Simulations Status Report



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Outline

Goals and Responsible Groups

Production Pipelines

- Detector Response
- Environmental Backgrounds
- Use For Other Samples

New Software Development

- Geometry
- Physics
- Performance
- Pipelines

Commissioning Support

Looking Forward



This talk will present the status of the CDMS sources/backgrounds simulation, including the production pipelines

The details of the detector response simulation (DMC) will be presented by Warren Perry in the next talk

Goals for CDMS Simulations

Simulations are designed to quantify backgrounds, reduce systematic uncertainties and optimize analyses as part of the Integrated Analysis Plan (IAP)

There are two simulation pipelines to make large datasets to achieve these goals:

- Environmental Backgrounds, to evaluate radioisotopes in the materials and components we used to build the experiment, and in the cavern around it
- **Detector Response** ("DMC"), to evaluate how the detectors respond to energy deposits, and what readout signals they should produce

Each are built in a modular way so they can support Special-Purpose Simulations



Production Pipelines

The two production pipelines are designed around different kinds of simulations:

Detector Response (used by <u>O.6.4.2</u>) – runs at Texas A&M

- Limited number of "in detector" or "signal-like" sources (Confluence)
- Source simulation+DMC+readout traces \rightarrow raw data \rightarrow RQs/RRQs
- Complete pipeline used for Data Challenge 3

Environmental Backgrounds (used by <u>O.6.4.3</u>) – runs on DRAC

- Dozens of radioisotopes, thousands of component volumes/surfaces
- Source simulation only, based on cavern measurements and assay results
- Goal is 10× SNOLAB final data set, about "fifty years" of exposure
- Long-term campaign ongoing with geometry improvements

Both pipelines can be used by collaborators to produce special purpose samples

Detector Response

Includes complete job control and data management system, covering all stages of the simulations from sources, through DMC, raw data, and reconstruction. Analysis of RQs/RRQs using standard "real data" tools.

SimWorkFlowTools

Job control, completion checks, catalog registration

SimProdMacro

Standard, modular macros for SuperSim/DMC

DAQSim

DAQ simulation, raw data formats (both Soudan and SNOLAB) cdmsbats_config

CDMSbats configuration files



Detector Response: DC3

Started late 2023, completed September 2024

• Many iterations and updates (15~20k events)

Exercised complete production pipeline

- Job control, checks, catalog registration
- SuperSim/DMC with standardized macros
- DAQ simulation, Midas raw data format
- CDMSbats processing with configuration files



Generated and published 220,000 events with full detector response in 16 days

- Single detector (all four types) ER, NR, WIMP, Ge-71 (Ge only)
- Full SNOLAB geometry (24 detectors) Ba-133, Cf-252
- All available in Data Catalog for analysis, using standard analysis tools

Data quality reviewed with Jupyter notebooks; will inform commissioning checks

Environmental Backgrounds

Production pipeline

• BGExplorer

 Calculates component emission rates from assays, mass and surface area

• SNOLABBackgroundMacros

- Macros for each component
- Scripts for file/directory management, job submission, validation, processing
- SuperSim
 - Propagates particle tracks, records hits
- supersim_analysis
 - ROOT and Python utilities for event selection and ROI counting
- BGExplorer
 - Calculates expected BG rate in ROI from simulated spectra

June 2024 \rightarrow June 2025



Environmental Backgrounds

Current status and progress

• BGExplorer

- Many component additions, mass and surface area updates
- Some components still awaiting fixes
- SNOLABBackgroundMacros
 - Special additions (²¹⁰Pb, cavern) done
 - Ready to read in BGE's run list
- SuperSim
 - Updated "Oct24" geometry released
- supersim_analysis
 - Ready to process all simulations (incl. importance biasing)

Production pipeline successfully tested with latest Apptainer release on Cedar, DRAC

June 2024 \rightarrow June 2025



Single-Purpose Samples

Both simulations pipelines can be used for smaller scale samples, managing the processing and data organization, even (optionally) registering the output into the Data Catalog for general use

Detector Response has been used for several large scale DMC samples for studies, validation, and thesis topics

- iZIP5 and CDMSlite (A&M, Karlsruhe)
- HV100mm Mock Analysis (A&M)

- DMC tuning with CUTE Tower3 (U of T)
- iZIP crosstalk with CDMSbats (A&M)

Environmental Backgrounds is being used to produce large-scale samples for CUTE Tower3 analyses (via **CUTEBackgroundMacros** package)

If there are dedicated production-scale samples which would be useful for your analysis, please reach out to the Simulation WG

Software Development

The simulation software, and the pipeline packages, are in a cycle of continuous improvement

- Issue tracking (JIRA, e-Log) supports bug reports and new features
- Consistent use by many people exercises all of the features

Rather than enumerating hundreds of individual issue tickets, we will show four (non-DMC) categories where significant work has been done in the past year

- Updating the Experiment geometry
- Additions/upgrades to physics processes
- Improving efficiency, speed and memory
- Improvements to the Production Pipelines

Detector Geometry Improvements

Full "as built" (so far!) SNOLAB apparatus, with better cavern

- Final engineering documents wherever possible
- Update as needed with in situ measurements or modifications from I&I
- Released in April 2025 (V16-00-00) to be used with commissioning
- Labelled as "Oct24" because that's when we started work

CUTE Tower3 geometry via macro file

- All six specific crystals (with individual DMC configurations) in position
- Can run with or without shielding and infrastructure as desired

Associated R&D (e.g., QUTEbits; ask Stefan!) is well integrated into SuperSim

- Flexible chip designs and macro-configurable layout
- All our test facilities already supported



Physics Process Improvements, Big and Small

Low energy optical physics

- Coupled transition radiation and Cherenkov
- Physics has been validated and deployed, needs performance improvements

Coherent photon scattering

- JAEA model adapted from Geant4 with improvements
- Final tuning and fixes in process

Custom radioactive decay files

- Already have some of these in place for Ge X-ray intensities
- Now have macro command support and special SF-only Cf-252 file
- Might be useful for Ge-71 activation studies

Software Performance Improvements

Reduced memory usage

- Reduced memory buffers for ROOT (trade-off with I/O job time)
- Global singleton for electric field models (smaller footprint up to ×10)

Importance Biasing (arXiv:2503.00585, submitted to NIM A)

- Clone and reweight tracks passing through thick shielding
- Generates multiple trajectories based on scattering effects
- Significantly increases backgrounds job efficiency: $O(10^4)$

Parameterized detector response (FastDMC)

- Models channel response (energy sharing) with approximations
- Runs as fast as SourceSim, not like full G4DMC
- Backgrounds WG investigating utility for analysis

Detector Response Pipeline Improvements

Basic structure and performance was validated with DC3, improvements since then to support Commissioning and beyond, including

- Significant memory reduction and speed improvement for DAQSim
- Support for complete SNOLAB and Soudan apparatus (multiple towers, multiple detector types, in single processed event)
- Both iZIP5 and CDMSlite runs
- Support for crystal-specific or "general/ideal" CDMSbats configurations

Job control and file management (**SimWorkFlowTools**) only functions at A&M, due to Slurm and directory structure specificity. Adding multi-site modularity would be a welcome improvement, if some group has a need and interest

Commissioning

All of the pre-commissioning tasks identified for Simulations are complete, and the pipelines are ready to run.

- Environmental Backgrounds campaign is continuing using the new Oct24 geometry, and will support Commissioning
- Source simulations are being used to generate models for calibration source placement and rates, to inform duration of calibration runs, and to calibrate source activity
- Detector Response pipeline is being used by CUTE Tower3 Analysis group to generate samples supporting their efforts

If there are production-scale Detector Response samples which would be of interest to Commissioning and the SNOLAB Analysis Sub-WG, please coordinate with the Analysis WG who will work with O.6.4.2

Backgrounds Modelling

Will use new geometry and Environmental Backgrounds campaign

- Inform detector expectations before
 Commissioning
- Help fit backgrounds in energy spectra taken during Commissioning



There is interest in developing good parameterizations in FastDMC to support high statistics, rapid turnaround backgrounds studies which include some level of detector response (pulse sims \rightarrow DAQSim \rightarrow CDMSbats)

See Maddy's Backgrounds plenary talks after lunch

Calibration Strategy Studies

Using full geometry, simulating possible source positions and activity/duration, with resulting detector rates and spectra (SourceSim only, no DMC required)



See Stefan's Calibrations plenary talk tomorrow

Calibration Source Activity

Using CUTE Tower3 data, connect Ge-71 decays seen in data with activation from Cf-252 source exposure. Simulations show activation vs. unit source activity



Cf-252 source reference (Mar 2020) 37 ± 5.6 kBq $\rightarrow 34.6\pm5.1$ kBq (est.)

Warren Perry, UofT (in progress)

Looking Forward

Beyond Commissioning, there will be more things for Simulations to consider and to contribute to for SuperCDMS

- What is needed for Simulations to contribute effectively to Early Science (and to Science Running)?
- What projects do we have in the short and medium term to be ready for those later contributions?

Early Science Publications

There have been no specific requests for Detector Response sample, or for special-purpose Environmental Backgrounds, for the early science analyses.

- Environmental Backgrounds production will be available and stable with the as-built detector geometry.
- Detector Response simulations could inform questions of efficiency, fiducialization, etc.

If there are production-scale Detector Response samples which would be of interest to the G2 Science Planning or Analysis WGs, please coordinate with O.6.4 to get them on our list

Upcoming Work and Campaigns

Environmental Backgrounds

• Ongoing: backgrounds affected by geometry changes are being regenerated

Calibration Strategy Studies

• First round completed: new runs based on feedback, focused studies

Detector Response Simulations

- No currently scheduled campaigns for Commissioning or Early Science
- Few weeks to prep and validate configurations on small samples
- 2-3 days per 10k events per source, can run in parallel

Continuous Software Development as needed

Open Projects, Open Tickets

Minor additions to SNOLAB geometry, improved class structures

Software bug fixes which don't affect production (multi-run jobs, scorer overlaps)

Improvements to Python utilities for DMC data access and plotting

Numerous DMC-related projects, not discussed here (See Warren's talk)

Many other things, several self-contained, good "student startup" projects

- <u>Current Simulations Topics</u>
- SuperSim Open Issues
- <u>All open e-Logs</u>

Summary and Conclusions

Simulations development is in the "cycle of continuous improvement"

Simulation pipelines are fully operational for large production campaigns

SNOLAB geometry is implemented and up to date with installation as of April

We have completed all of the tasks identified in preparation for Commissioning to begin, and for Simulations to support it

Well integrated with Analysis, Backgrounds, Software and Operations O.6

• On target to achieve the Collaboration's Early Science and Science goals

Extras

Running the Production Pipelines

The packages for both production pipelines are part of the Integrated Software Plan, and are included in Offline Release containers where appropriate

However, each one can only be used at a particular analysis site, because of the customizations required for Slurm job submission and local directory management

Detector Response (SimWorkFlowTools)

Runs on the Grace and Faster clusters at Texas A&M

Environmental Backgrounds (SNOLABBackgroundMacros)

Runs on the Cedar and Niagara clusters of ComputeCanada/DRAC

If you are interested in generating your own samples, or would like to work on modularizing the pipelines to run at additional sites, please contact the Simulations *WG*

Full SNOLAB "Oct24" Geometry





Fridge on a stand