has yet to determine if the race condition is a Geant4 problem or nEDM Problem

Currently running single threaded with 1 MPI rank per core (16 per node), results in:

- 16x number of files (meta-data) for the same number of events.
- Inefficient memory usage, many objects can be shared with multiple threads.
- Increased startup overhead.

The workaround also exposed a memory leak due to the reduced memory per rank (2 GB).

- Problem fixed, but caused further delays.

Panda Submission

monitor-bigpanda.apps.ccs.ornl.gov/job?pandaid=477

Search

PanDA | Dash | Tasks | Jobs | Errors | Users | Sites | Incidents | Search | Admin | VO | Help

PanDA logger

Job details for PanDA job **477**

monitor-5-tqrbw Built 20:33, cache 3' Actual version

PandaID Attempt#	Owner / VO	Request Task ID	Status	Created	Time to start d:h:m:s	Duration d:h:m:s	Modified	Site	Priority
477 Attempt 10	/ST=TXRuslan Mashinistov / lqcd	2	finished	2018-01-16 17:14	0:0:00:21	0:3:06:26	01-16 20:25	ANALY_ORNL_Titan_nEDM	933

Job name: 802e2f67-6a66-423a-83c3-1c135e96a6cf **transformation:** #json#

Datasets: **Out:** panda.destDB.548c0c8a-8eab-4f51-acab-eac5dc72d563

Dataset summary: log: 1

This is attempt number 10 for this job. To see a history of job attempts click on the job name above.

Show script to re-create job for offline debugging: 477

Job information | job stdoutoutputs | payload stdout | job cache tarball | pilot records | JEDI action logger | child jobs

1 job files

Filename (Type)	Scope	Size (MB)	Status	Attempt (max)	Dataset
802e2f67-6a66-423a-83c3-1c135e96a6cf.job.log.tgz (log)	None	0	ready		panda.destDB.548c0c8a-8eab-4f51-acab-eac5dc72d563 (destination block: panda.destDB.548c0c8a-8eab-4f51-acab-eac5dc72d563 rucio)

Other key job parameters

Last state change	to finished at 2018-01-16 20:25
Attempt number	10 of a maximum 2
Output destination	local
Job parameters	{"nodes": 200, "next": null, "command": "\ncd /lustre/atlas1/nph118/proj-shared/PanDAtest/Captures\npwd\nsource /ccs/proj/nph118/scripts/G4DataPaths.sh\naprun -n 3200 -N 16 /ccs/proj /nph118/nEDMSims/build-gcc/nEDMMeasurementCell/nEDMMeasurementCell_Capture /ccs/proj/nph118/scripts/run_captures.mac\n", "name": "captures", "walltime": "00:30:00"}
Pilot ID	xtestP001|PR|PICARD 59aRC2 (Titan)

Data Challenge Production

First wave of Mock Data Challenge has been prepared for Panda Submission

- 100 Billion Neutron Capture Events will be generated in 50 Panda jobs.
- Each job requests 200 nodes for 30 minutes.
- This will be completed by end of month and will exhaust remaining nph118 hours.

Second wave of Mock Data Challenge is in QA and will be ready for Panda submission soon.

- Multiple types of background will be produced.
- Total computational needs around 10x Neutron Capture simulations.
- If possible, begin submitting through nph118, continue after January with new DD project.

Future nEDM Computing needs

Mock Data Challenge 2.0 Analysis

- Currently setting up analysis codes on Rhea.
- Stalled due to ROOT installation difficulties.

Potential Mock Data Challenge 3.0 in discussion

- Explore larger parameter space.
- 2-3x computational needs of 3.0

nEDM Collaboration

Thank You!

Arizona State University

Bartoszek Engineering

Brown University

California Institute of Technology

Duke University

University of Illinois

Indiana University

University of Kentucky

Los Alamos National Laboratory

Massachusetts Institute of Technology

National Autonomous University of Mexico

Mississippi State University

North Carolina State University

Oak Ridge National Laboratory

Simon Fraser University

Tennessee Tech University

University of Tennessee

Valparaiso University

University of Virginia

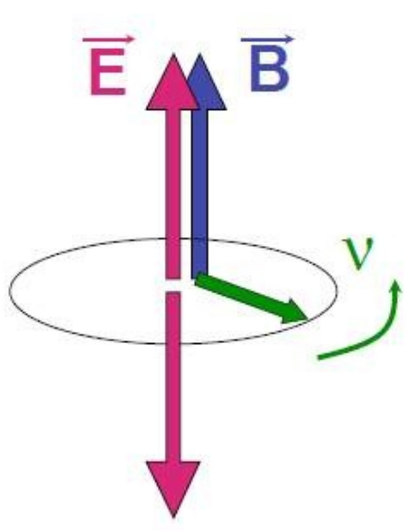
Extra Slides

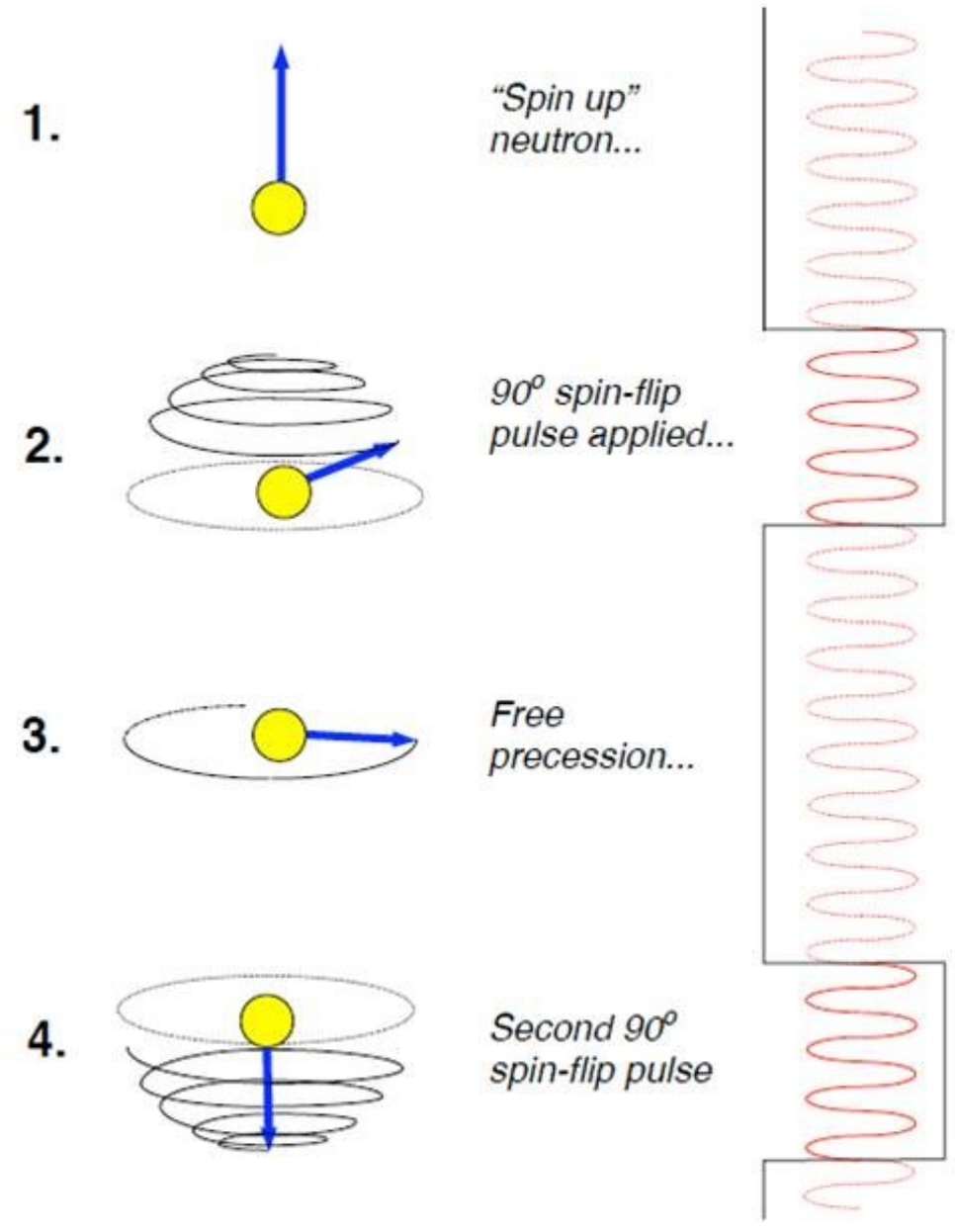
EDM Measurement Technique

- Measure change in precession frequency with parallel vs antiparallel **E**, **B** fields

$$\omega = \frac{2\vec{\mu}\cdot\vec{B} \pm 2\vec{d}\cdot\vec{E}}{\hbar}$$

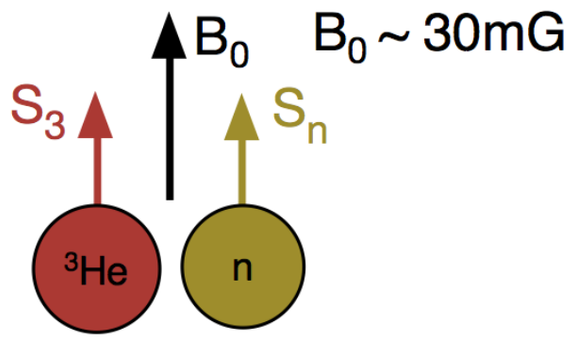
$$\Delta\omega = \frac{4dE}{\hbar}$$

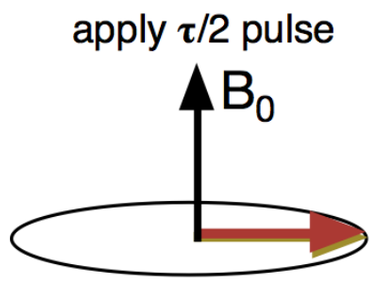


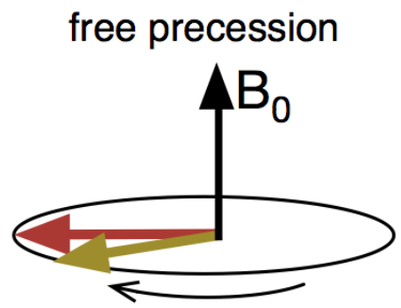


*Slide from Leah Broussard.

EDM Measurement Technique







^{3}He + n → p + ^{3}T (Q=764keV) has **spin-dependent** cross-section (@2200m/s):

Parallel spins: $\sigma_{\uparrow\uparrow} < 10\,\mathrm{b}$ Anti-parallel spins : $\sigma_{\uparrow\downarrow} \approx 11\,\mathrm{kb}$

Scintillation light signal: $1 - P_n\,P_3\,\cos\theta_{\mathrm{n3}}(t)$

← angle between n & ^{3}He spins

Effects of He-3 EDM suppressed by Schiff screening so that:

$$\theta_{\mathrm{n3}} = |\gamma_n - \gamma_3|B_0 t \pm \frac{e d_n |E|}{\hbar} t \qquad \gamma_3 \approx 1.1\,\gamma_{\mathrm{n}} \qquad \gamma_3 B_0/(2\pi) \approx 100\,\mathrm{Hz}$$

Measure ^{3}He precession $\gamma_3 B_0/(2\pi)$ with SQUIDS => sensitivity $\approx 5 \times 10^{-28}\,e.\mathrm{cm}$

Alternative dressed-spin technique: apply strong RF ($B_{\mathrm{rf}} \sim 1\,\mathrm{G}$ $\omega_{\mathrm{rf}}/(2\pi) \sim 3\,\mathrm{kHz}$) and increase sensitivity of exp.

*Slide from Ken Leung.