FlameNEST: powerful statistical inference for the LZ and XLZD experiments

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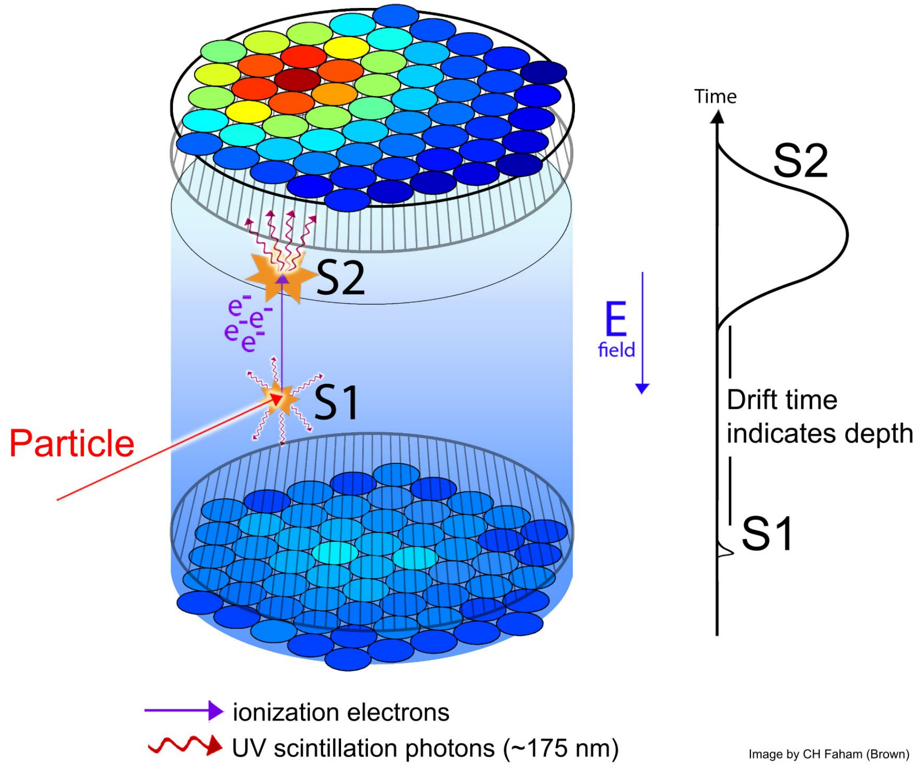
ARC CDM Annual Workshop 2023, Adelaide

Part I

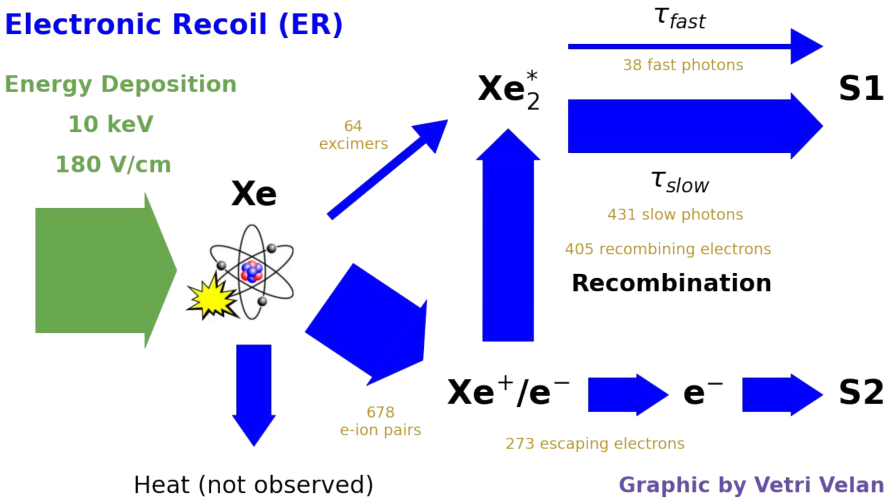
FlameNEST

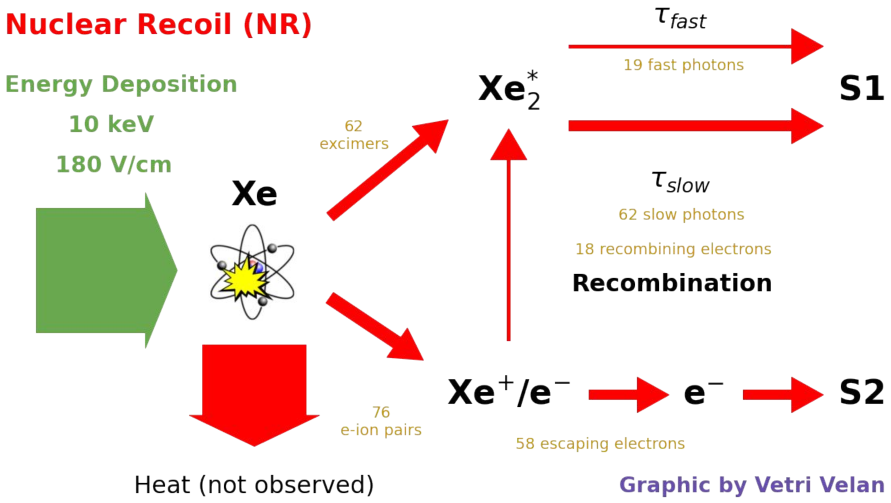
Direct detection with noble element TPCs



- Dual phase liquid xenon time projection chambers: leading technology for WIMP dark matter detection
- Particle interactions in the LXe → prompt scintillation photons (S1 signal) and ionisation electrons
- Ionisation electrons swept up by applied electric field, extracted into gaseous xenon → electroluminescence → delayed ionisation photons (S2 signal)
- Time difference between S1 and S2 allows z-position reconstruction
- S2 PMT hit pattern (top) allows for (x,y)-position reconstruction

Signal/background discrimination

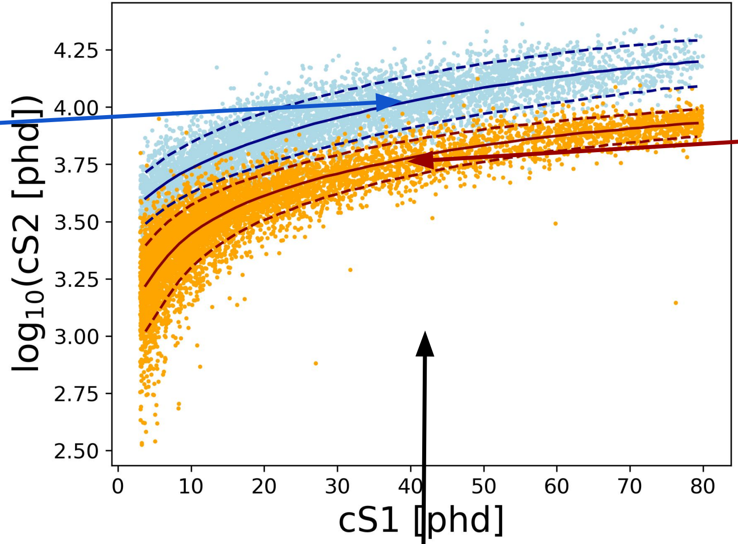




Signal/background discrimination

ER events

- Neutrino-electron scattering (pp, CNO, ^{7}Be solar neutrinos)
- β-decays (^{214}Pb, ^{212}Pb, ^{85}Kr from Rn plate-out, dust and contamination)
- ^{124}Xe / ^{136}Xe decay (2ν DEC / $2\nu\beta\beta$ decay)
- γ-decays from detector materials and rock → ‘detector ER’



NR events

- Coherent elastic neutrino-nucleus scattering (^{8}B + hep solar neutrinos, atmospheric neutrinos, DSNB neutrinos)
- Neutron scattering (^{238}U spontaneous fission, (α,n) reactions on light nuclei) → ‘detector NR’

Other events

- Accidental S1/S2 coincidences → ‘accidentals’
- Decays in the PTFE wall of the TPC (charge loss → ER background shifted to NR band)

Enhancing signal/background discrimination

z spatial variation

- Finite electron lifetime → larger S2s at the top of the detector
- Reflections at the liquid/gas interface → larger S1s at the bottom of the detector
- Distinguishing top/bottom improves ER/NR discrimination

(x,y) spatial variation

- Certain backgrounds concentrated towards the edges of the detector (source distribution geometry, veto effects)
- Light collection variation across the PMT arrays
- Accounting for radial variation improves background discrimination

Temporal variation

- Galactic dark matter, solar neutrino event rates experience (different) annual modulations
- Certain backgrounds decay over time
- Temporal variation in detector conditions
- Time-dependent modelling can improve dark matter sensitivity

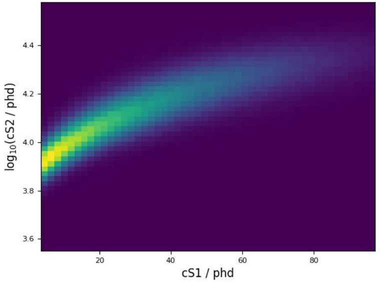
$$\mathrm{cS1} := \mathrm{S1}\frac{G_1(0,0,z_c)}{G_1(x,y,z)}$$

$$\mathrm{cS2} := \mathrm{S2}\frac{G_1^{\mathrm{gas}}(0,0)}{G_1^{\mathrm{gas}}(x,y)}e^{t_{\mathrm{drift}}/\tau_e}$$

Shape-varying nuisance parameters

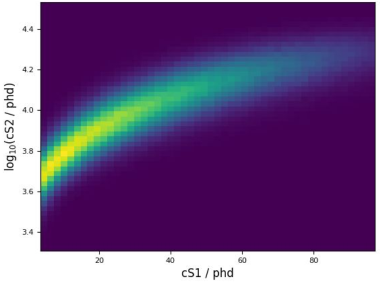
$$\mathrm{Q}_y(E,\mathcal{E},\rho) = m_1(\mathcal{E},\rho) + \frac{m_2 - m_1(\mathcal{E},\rho)}{[1+(\frac{E}{m_3})^{m_4}]^{m_9}} + m_5 + \frac{-m_5}{[1+(\frac{E}{m_7(\mathcal{E})})^{m_8}]^{m_{10}}}$$

$\langle m_2 \rangle + 1\sigma$



template for each m_2

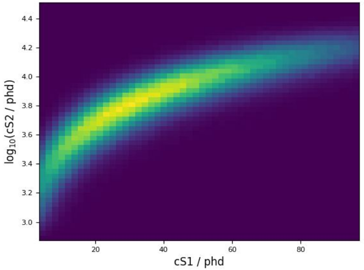
$\langle m_2 \rangle$



...

template for each m_5

$\langle m_2 \rangle - 1\sigma$



LZ CH_3T: simulation

The likelihood for rare event searches

$$\ln(L) = -\nu(\vec{\theta}) + \sum_e \ln\left(\sum_j R_j(\vec{d}_e; \vec{\theta})\right) + \sum_k \mathcal{C}_k(\vec{\theta})$$

(remnant of) Poisson term

'shape term':
differential rate

ancillary constraints

The goal:

utilise full
observable space

$$\vec{d} = \{\mathrm{cS1}, \mathrm{cS2}\}$$

$$\vec{d} = \{\mathrm{S1}, \mathrm{S2}, x, y, z, t\}$$

include
shape-varying
nuisance
parameters

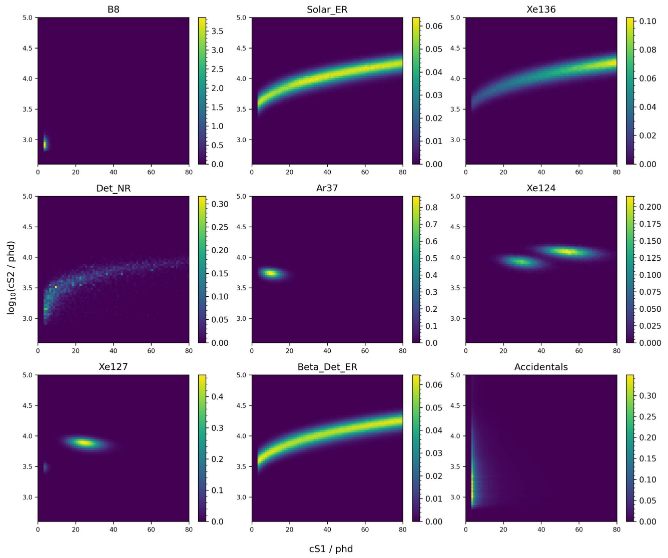
- Important where model uncertainties are large
- Important if a discovery claim were to be made

Likelihood evaluation with templates

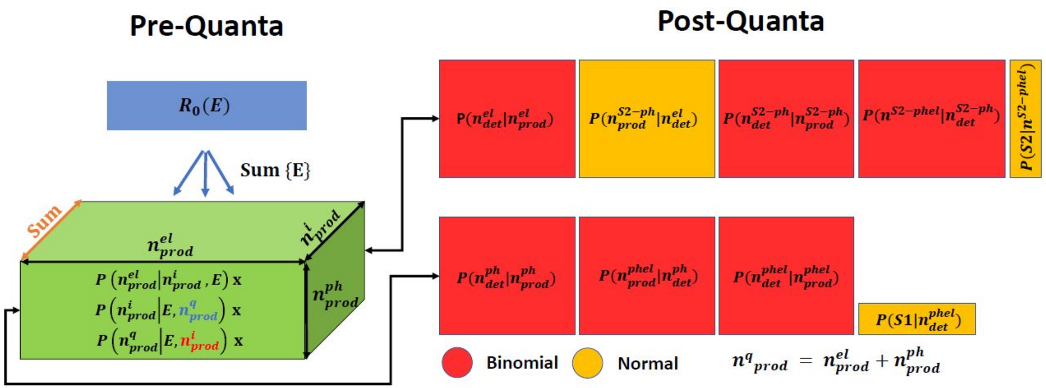
easy — difficult — easy

$$\ln(L) = -\nu(\vec{\theta}) + \sum_{e} \ln\left(\sum_{j} R_j(\vec{d}_e; \vec{\theta})\right) + \sum_{k} \mathcal{C}_k(\vec{\theta})$$

- Traditional method: Monte Carlo simulation for signal/background sources, fill histogram (template) with MC events, use to approximate differential rates
- Generation time for templates scales exponentially as dimensionality of observable space is increased
- Generation time for templates scales exponentially as additional correlated shape-varying nuisance parameters are added
- **Benchmark:** 6D observable space for one WIMP mass (80 S1/S2 bins, 10 spatial/temporal bins) would take 35,000 CPU minutes (LZ)



FlameNEST: analytic likelihood evaluation



- Analytic probability elements convolved together in single tensorflow multiplication
- Automatic differentiation → gradients + Hessian → vastly improved likelihood maximisation
- No scaling with 2D → 6D observable space
- Linear scaling with additional nuisance parameters
- State of the art NEST (Noble Element Simulation Technique) models included

this is our differential rate

photon yield - > S1 detector response

energy -> electron/photon yields

electron yield - > S2 detector response

$$\sum_{E,e,\gamma,i,j,k,l,m,n,\dots} \overbrace{P(S1|i)P(i|j)P(j|\dots)\dots P(k|\gamma)}^{\text{photon yield -> S1 detector response}}\overbrace{P(e,\gamma|E)R^j(E)}^{\text{energy -> electron/photon yields}}\overbrace{P(l|e)\dots P(m|\dots)P(n|m)P(S2|n)}^{\text{electron yield -> S2 detector response}},$$

Code availability, outlook

- Now being used by the LZ collaboration for all statistical inference for the LZ experiment

- Work within the XENONnT collaboration towards utilising for inference

flamedisx paper: J. Aalbers et al. "Finding dark matter faster with explicit profile likelihoods". *Physical Review D* **102** 072010 (2020)

FlameNEST paper: R. S. James et al. "FlameNEST: explicit profile likelihoods with the Noble Element Simulation Technique". *Journal of Instrumentation* **17** P08012 (2022)

Code repository: github.com/FlamTeam/flamedisx

- Beginning to be used within the XLZD consortium for sensitivity studies

- Now have O(10) people actively working on development across the two collaborations

- Work in LZ towards further speed optimisations, incorporation of more complex detector effects, higher-order asymptotic inference

Part II

Applications to LZ

The LUX-ZEPLIN experiment

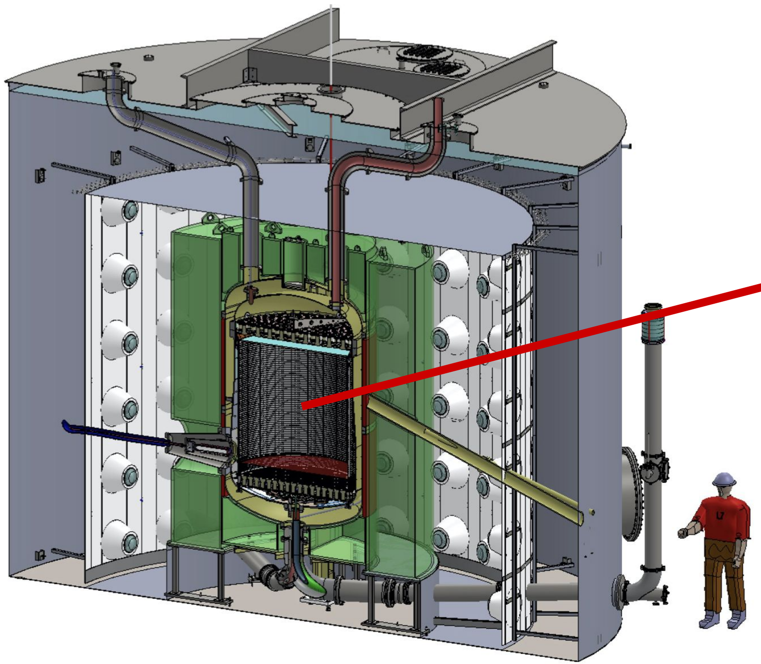
- More than 250 collaborators spread across 4 continents, 5 countries, 37 institutions

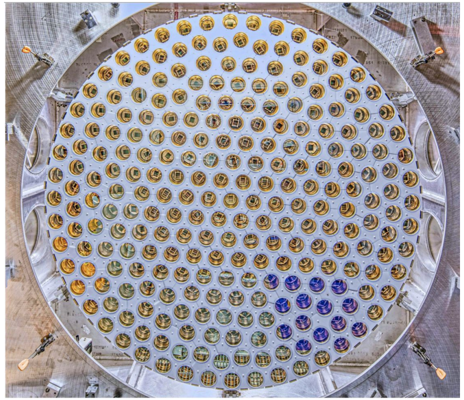
- Located 1 mile underground at the Sanford Underground Research Facility, Lead, SD, USA

- First science results released in 2022. Engineering run to demonstrate detector performance, also set current world-leading WIMP constraints

- Currently running in discovery mode, collecting data over a much higher exposure, next results expected in 2024

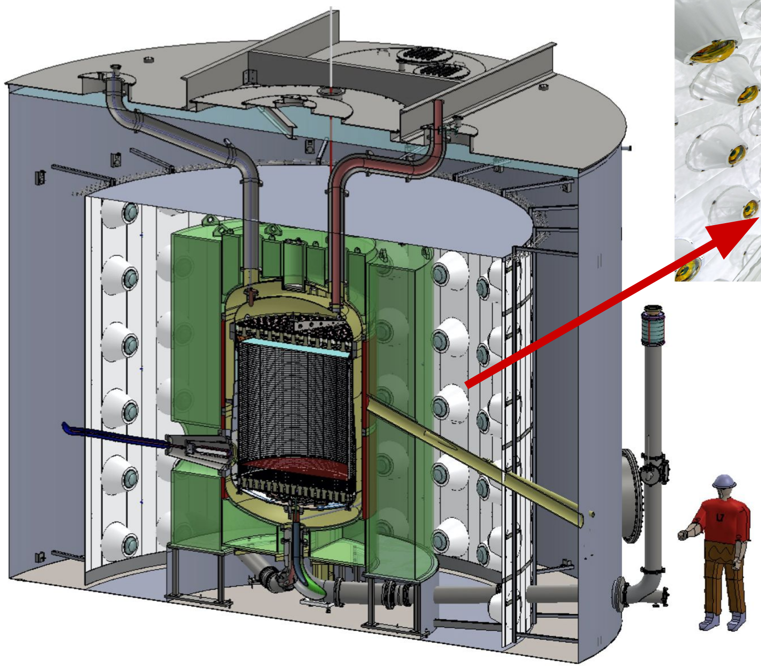
The LUX-ZEPLIN experiment: TPC

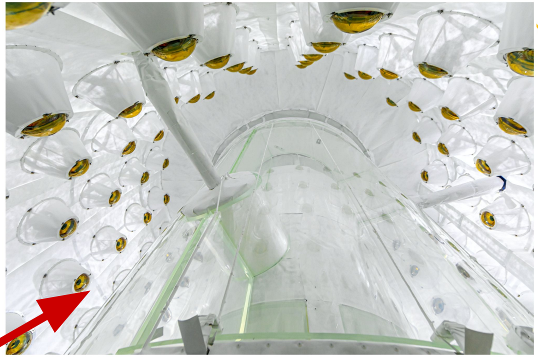


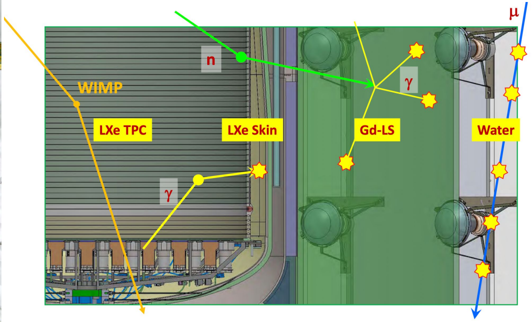


- 7 t active liquid xenon volume
- 494 Hamamatsu R11410 PMTs across two arrays
- Four grids maintaining drift field, extraction field, reverse field region

The LUX-ZEPLIN experiment: veto systems







- **Skin region:** 2 t additional liquid xenon, optically decoupled
- Primarily acts as a γ-ray veto

- **Outer detector:** 10 acrylic tanks filled with GdLS, imaged with 120 Hamamatsu R5912 PMTs
- Primarily acts to veto neutron backgrounds

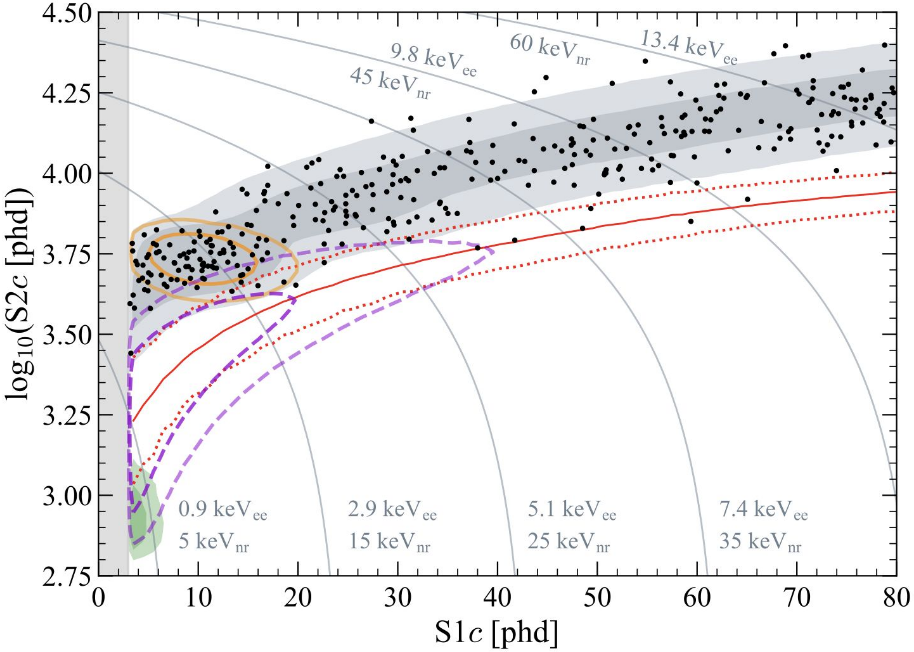
SR1: run parameters

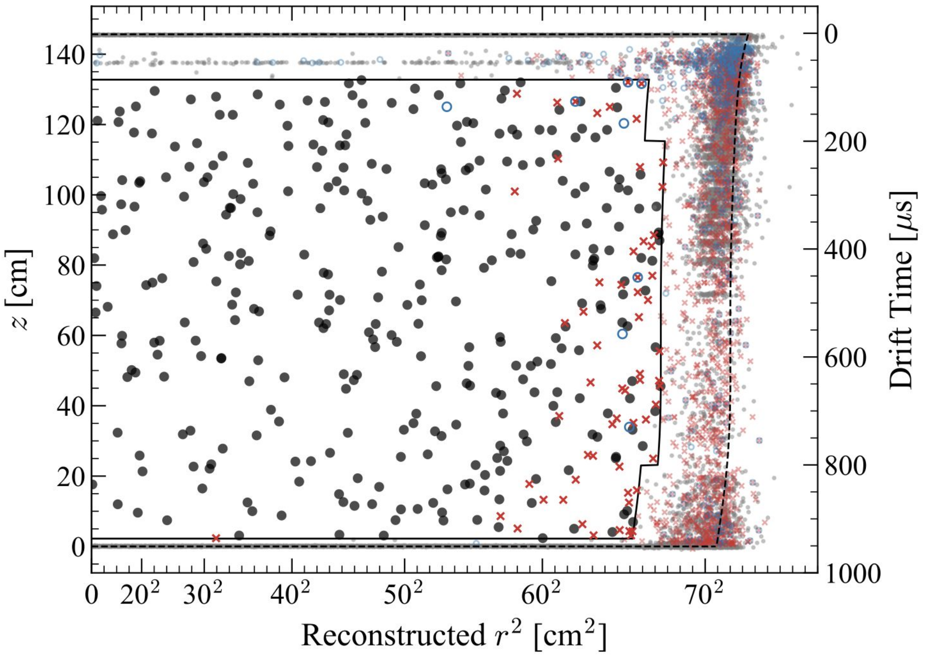
- S2-triggered data acquired between 23rd December 2021 - 11th May 2022

- Cuts applied
  - Veto
  - Fiducial volume
  - Livetime
  - Region of interest
  - Data quality
- After cuts, 335 events observed within a 5.5 t fiducial volume and 60 day total livetime

- Stable detector conditions throughout: 173.1 K temperature, 1.79 bar pressure, 193 V / cm drift field, 7.3 kV / cm extraction field

LZ SR1 WIMP search data



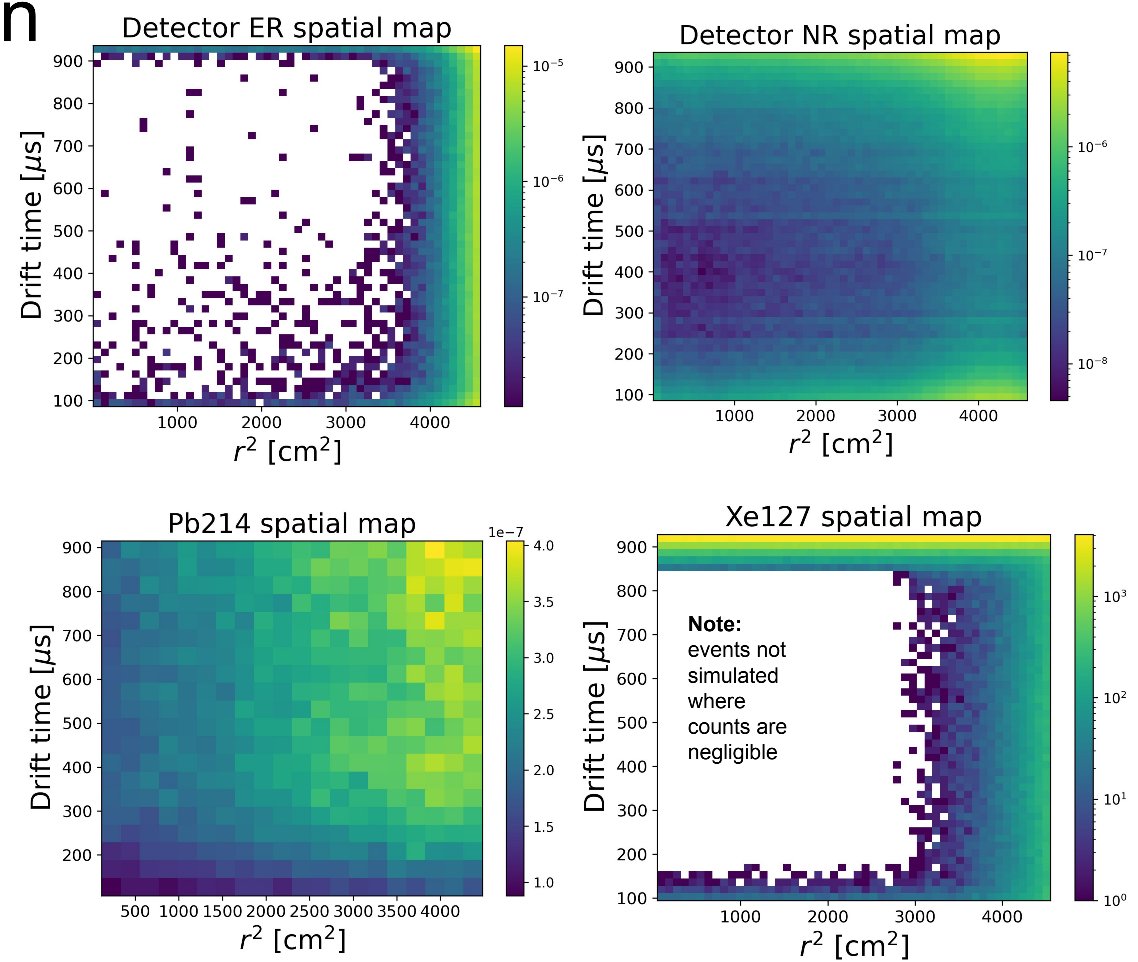


SR1: spatial variation

- Key backgrounds present with spatial non-uniformities throughout the detector
- Including this information in the inference improves discrimination

- Relevant for the primary ER background (^{214}Pb) and primary NR background (neutrons)

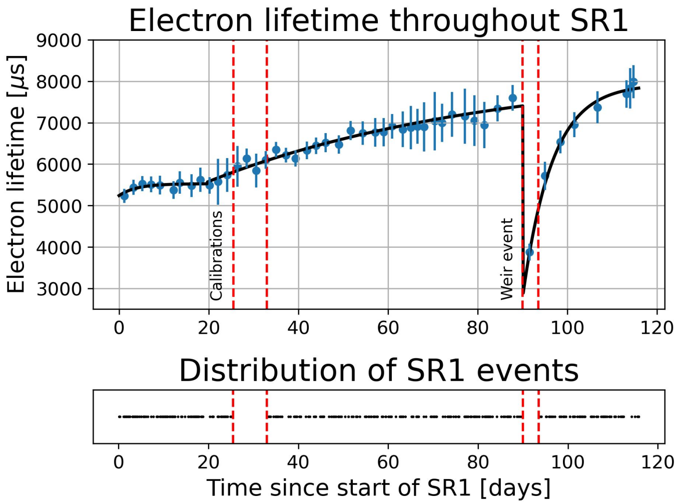
- Additional spatial variation in light collection efficiency
- Using raw S1/S2 in the inference along with spatial information further enhances ER/NR discrimination power

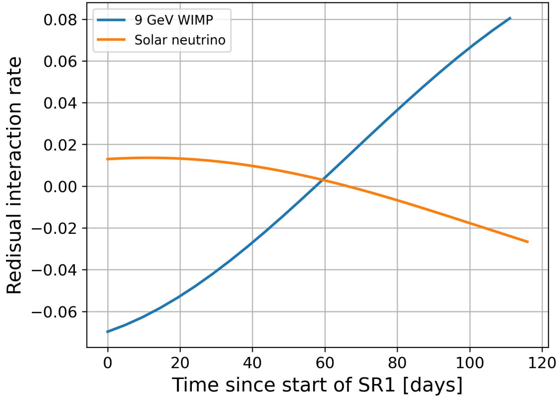


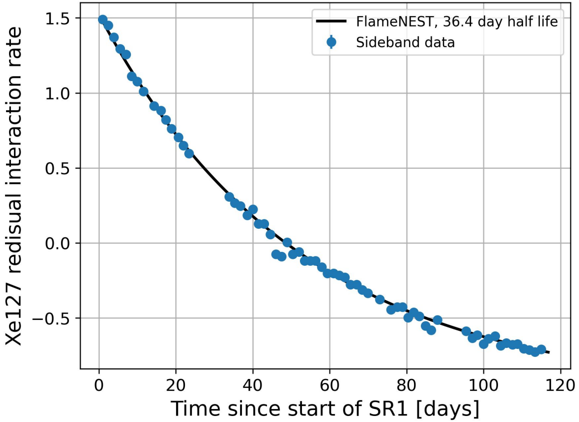
SR1: temporal variation

- SR1 was very stable with respect to detector conditions, but longer future runs have potential for variation
- Electron lifetime variation fully captured in 6D inference: example of how FlameNEST can be used to capture changing detector conditions

- Key background rate present with time dependence, in addition to modulation of dark matter signal
- Capturing this in the inference further enhances discrimination

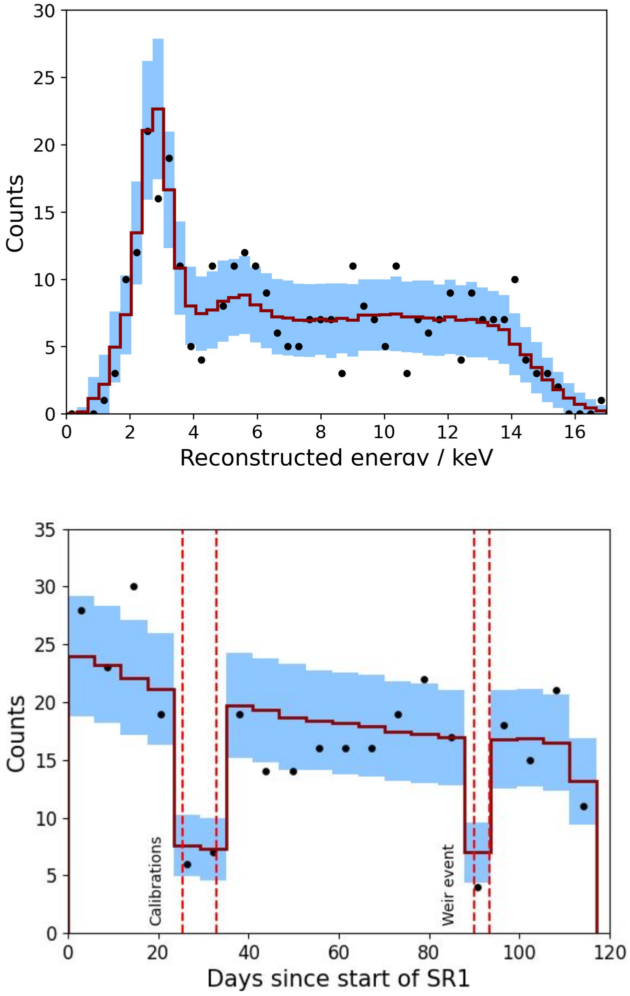




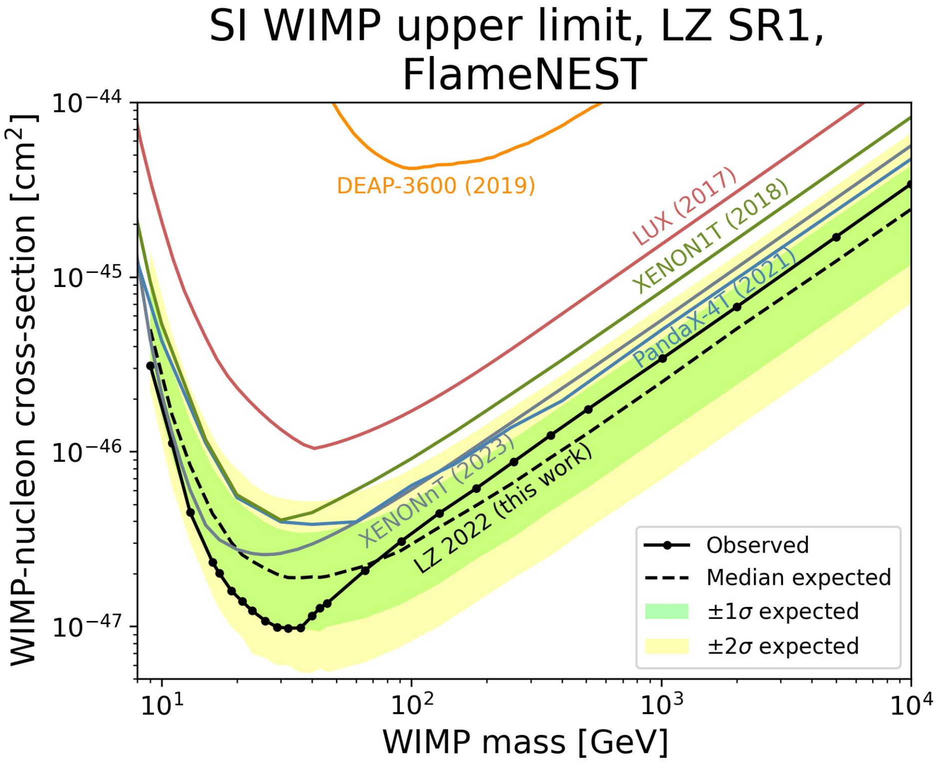


SR1 fit results with FlameNEST

Source	Counts	Uncertainty
ν ER (pp+CNO+^{7}Be)	27.4	1.6
ν NR (^{8}B)	0.143	0.009
^{214}Pb	168	17
Detector ER	1.24	0.32
β	52.9	6.9
^{124}Xe	5.34	1.39
^{136}Xe	15.5	2.4
^{127}Xe	8.77	0.82
^{37}Ar	53.2	+9.3, -8.3
Detector NR	0.1	+0.2, -0.1
Accidentals	1.17	0.26
30 GeV WIMP	0.0	+0.7, -0.0



SR1 limit curve with FlameNEST



- LZ has set current world-leading spin-independent WIMP-nucleon constraints
- First demonstration of inference in a liquid xenon TPC using a 6D observable space, without the need for computationally expensive Monte Carlo simulation

- Future LZ results utilising FlameNEST will benefit from an expanded fiducial volume and lower ROI threshold
- Enhanced discrimination power can greatly enhance discovery significance
- Ability to incorporate many correlated shape-varying nuisance parameters will aid robustness of potential discovery claim

Part III

Applications to XLZD

The XLZD consortium

- More than 450 people spread across 4 continents, 15 countries, 52 institutions

- First meeting in Karlsruhe in summer 2022, second at UCLA in spring 2023

- Joint effort across LZ, XENONnT and DARWIN collaborations to work towards the ultimate next-generation observatory for dark matter and neutrino physics

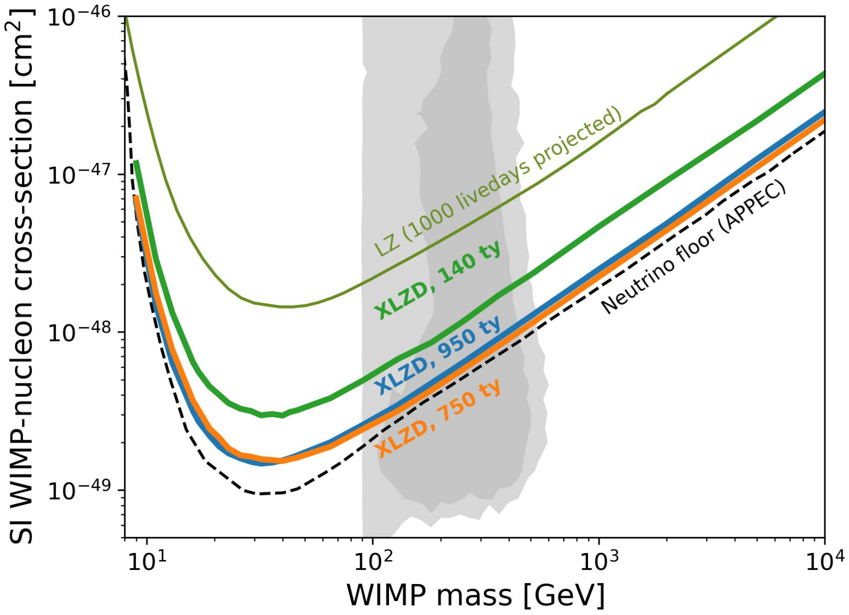
- Design book in preparation, will shortly begin broad programme of in-depth sensitivity studies

WIMP sensitivity: exposure

- **Early science:** run 40 t for ~5 years → 140 ty exposure
- **Nominal:** run 60 t for ~14 years → 750 ty total exposure
- **Opportunity:** run 80 t for ~14 years → 950 ty total exposure

- **Goal:** probe WIMP dark matter down to the neutrino floor

- Clear opportunity for strong science in initial phase
- 80 t option not well-motivated for WIMP case: background limited, taller detector offers worse discrimination

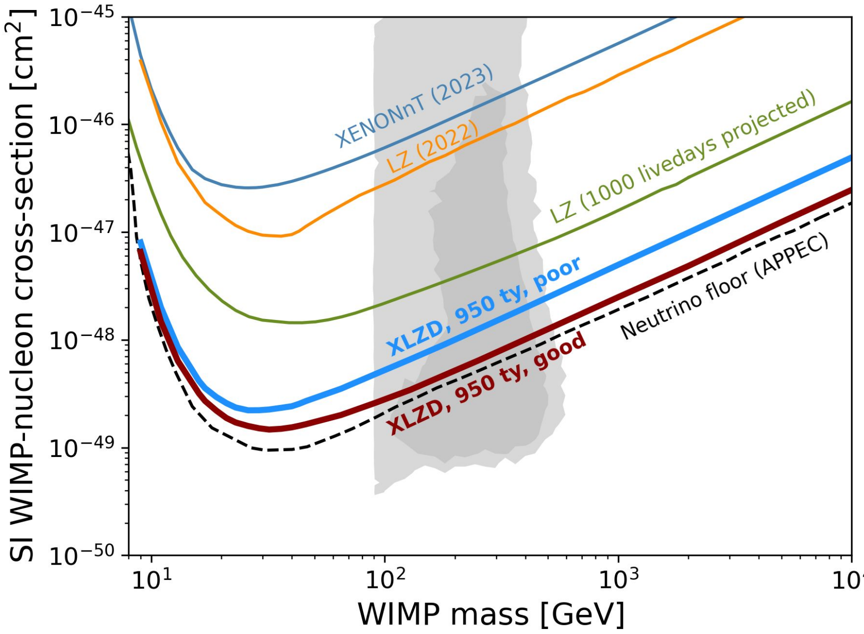


WIMP sensitivity: conditions

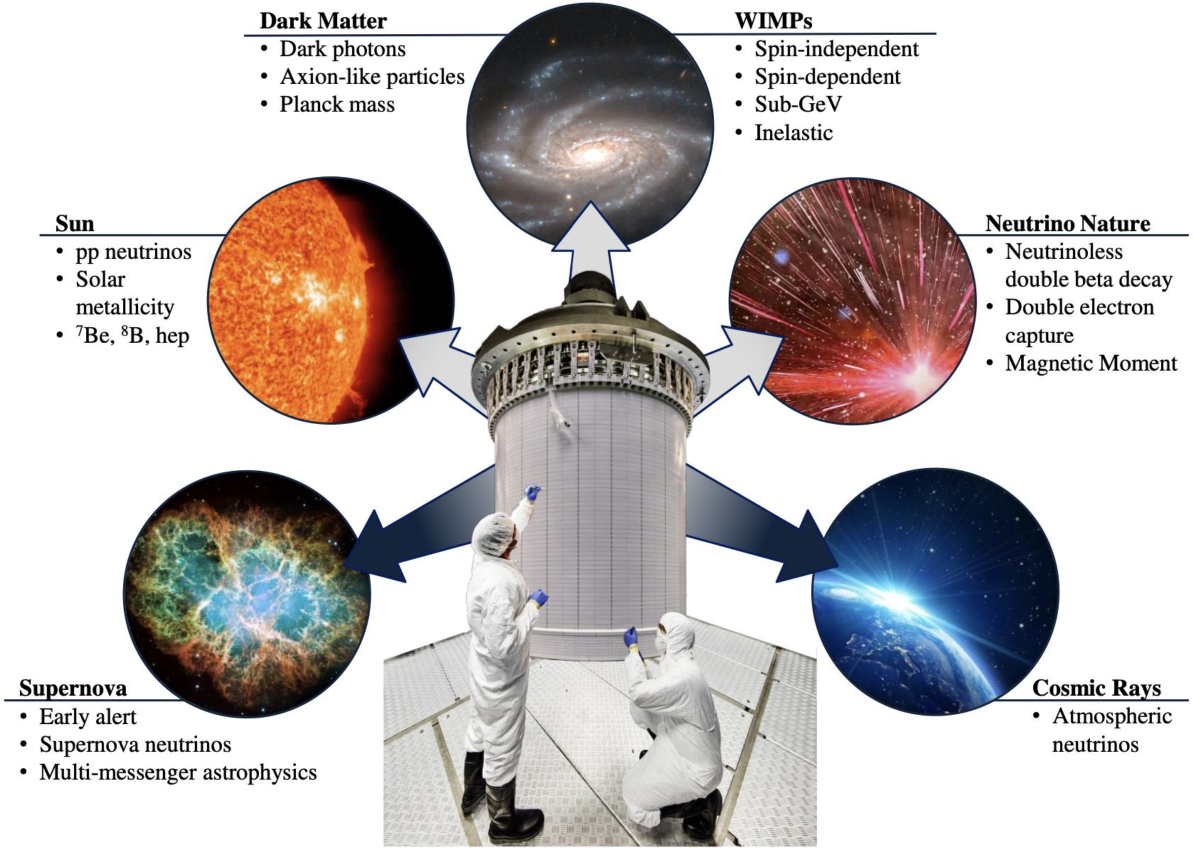
- **Good:** 10 ms electron lifetime, 7.5 kV / cm extraction field, 0.27 PMT QE, 80 V / cm drift field
- **Poor:** 10 ms electron lifetime, 7.5 kV / cm extraction field, 0.25 PMT QE, 25 V / cm drift field

- If XLZD is to probe down to the neutrino floor, clear requirement to meet sufficient ER/NR discrimination level
- Significant R&D needed to achieve required drift field, in particular

- **Future studies:** ensure other physics searches aren't compromised by choice of conditions

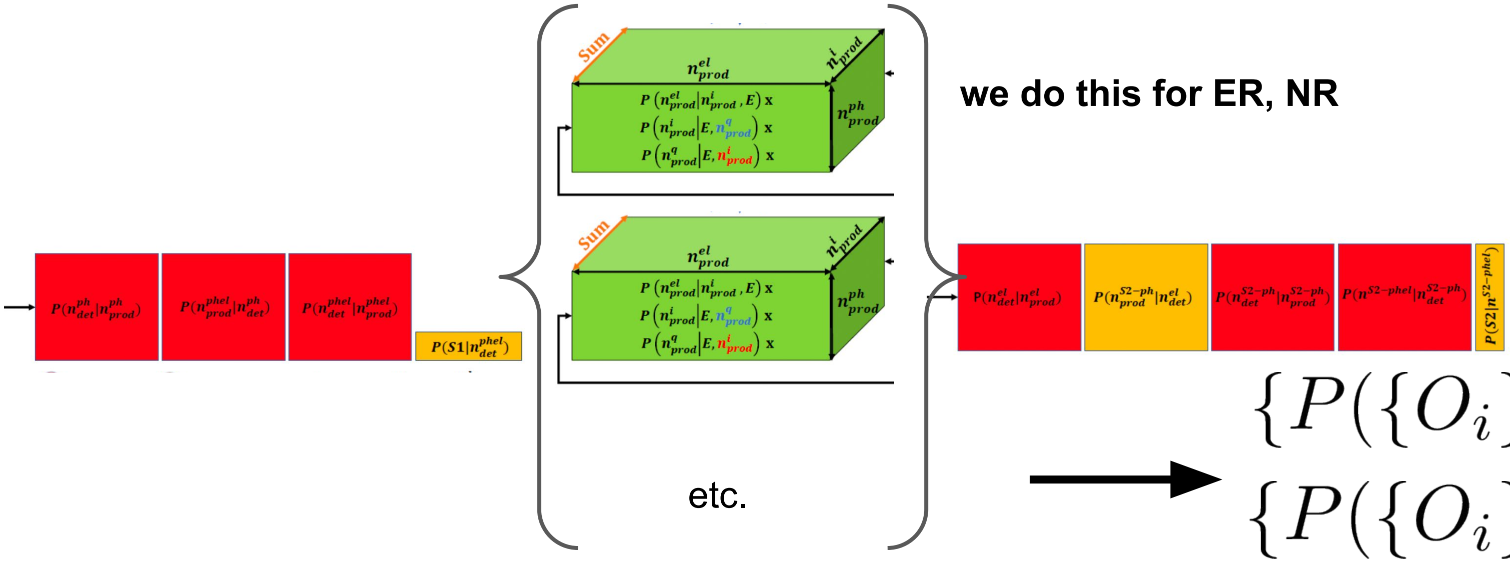


A broad science programme

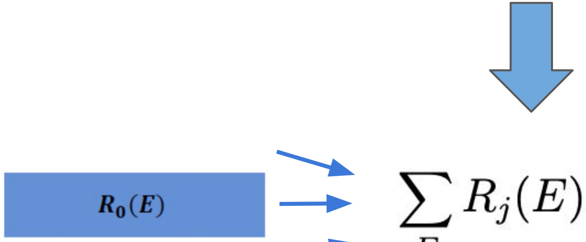


Enabling rapid sensitivity scans

we do this for ER, NR



$$\{P(\{O_i\}|E_1)\}$$
$$\{P(\{O_i\}|E_2)\}$$

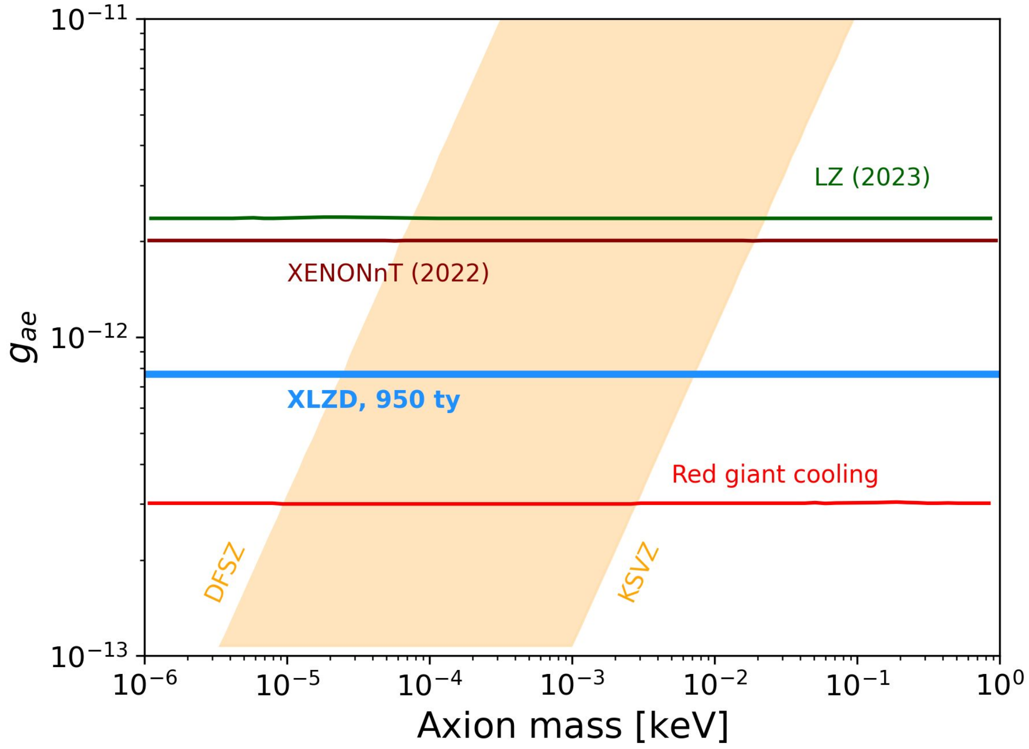


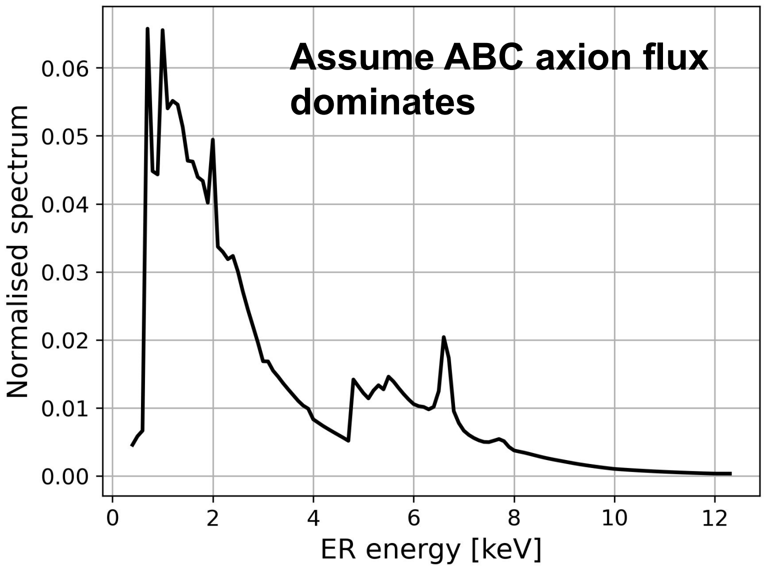
$$\sum_E R_j(E)P_j(S1, S2|E)$$

Example: solar axions

$$\mathcal{L}_{\rm int} = -\frac{\partial_\mu a}{f_a}\bar{\psi}\gamma^\mu\gamma^5\psi$$

$$\sigma_{ae}(E) = \sigma_{pe}(E) g_{ae}^2 \frac{E^2}{8\pi\alpha m_e^2}$$





XLZD in Australia

- University of Melbourne:
  - Myself, Phillip Urquijo, Elisabetta Barberio, Owen Stanley, Nicole Bell, Jayden Newstead, Yajing Xing (next year)
- University of Sydney
  - Theresa Fruth, Ciaran O'Hare, Celine Boehm

- Collaboration with Subatech, France
  - Sara Diglio, Marina Bazyk, Lorenzo Principe

- Plans to continue sensitivity studies within this collaborative group to further optimise detector design and demonstrate XLZD physics potential using common design goals and assumptions

Conclusions and outlook

- FlameNEST allows for likelihood evaluation that negates the need for Monte Carlo simulation: higher dimensional observable space, good scaling with additional shape-varying nuisance parameters
- Enhanced discrimination power and robustness of inference
- State-of-the-art NEST models used, enabling acceptance across collaborations

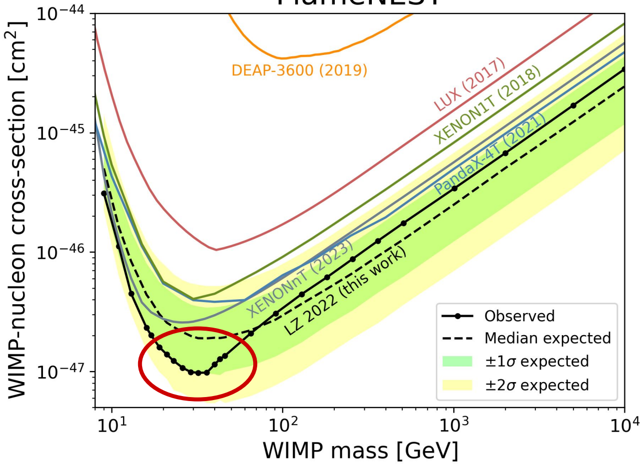
- First demonstration of real use case for LZ SR1 science data
- Additional analyses performed (not shown here), including
  - Fermionic dark matter absorption by nuclei
  - Search for Migdal effect with DD neutrons (8 shape-varying nuisance parameters incorporated)

- Being used for rapid sensitivity studies within the XLZD consortium

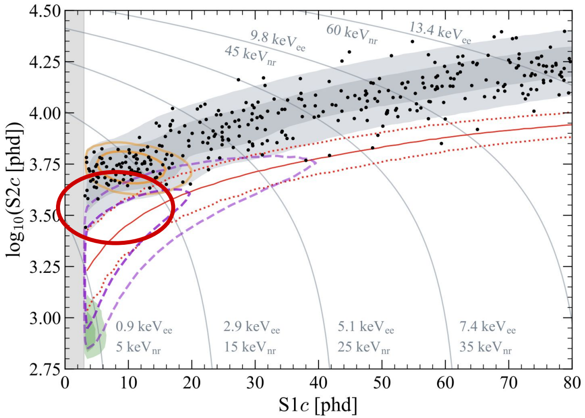
Backup slides

Power constraint and under-fluctuation

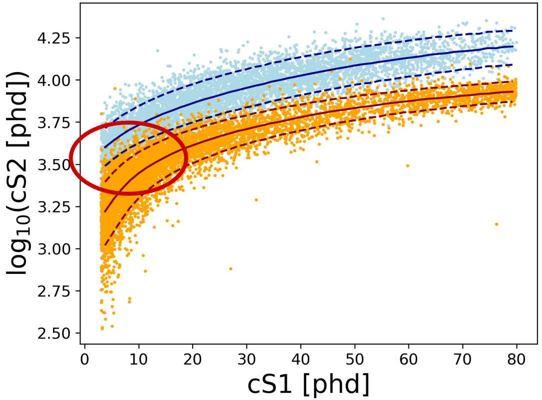
SI WIMP upper limit, LZ SR1, FlameNEST



Limit curve here falls below -1σ band (power constraint applied)...

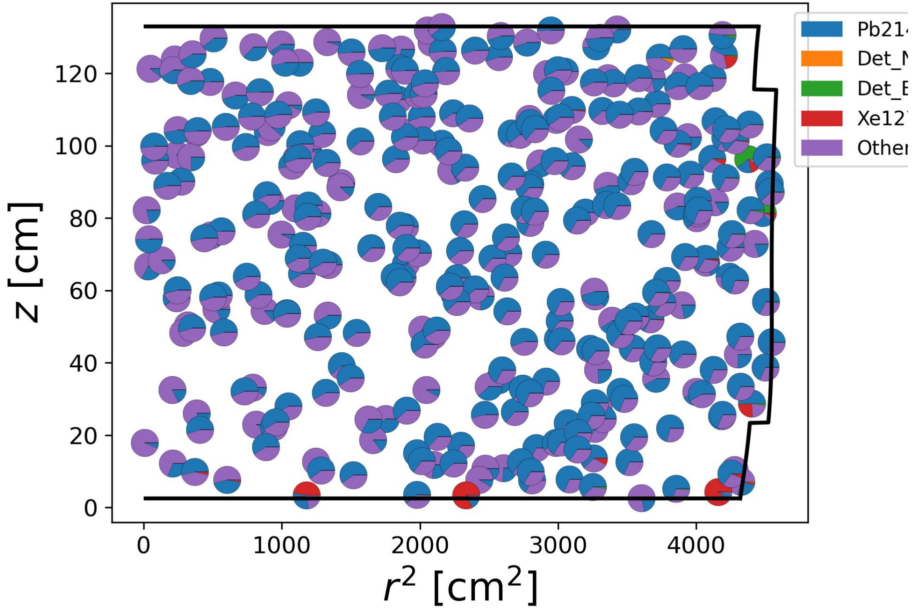


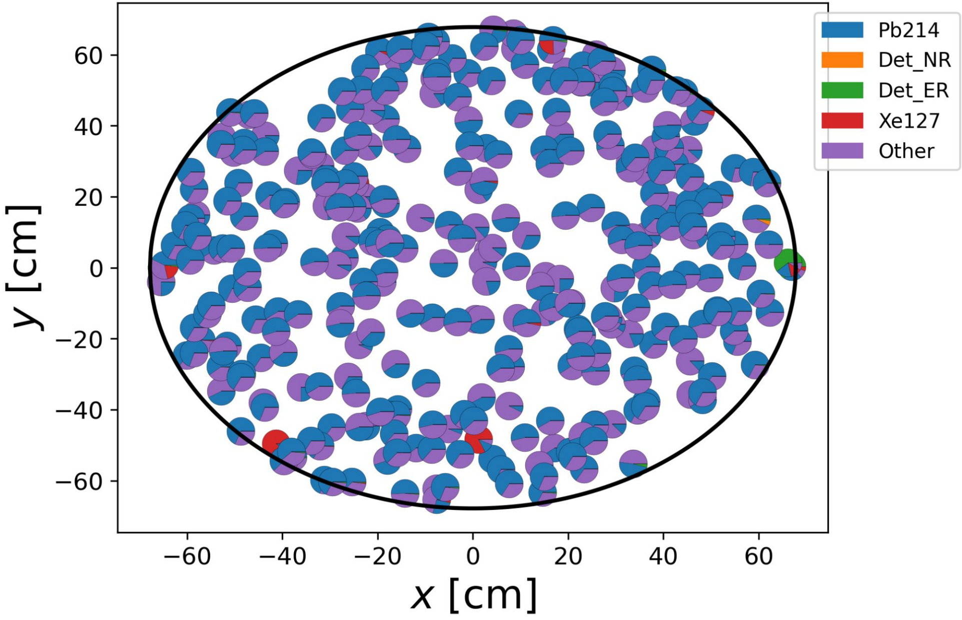
…hypothesised to be due to background under-fluctuation...



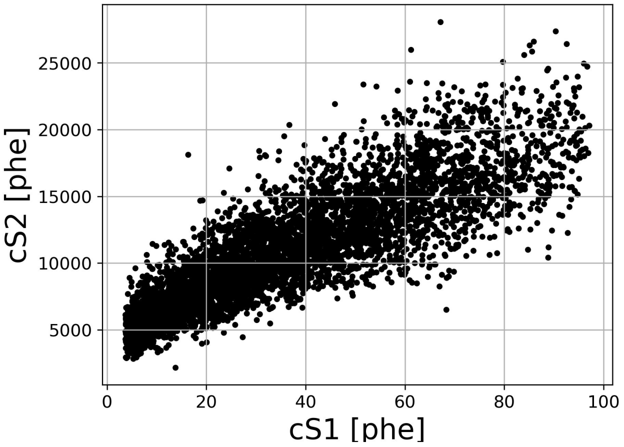
…consistent with the fact that modelling here agrees very well with calibration data.

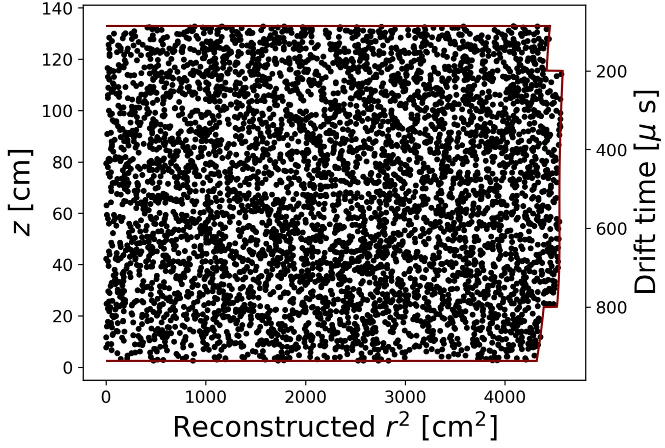
Spatial event probability distributions



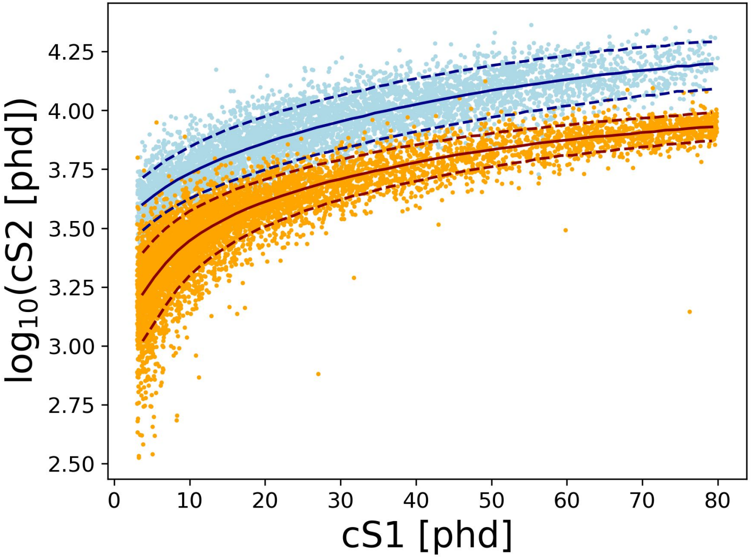


Detector parameter fitting with FlameNEST

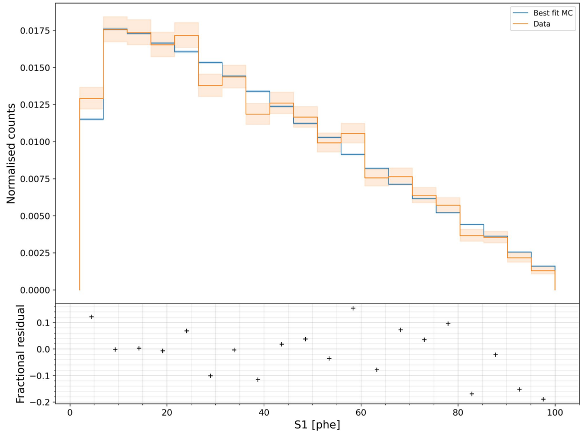


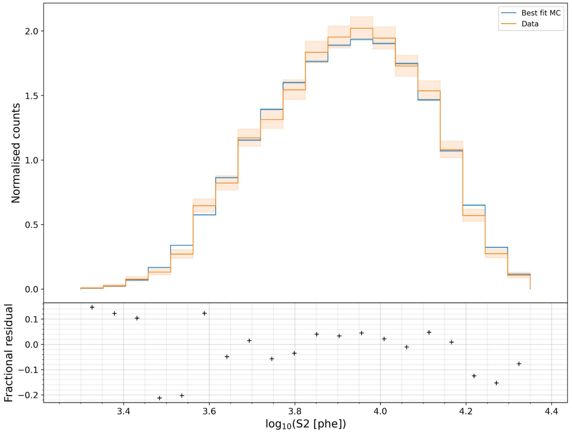


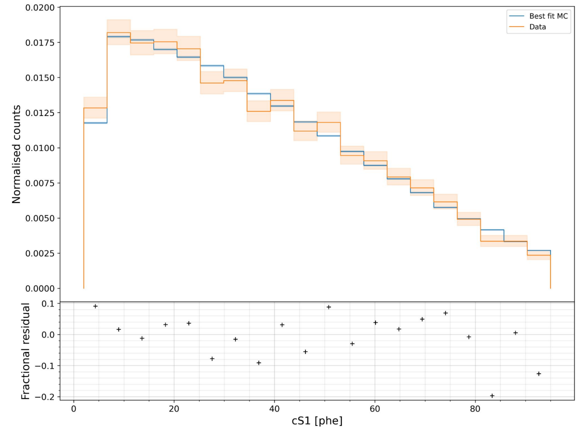
Parameter	Fit result
g1	0.114 ± 0.001
$g1_{gas}$	0.0929 ± 0.0005

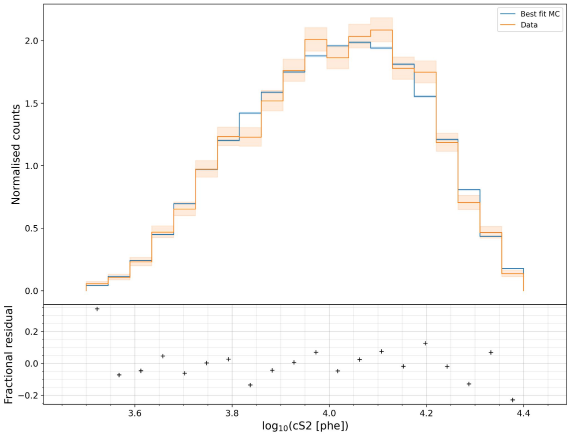


Goodness of fit results: calibrations









Variable	**p-value (KS)**	**p-value (Anderson-Darling)**
S1	0.36	0.17
$\log_{10}$(S2)	0.45	0.24
cS1	0.4	0.24
$\log_{10}$(cS2)	0.41	0.25

XLZD staged approach

- Choice depends on:
  - Physics potential (dark matter, neutrinoless double beta decay)
  - Xenon procurement (availability, cost)
  - Construction considerations (e.g. grid voltages to maintain fields)
  - Timeline for the experiment: how long would we need to run for?