Simulations of the LUX-ZEPLIN (LZ) experiment using Geant4

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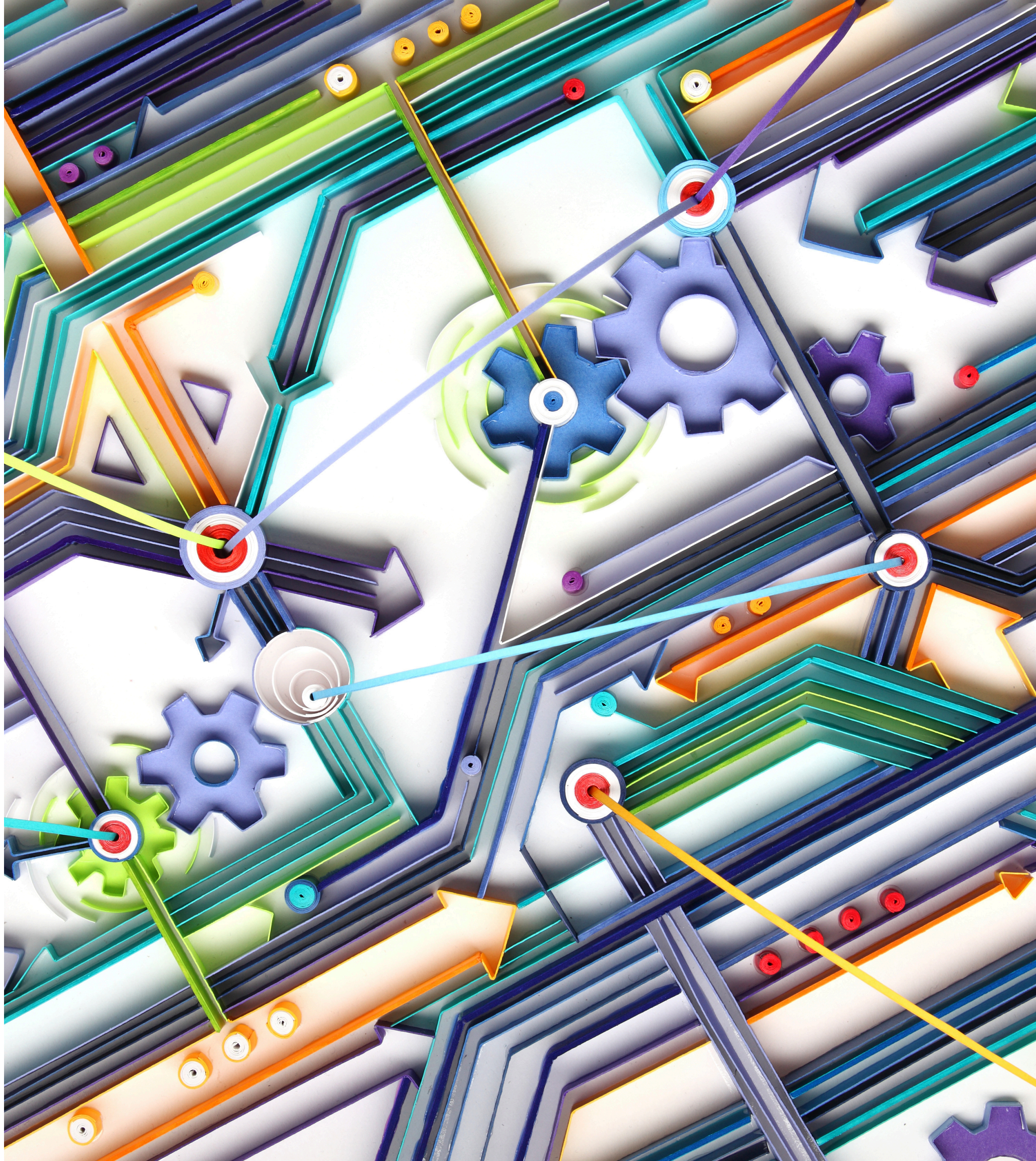
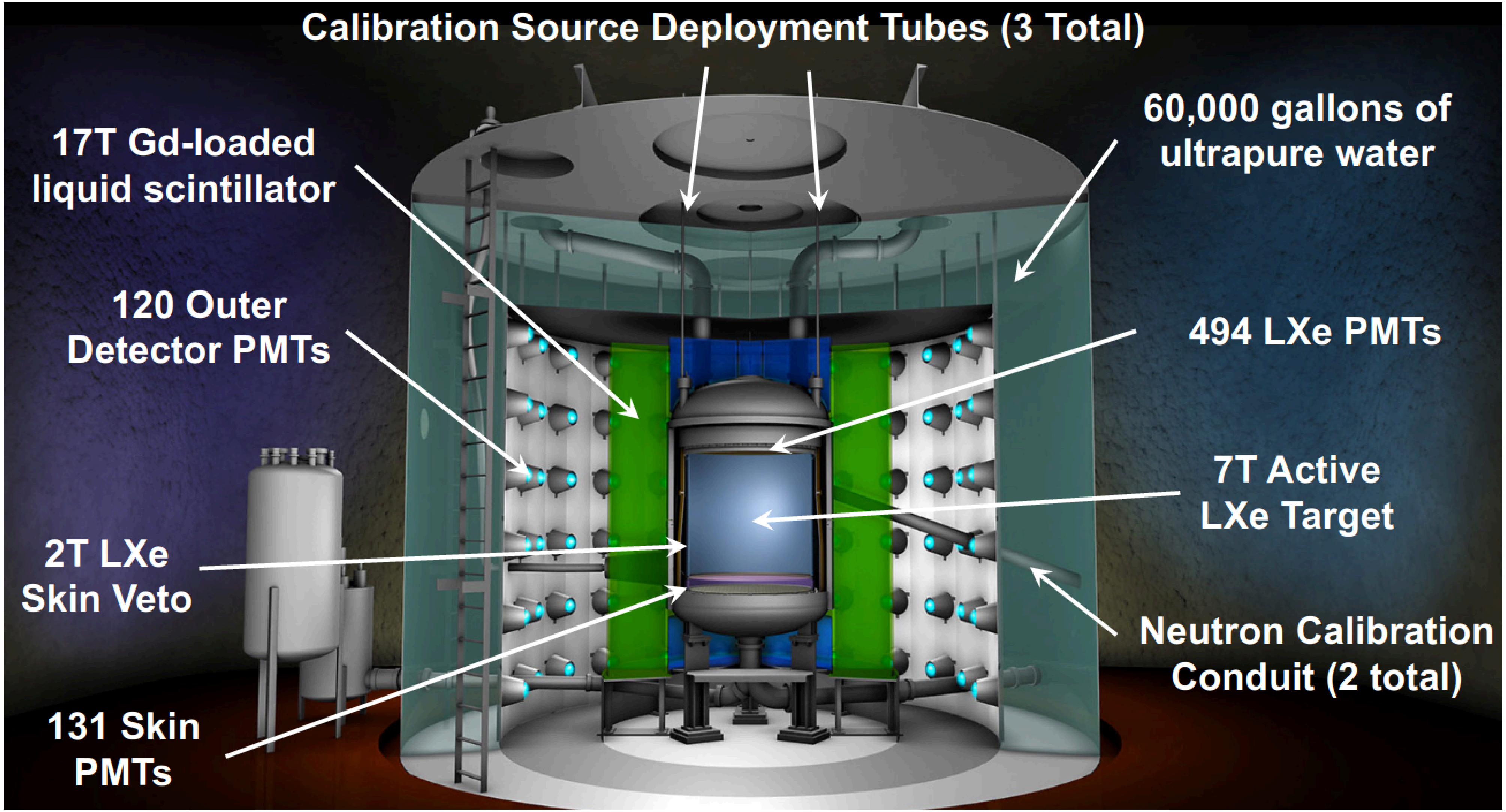
VIEWS

April 2024

LZ simulation paper | Astropart. Phys.125

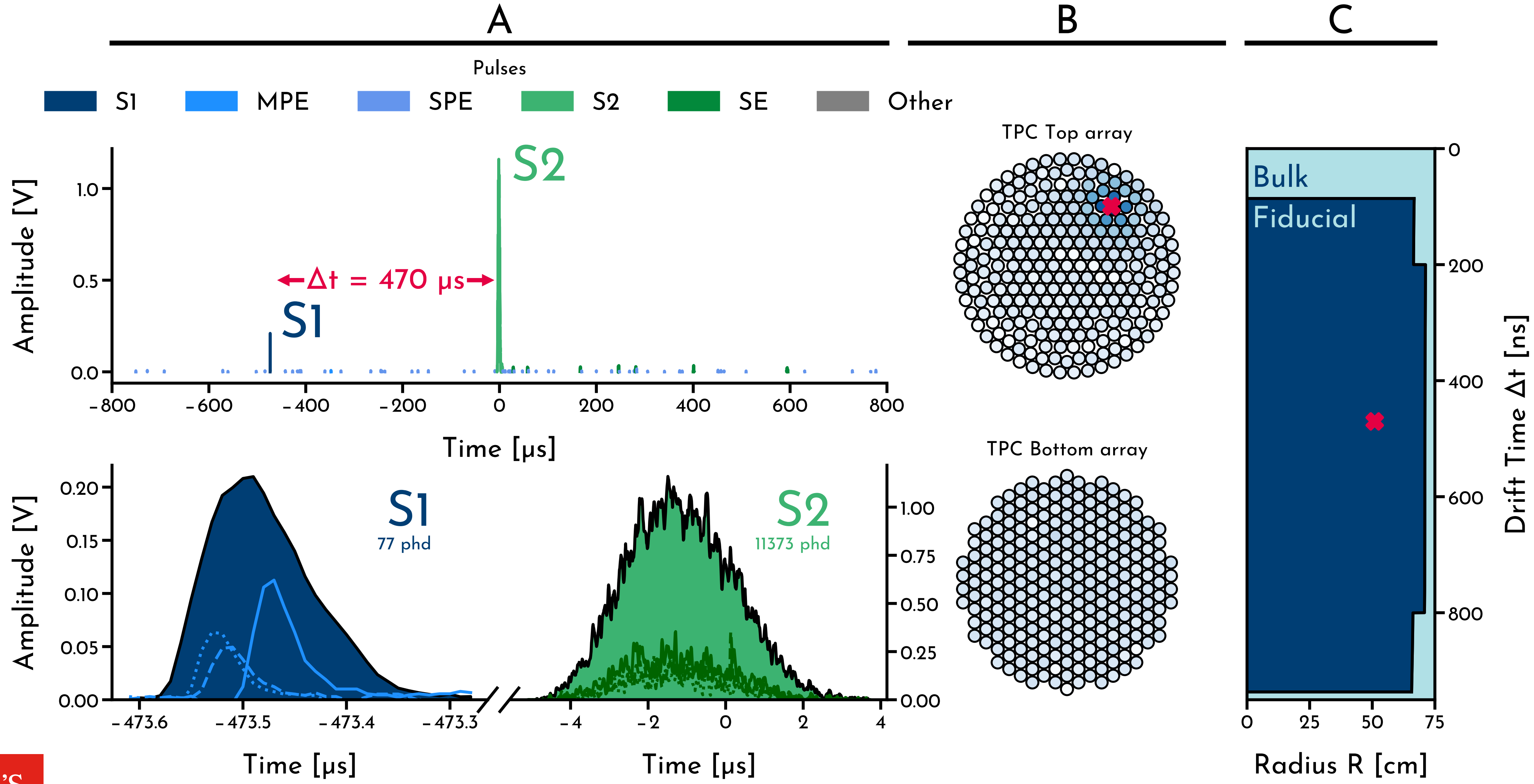


LUX-ZEPLIN



Calibration Source Deployment Tubes (3 Total)
17T Gd-loaded liquid scintillator
120 Outer Detector PMTs
2T LXe Skin Veto
131 Skin PMTs
60,000 gallons of ultrapure water
494 LXe PMTs
7T Active LXe Target
Neutron Calibration Conduit (2 total)

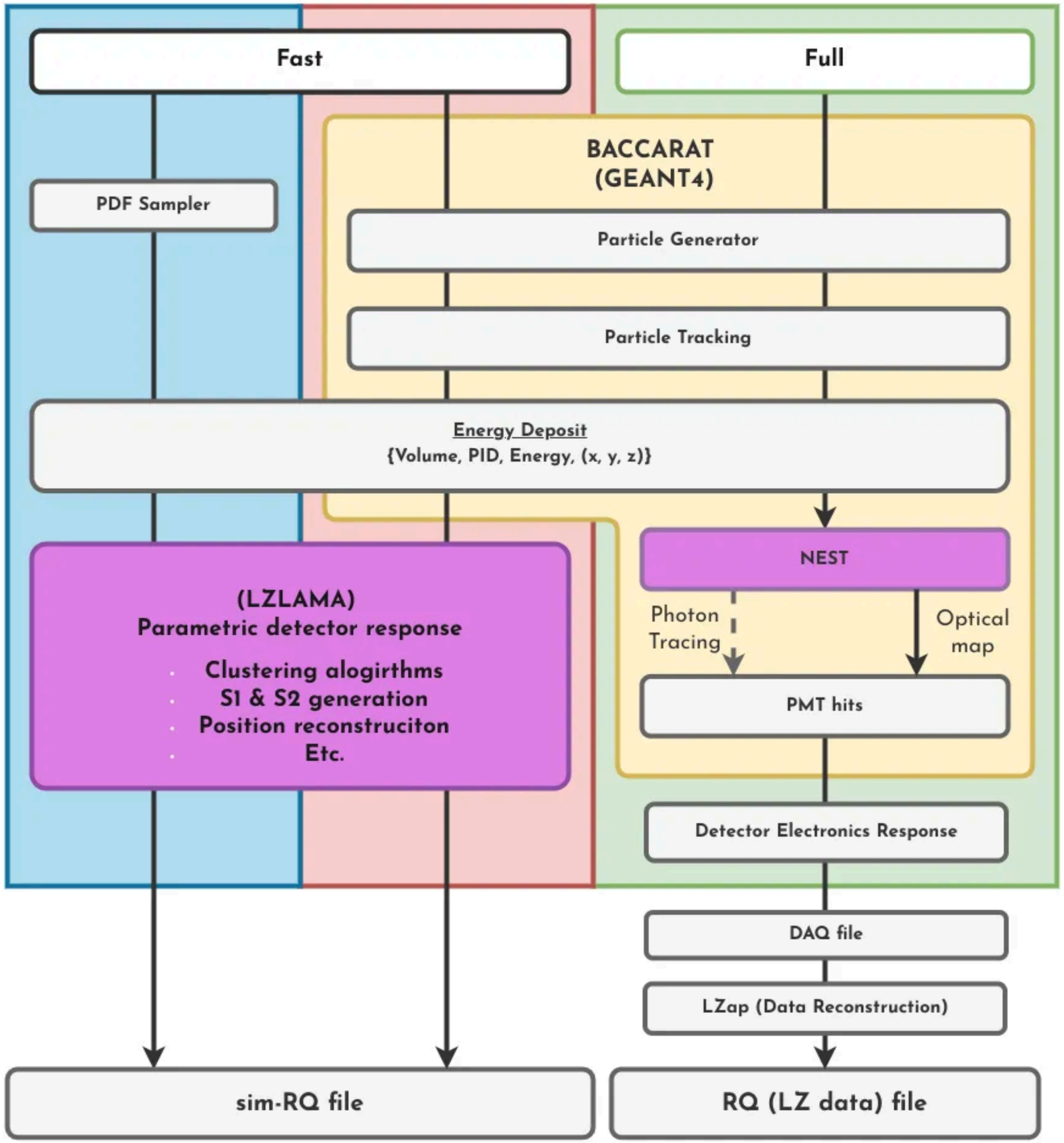
LUX-ZEPLIN



A
B
C
Pulses
S1
MPE
SPE
S2
SE
Other
S2
←Δt = 470 μs→
S1
Amplitude [V]
1.0
0.5
0.0
-800
-600
-400
-200
0
200
400
600
800
Time [μs]
TPC Top array
TPC Bottom array
Bulk
Fiducial
0
200
400
600
800
Drift Time Δt [ns]
0
25
50
75
Radius R [cm]
S1
77 phd
S2
11373 phd
Amplitude [V]
0.20
0.15
0.10
0.05
0.00
-473.6
-473.5
-473.4
-473.3
Time [μs]
1.00
0.75
0.50
0.25
0.00
-4
-2
0
2
4
Time [μs]

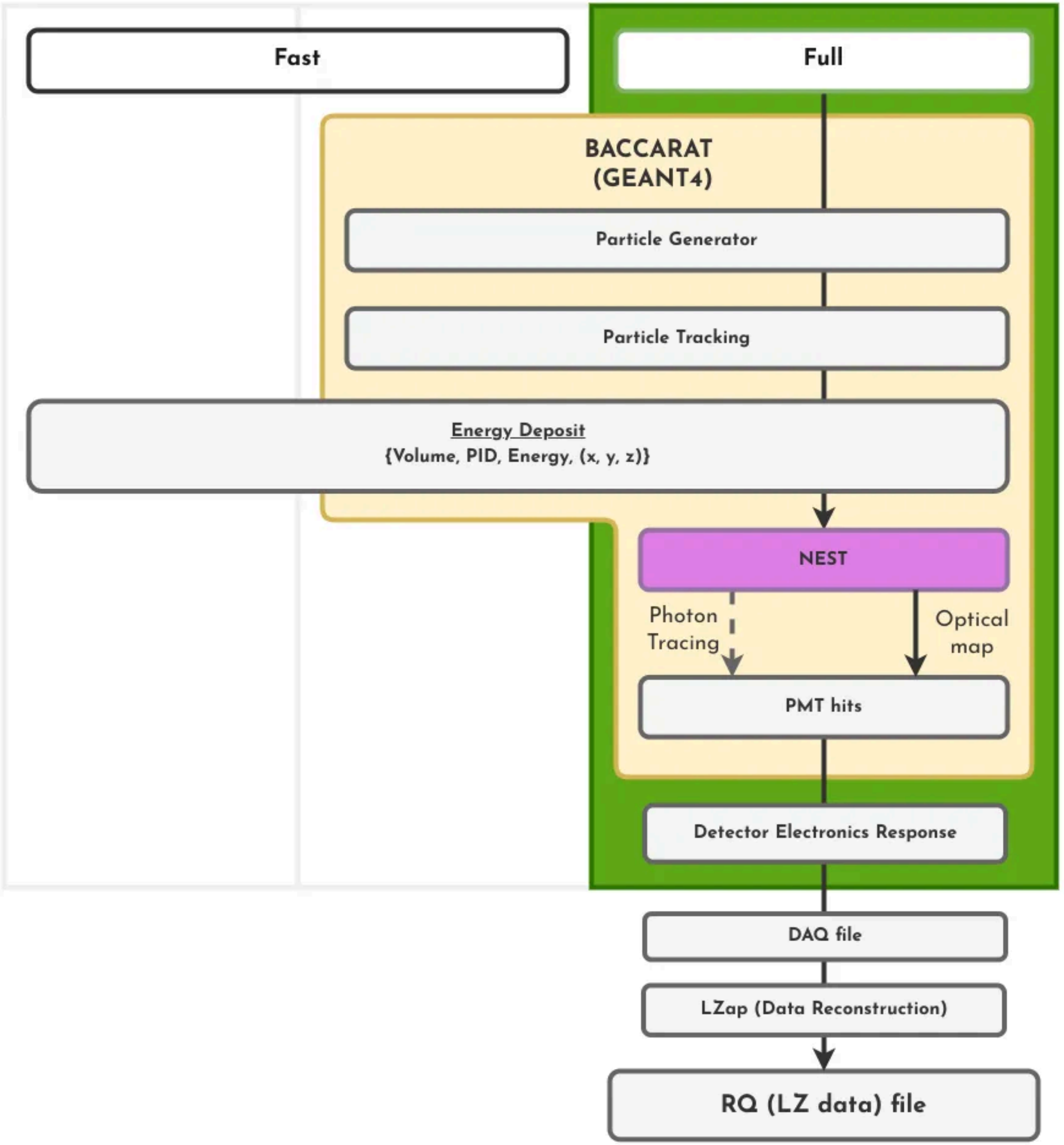
The Simulation Chains

- LZ has two simulations chains
  - Fast
    - < 0.3 s / event
    - Signal and background PDF generation
  - Full
    - 4–50 s / event with photon tracing
    - Least used, for full detector response
- All deployed via gitlab CI/CD
  - Easily support multiple computing environments
  - Uses containers
    - No installing of any software or dependencies
  - User friendly for analysers



Full Chain

- Uses Geant4 to simulate energy deposits
- Ray tracing or map for photon detection
  - Tracing is a bottleneck
  - Exploring GPU tools for this (OPTICKS)
- Detector electronics response (DER) model
  - Pulse and PMT level simulations
- Creates DAQ-like file
  - Treated just like real data
- Used to generate mock data challenges (MDC) prior to detector construction and commissioning
- XLZD have been using BACCARAT for some studies



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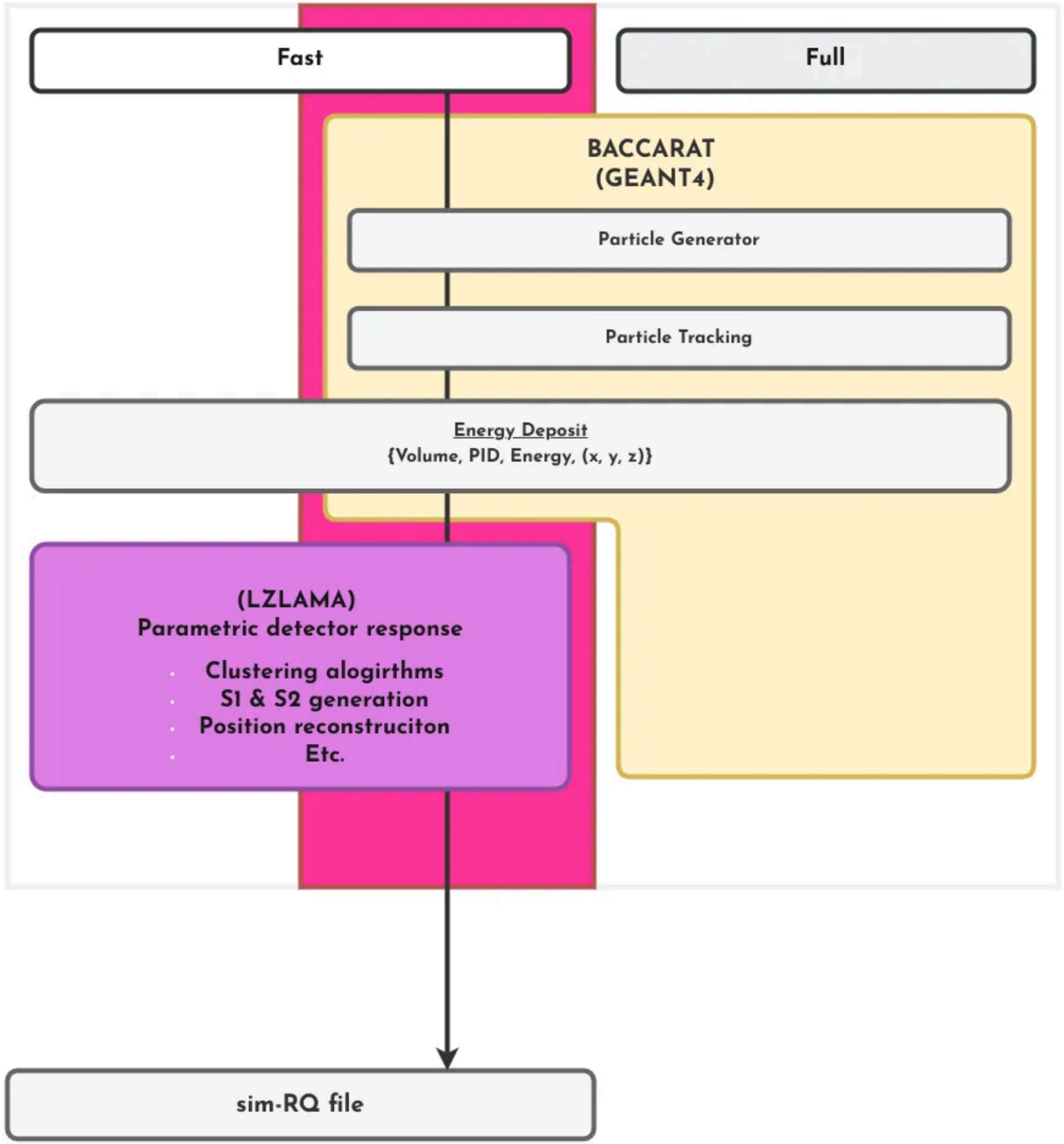
Fast Chain

- Uses Geant4 to simulate energy deposits
- Allows us to use a very flexible detector model (LZLAMA)
  - Generates data similar to LZ data
    - TPC only has scatter info
      - No pulses or PMTs
- Used to make PDFs / templates for statistical tests



Geant4

Options	Value
G4 Version	10.3
Threading	Single only
CXX	C++17
g++	8.2.0

- All deployed via gitlab CI/CD
  - Allows us to build, deploy and test our codebase against multiple Geant4 versions

Physics Lists	Notes
G4EmLivermorePhysics	
G4EmExtraPhysics	
G4RadioactiveDecayPhysics	
QGSP_BIC_HP	Modified Gd neutron capture using DICEBOX Updated thermal neutrons scattering on H in water/GdLS
G4Cherenkov	
G4OpAbsorbtion	Updated absorbtion lengths of LXe/GdLS
G4OpRayleigh	Updated scattering lengths of LXe/GdLS
G4OpBoundaryProcess	
G4OpWLS	
Custom LXe list	Built on NEST

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Thermal Neutron Scattering

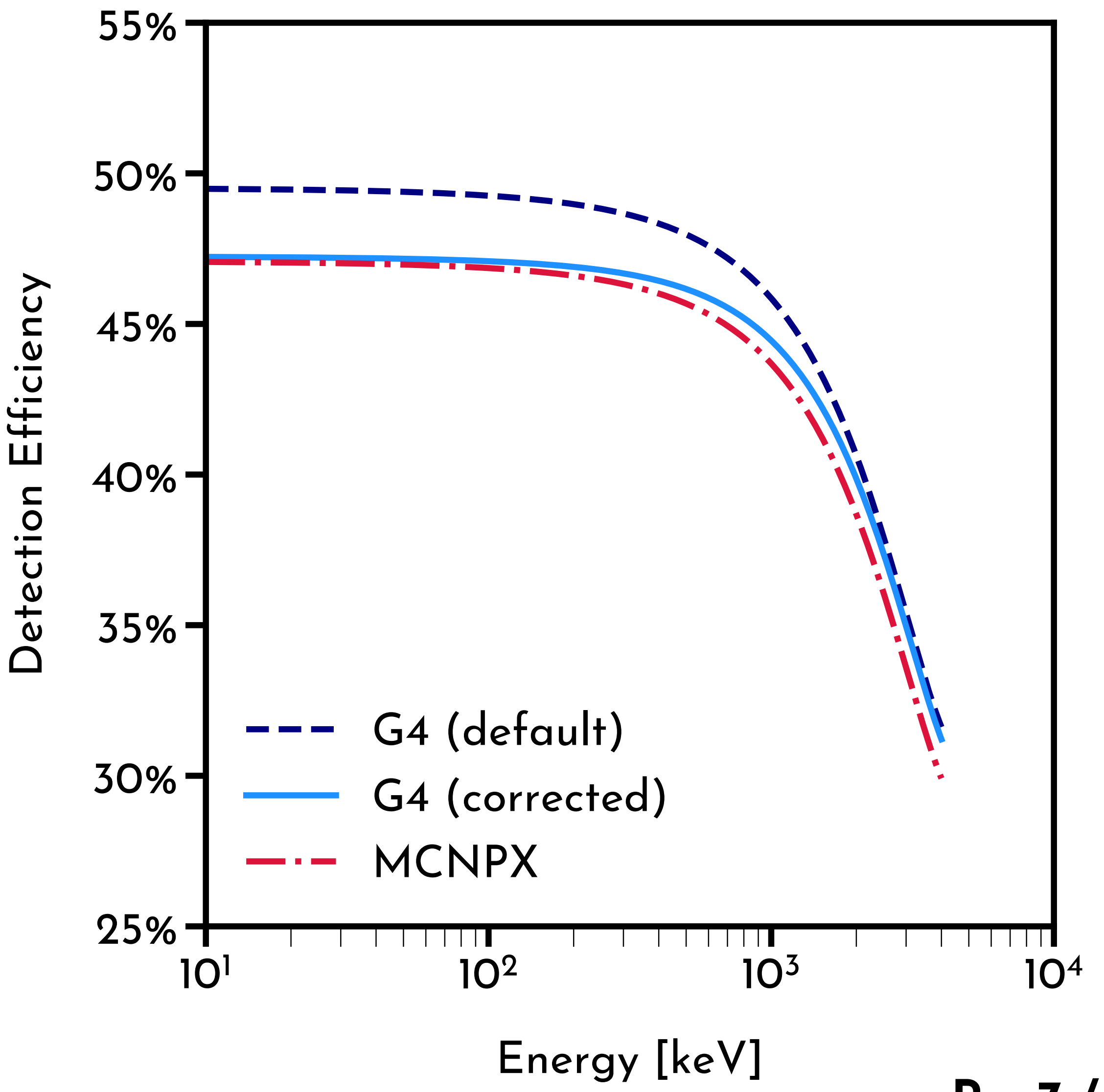
- Using procedure from presentation indico
- Default G4 overestimates detection eff. from neutrons in the OD
  - Wrong neutron (maxwellian) temperature
  - Incorrect interpolation points

```
auto H_PE = new G4Element(
  "TS_H_of_Polyethylene", "h_polyethylene", 1., 1.0079 * g / mole
);
auto H_W = new G4Element(
  "TS_H_of_Water", "h_water", 1., 1.0079 * g / mole
);

auto hel = mainElasticBuilder->GetNeutronProcess();
hel->RegisterMe(hp);
hel->AddDataSet(new G4NeutronHPElasticData());

auto hp = new G4NeutronHPElastic();
hp->SetMinEnergy(4. * eV);

auto thermal = new G4NeutronHPThermalScattering();
            hel->RegisterMe(thermal);
            hel->AddDataSet(new G4NeutronHPThermalScatteringData);
            thermal->SetMaxEnergy(4.0 * eV);
```



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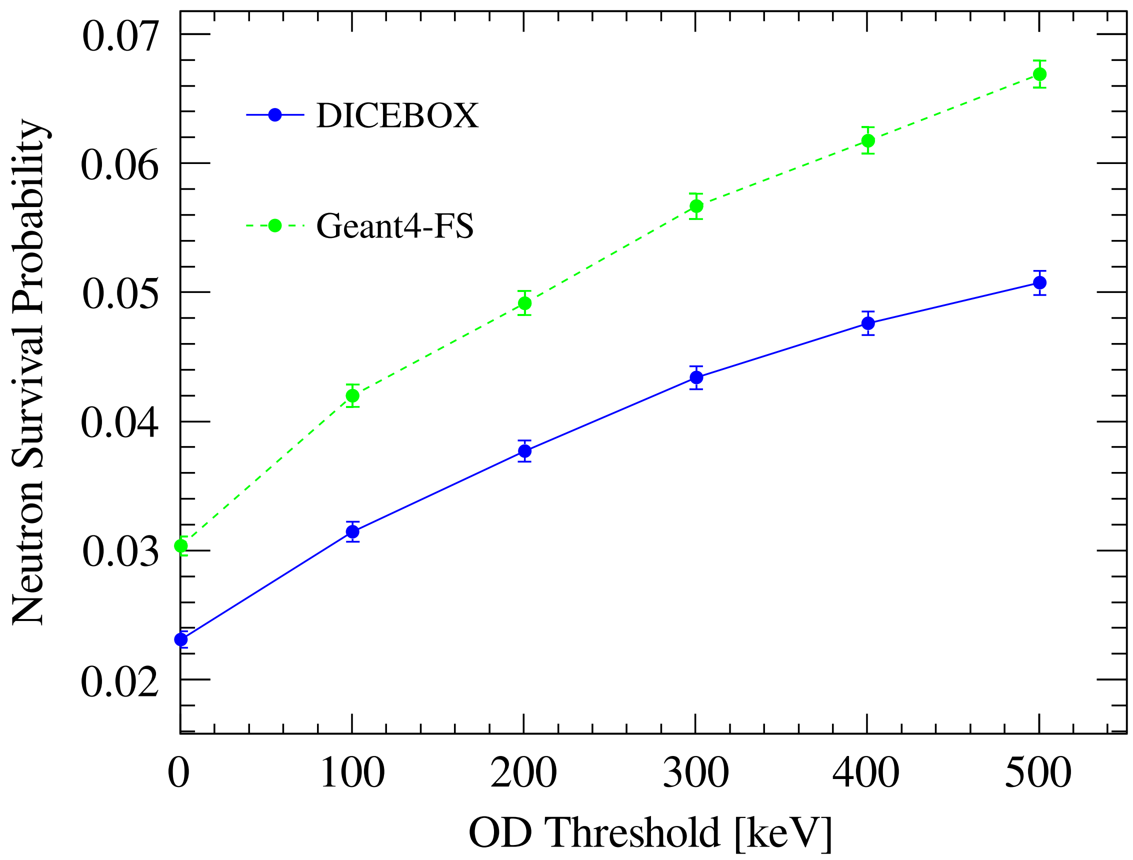
Gd neutron capture using DICEBOX

- LZ's outer detector (OD) it too small to capture all the deposited energy
  - Sensitive to specifics de-excitation processes
  - Larger detectors capture all the energy so do not care how the de-excitation happens
- DICEBOX (NIM-A 417 (2–3) pg. 434-449)
  - Statistical approach to model the γ-cascade
  - Correctly conserves energy
  - Better agreement with data
- Increased simulated veto efficiency from<n *95.1%* → *96.2%*

LZ simulation paper Astropart. Phys.125



Neutron Inelastic Scattering

- Observed discrepancy in inelastic neutron scattering off xenon
- Inelastic scatters can be easily tagged by the high-energy γ-ray
- We are seeing about 1/10th of the rate expected from Geant4
    - Origin of this is unknown

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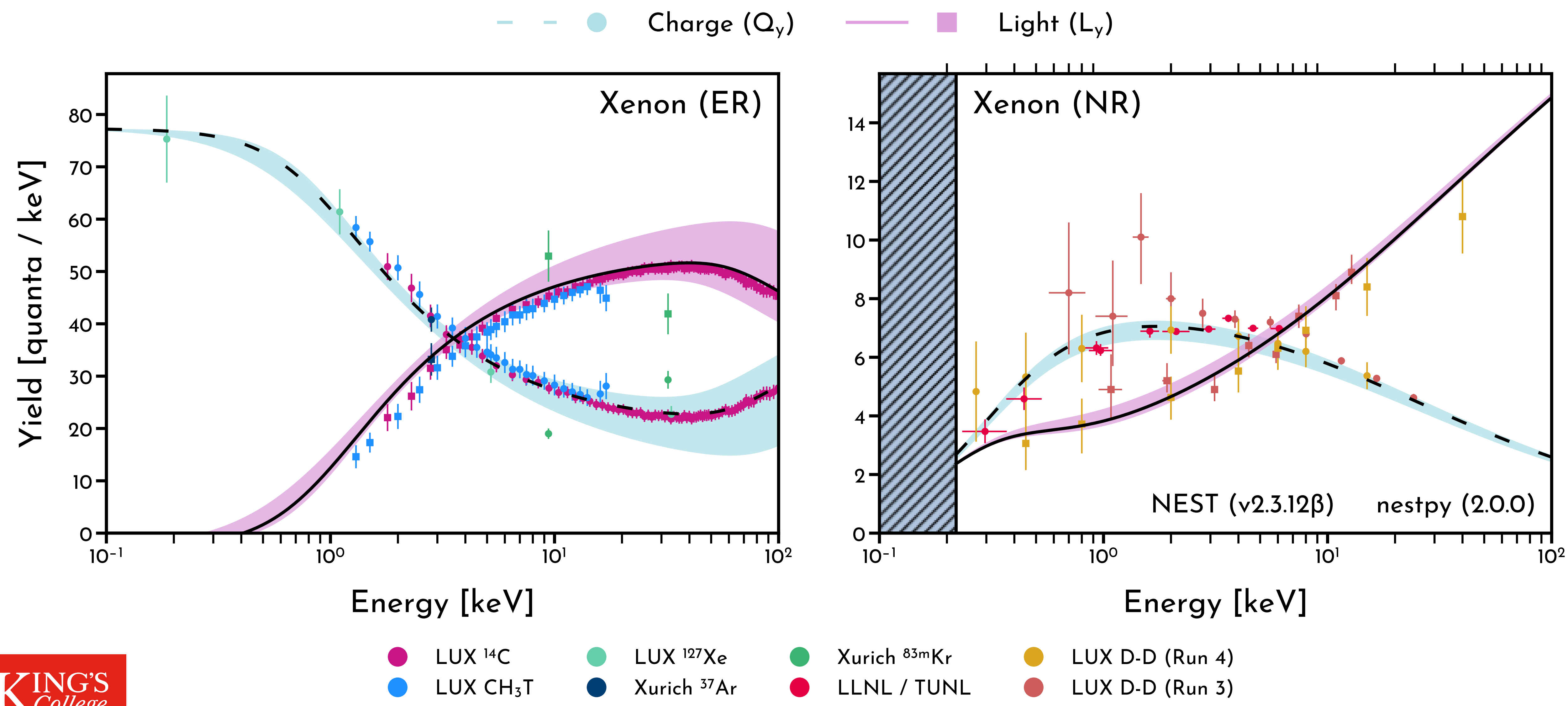
NEST

- Noble Element Simulation Technique
- We are wholly reliant on our xenon yield model
  - Geant4 does not get this right
- Semi-empirical collection of yield models
  - Based on calibration and "science" data from current and previous experiments
- C++ package for generating ER and NR light and charge yields in xenon (& recently argon)
  - Open source (NEST latest, DOI 10.5281/zenodo.8215927)
    - Support from multiple experiments
  - Python bindings available (NESTpy latest, DOI 10.5281/zenodo.10582363)
  - Inbuilt Geant4 interface
    - LZ has written a custom one by subclassing **G4VRestDiscreteProcess**
- Can simulate S1 and S2 observables given a detector model
  - LZ detector model is public: LZ detector model
  - Can even perform basic sensitivity studies

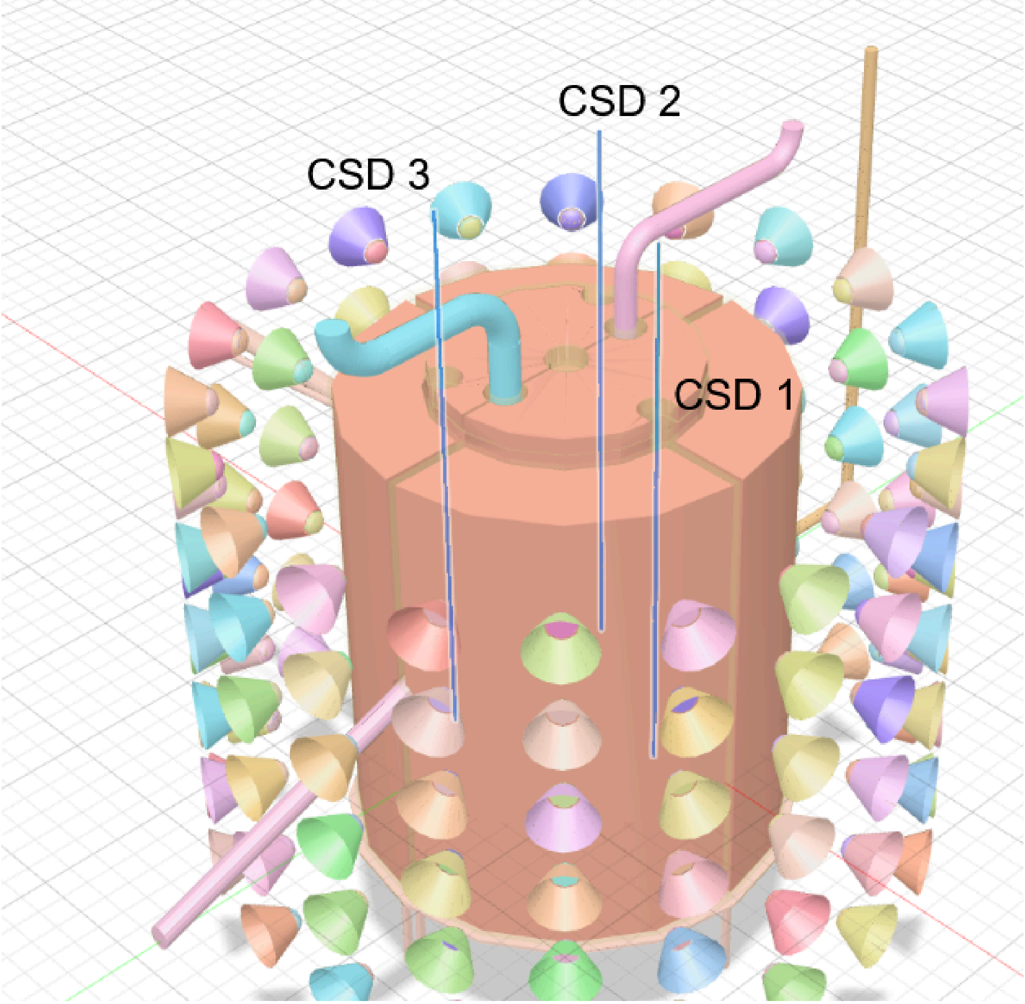
NEST Yields

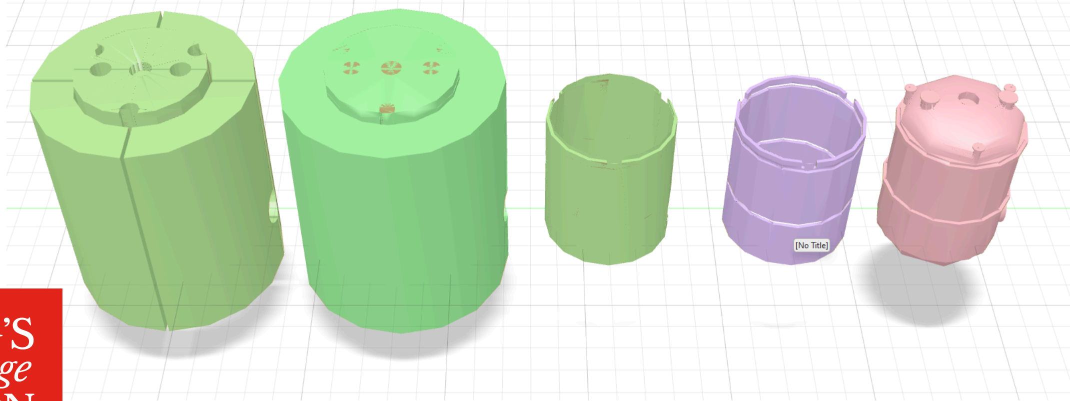


Charge (Q_y)
Light (L_y)
Xenon (ER)
Yield [quanta / keV]
Energy [keV]
Xenon (NR)
NEST (v2.3.12β)
nestpy (2.0.0)
Energy [keV]
LUX ^{14}C
LUX CH_3T
LUX ^{127}Xe
Xurich ^{37}Ar
Xurich ^{83m}Kr
LLNL / TUNL
LUX D-D (Run 4)
LUX D-D (Run 3)

Geometry and validation

- LZ geometry built "by hand"
    - Direct creation of G4Solids, very time-consuming
- Can validate geometry by exporting to *.obj* file via GDML using pyg4ometry
    - pyg4ometry latest, DOI 10.5281/zenodo.10471878
- Can compare G4 model to CAD and as-built designs
    - Should be useful for outreach materials
- XLZD have used pyg4ometry to directly design/control geometry for some Skin/OD models





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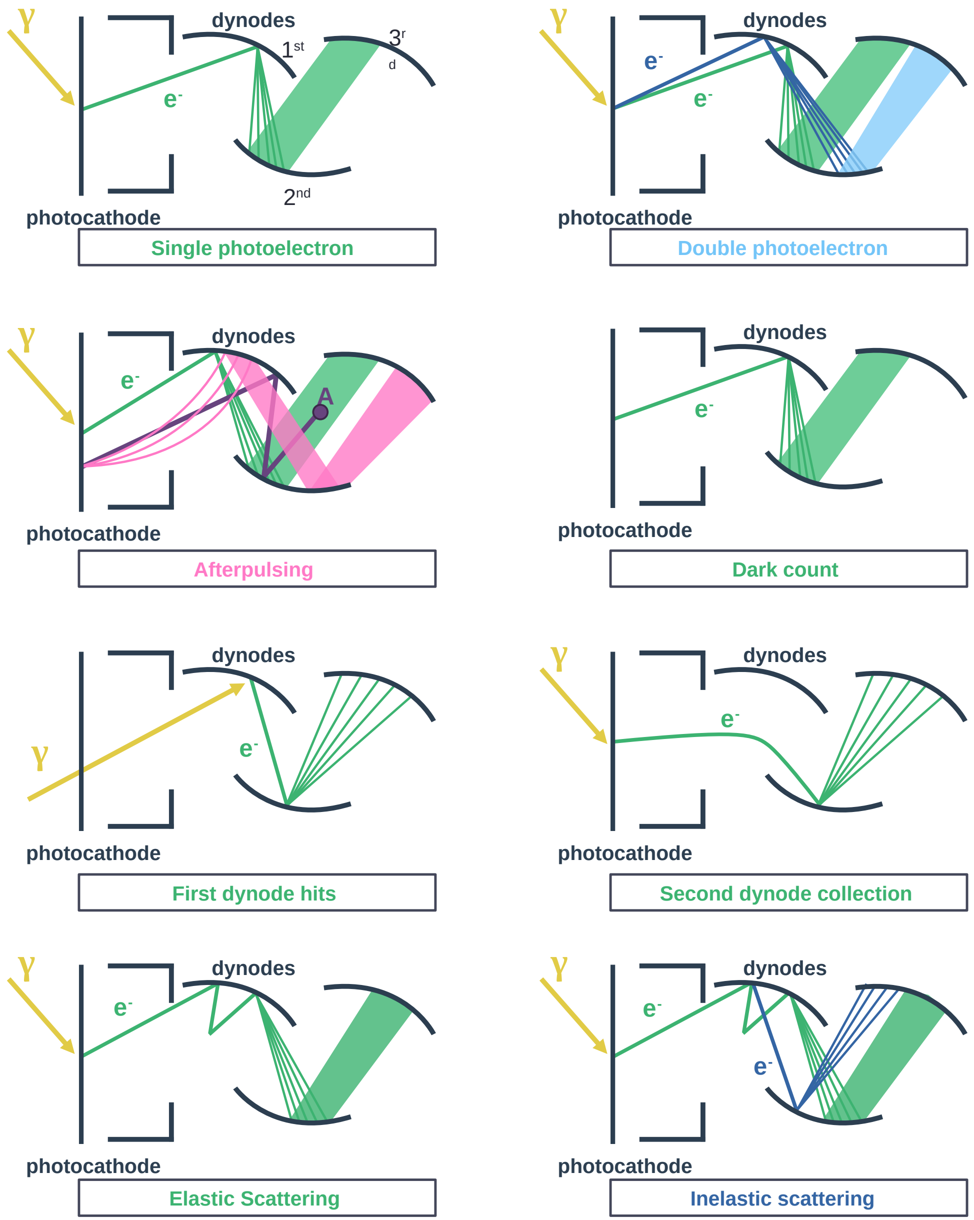
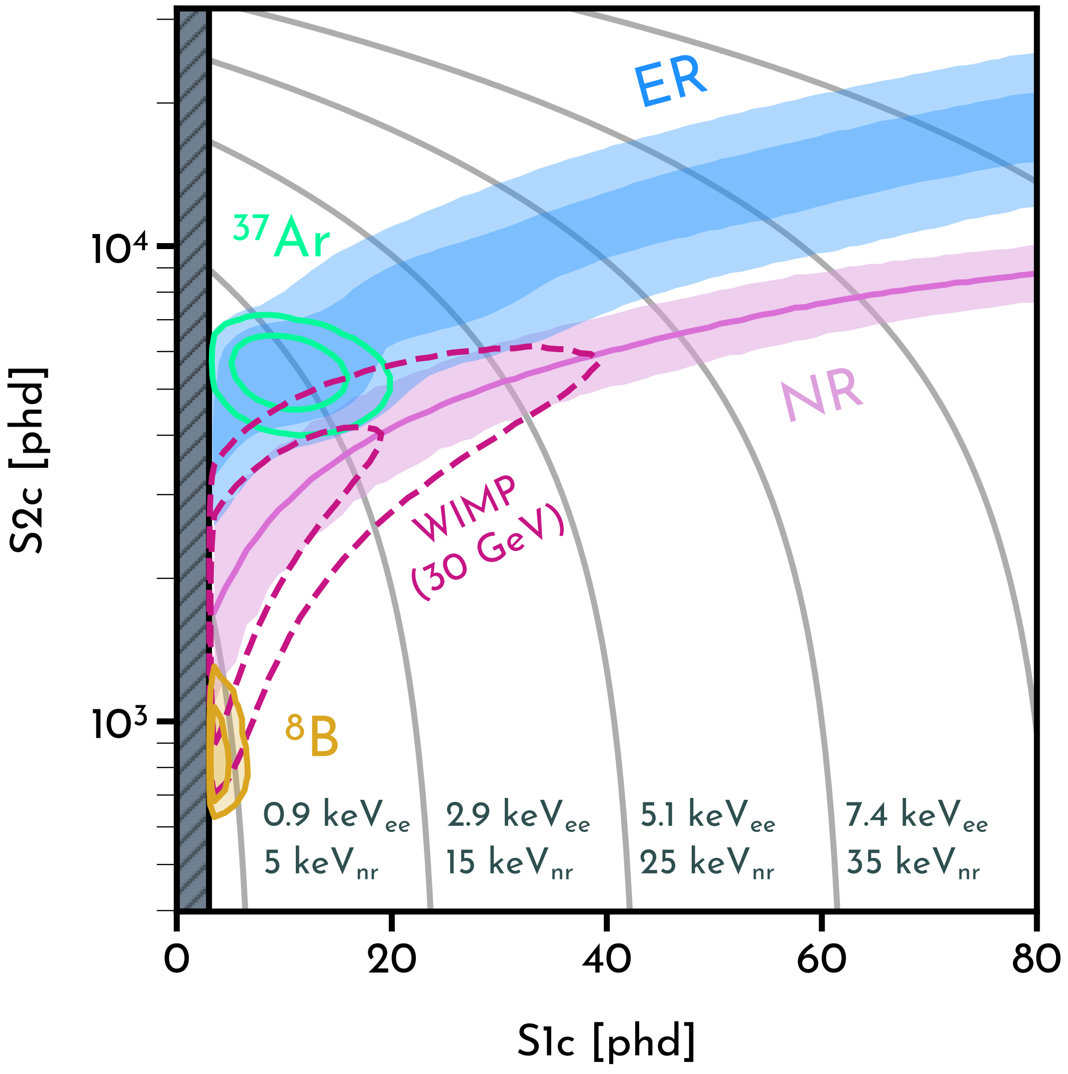
Detector Electronics Response (DER)

- Detector Electronic Response
  - Converts PMT hits into waveforms
  - Accounts for several PMT detection mechanisms
    - SPE
    - DPE
- Outputs raw-data format
  - Can be processed like real data
  - Used to produce large mock data challenge (MDC) datasets



LZLAMA

- A customisable NEST interface
- Very flexible to tune detector modeling
  - Correction maps
  - E-field maps
  - Clustering
  - NEST parameters
- Produces a subset of the detected variables:
  - limited to scatter level quantities
    - S1, S2, (x, y, z) etc.
- Used to generate S1–S2 PDFs for PLR analysis



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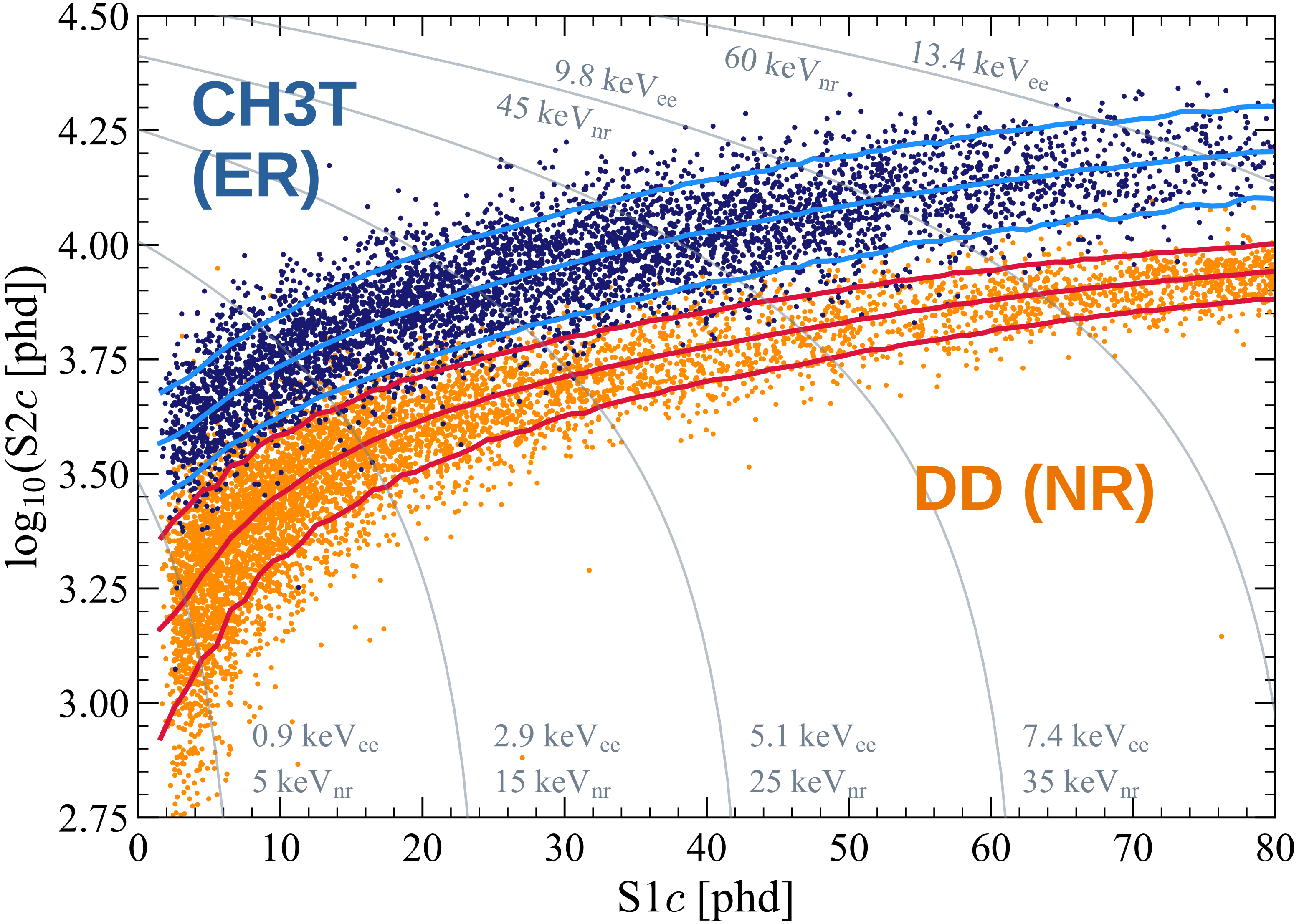
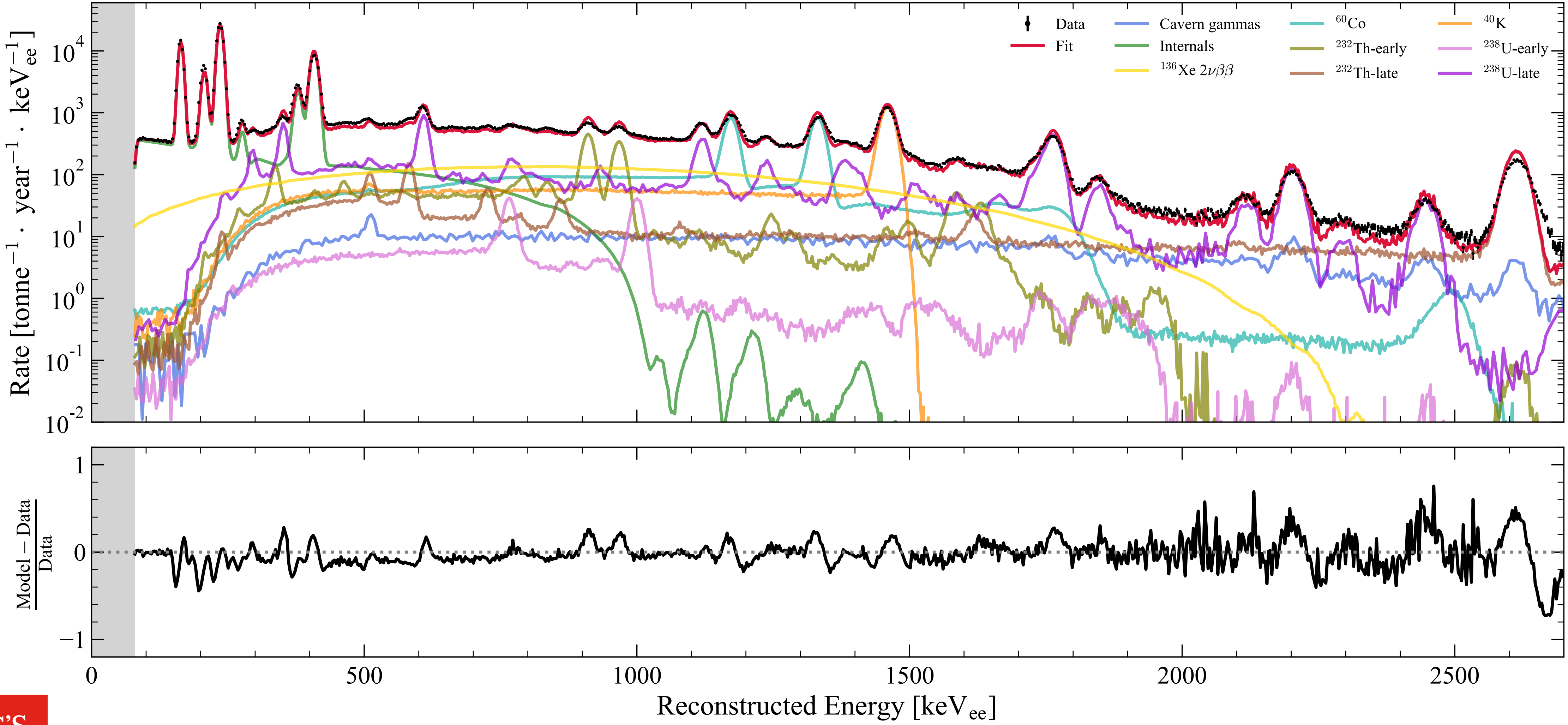
Calibration

LZ SR1 paper Phys. Rev. Lett. 131, 041002



Background Model

LZ simulation paper | Phys. Rev. D 108 012010



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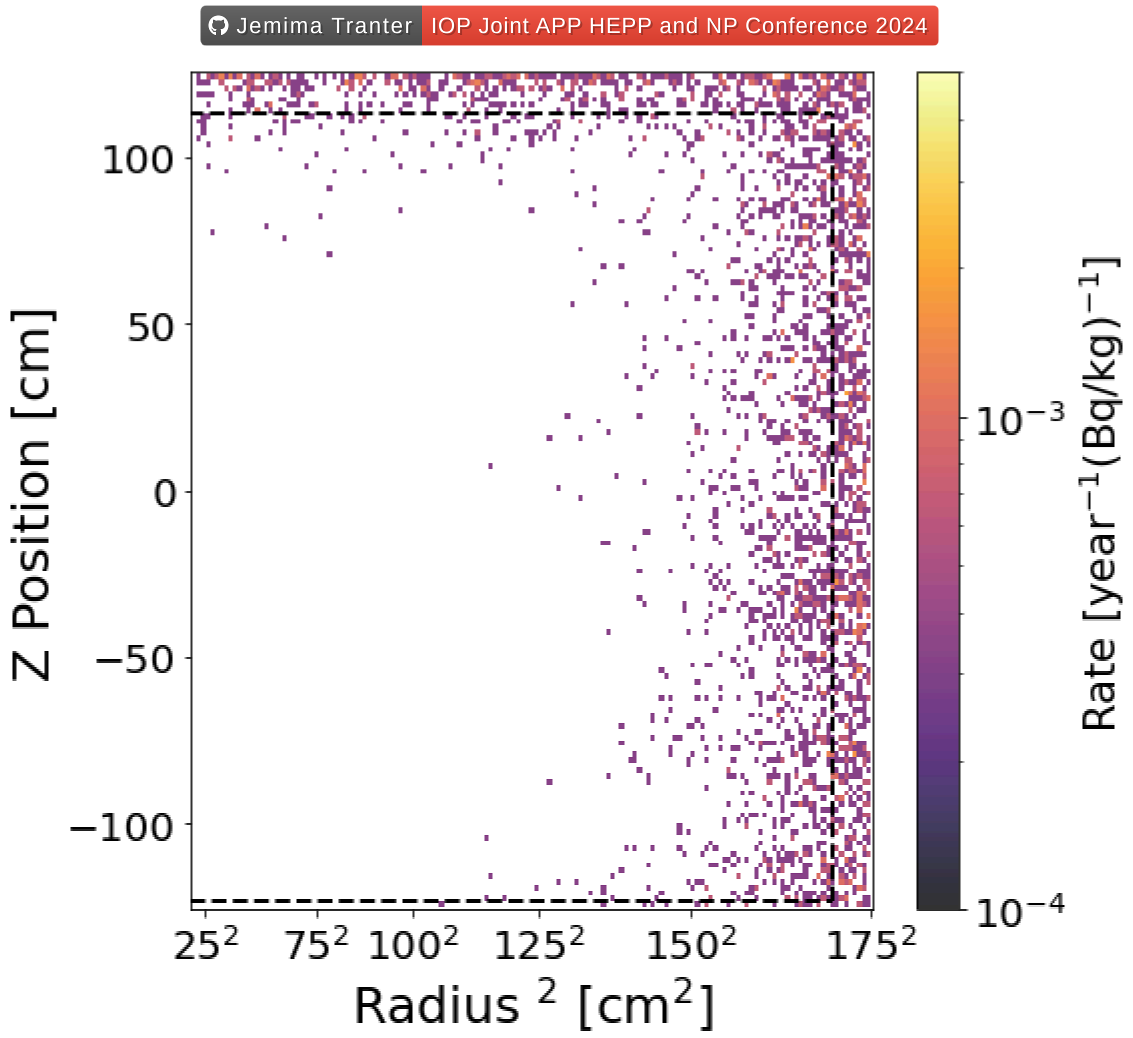
Shielded Detectors

- These shielded detectors minimise external backgrounds
  - Particularly γ-rays
  - Makes it much harder to simulate the central volume
- In LZ this is already a problem
  - $\sim 10^{-9}$ of events reach TPC (post-cuts)
- Will be lower in XLZD's proposed O(60 t) detector
  - $\sim 10^{-12}$ of events reach TPC (post-cuts)
- Current method:
  - Resample good tracks at detector boundaries



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Conclusion

- LZ can simulate at parametric and full detector electronics (PMT) levels
  - Parametric uses a NEST interface and used to produce PDFs for statistical analysis
  - Full detector creates DAQ-like files compatible with full LZ data processing
    - This was used to create mock datasets prior to commissioning
- We use a custom set of xenon yield functions using NEST
- We use a custom Gd neutron capture model using the DICEBOX algorithm
  - Increased simulated veto efficiency: 95.1% → 96.2%
- Have been making use of pyg4ometry to validate and build geometry
- Simulating such shielded detectors can be difficult
  - 1 in a billion simulated γ-ray events are interesting

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Acknowledgements

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38 Institutions, 250 scientists, engineers, and technical staff

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- Lawrence Livermore National Lab.
- LIP Coimbra
- Northwestern University
- Pennsylvania State University
- Royal Holloway University of London
- SLAC National Accelerator Lab.
- South Dakota School of Mines & Tech
- South Dakota Science & Technology Authority
- STFC Rutherford Appleton Lab.
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