

# FlameNEST: powerful statistical inference for the LZ and XLZD experiments

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ARC CDM Annual Workshop 2023, Adelaide

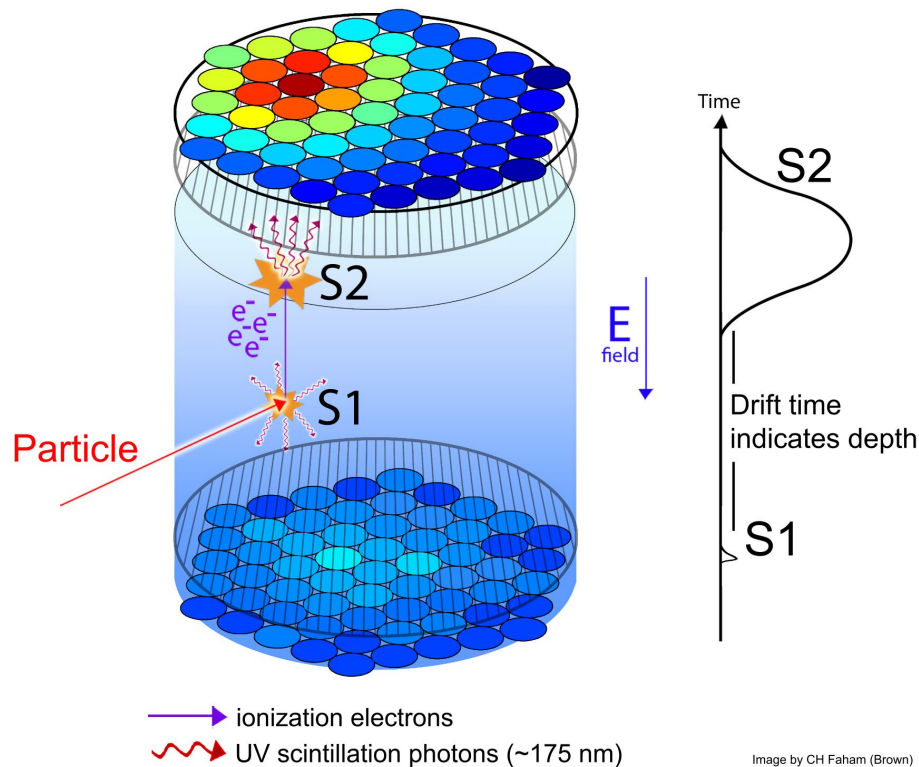




## Part I

# FlameNEST

# Direct detection with noble element TPCs



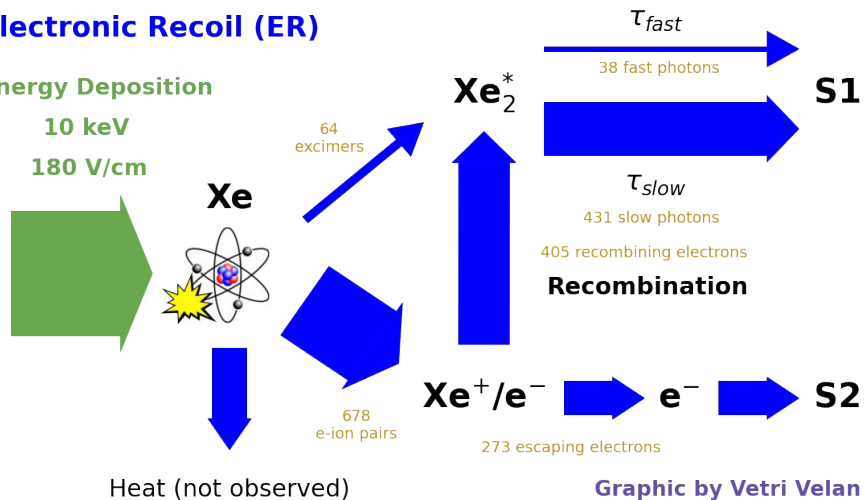
- Dual phase liquid xenon time projection chambers: leading technology for WIMP dark matter detection
- Particle interactions in the LXe → prompt scintillation photons (S1 signal) and ionisation electrons
- Ionisation electrons swept up by applied electric field, extracted into gaseous xenon → electroluminescence → 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

## Electronic Recoil (ER)

### Energy Deposition

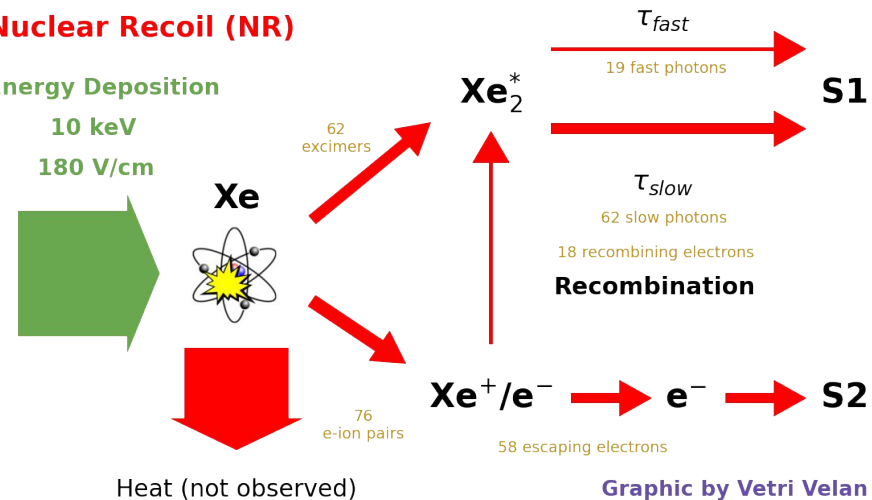
10 keV  
180 V/cm



## Nuclear Recoil (NR)

### Energy Deposition

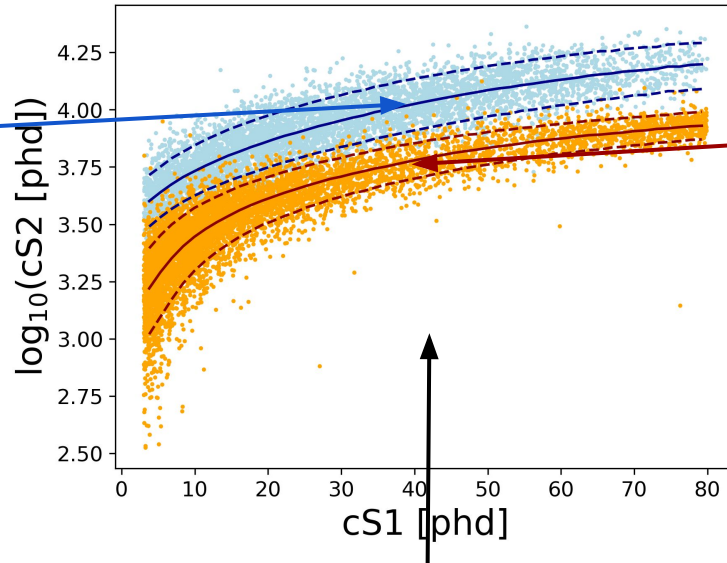
10 keV  
180 V/cm



# Signal/background discrimination

## ER events

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



## NR events

- Coherent elastic neutrino-nucleus scattering ( $^8\text{B}$  + hep solar neutrinos, atmospheric neutrinos, DSNB neutrinos)
- Neutron scattering ( $^{238}\text{U}$  spontaneous fission, ( $\alpha, n$ ) reactions on light nuclei)  $\rightarrow$  'detector NR'

## Other events

- Accidental S1/S2 coincidences  $\rightarrow$  'accidentals'
- Decays in the PTFE wall of the TPC (charge loss  $\rightarrow$  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

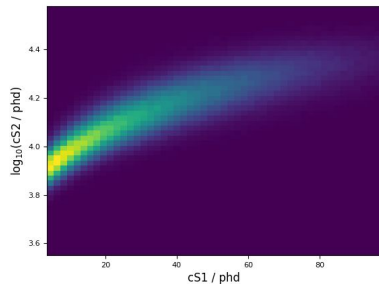
- Galactic dark matter, solar neutrino event rates experience (different) annual modulations
- Certain backgrounds decay over time
- Temporal variation in detector conditions
- Time-dependent modelling can improve dark matter sensitivity

$$cS1 := S1 \frac{G_1(0, 0, z_c)}{G_1(x, y, z)}$$
$$cS2 := S2 \frac{G_1^{\text{gas}}(0, 0)}{G_1^{\text{gas}}(x, y)} e^{t_{\text{drift}}/\tau_e}$$

# Shape-varying nuisance parameters

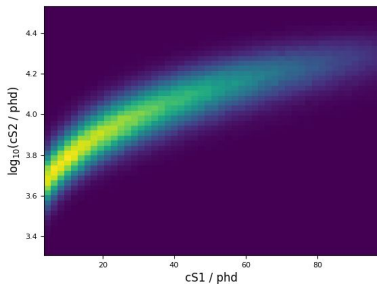
template  
for each  $m_2$

$\langle m_2 \rangle + 1\sigma$



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

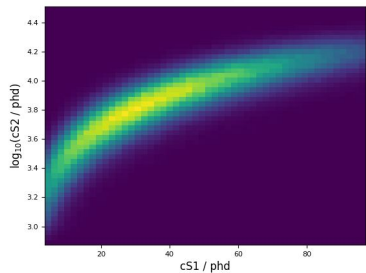
$\langle m_2 \rangle$



...

template for  
each  $m_5$

$\langle m_2 \rangle - 1\sigma$



**LZ CH<sub>3</sub>T:  
simulation**



# The likelihood for rare event searches

$$\ln(L) = \underbrace{-\nu(\vec{\theta})}_{\text{(remnant of) Poisson term}} + \underbrace{\sum_e \ln \left( \sum_j R_j(\vec{d}_e; \vec{\theta}) \right)}_{\text{'shape term': differential rate}} + \underbrace{\sum_k C_k(\vec{\theta})}_{\text{ancillary constraints}}$$

(remnant of) Poisson term

'shape term':  
differential rate

ancillary constraints

## The goal:

utilise full  
observable space

include  
shape-varying  
nuisance  
parameters

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

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

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

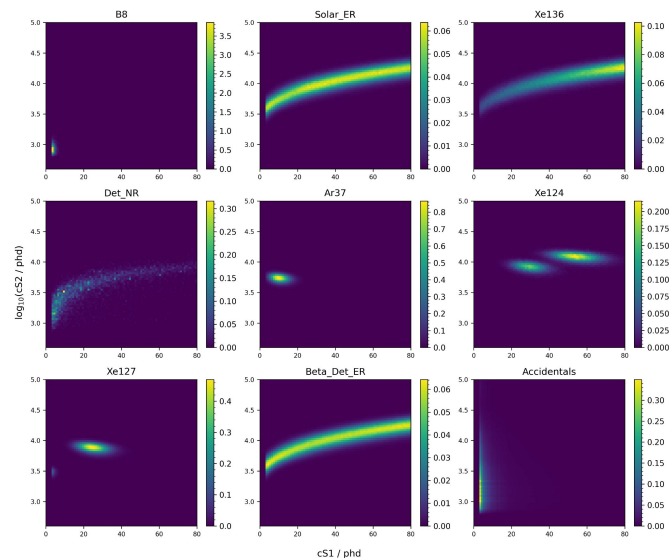




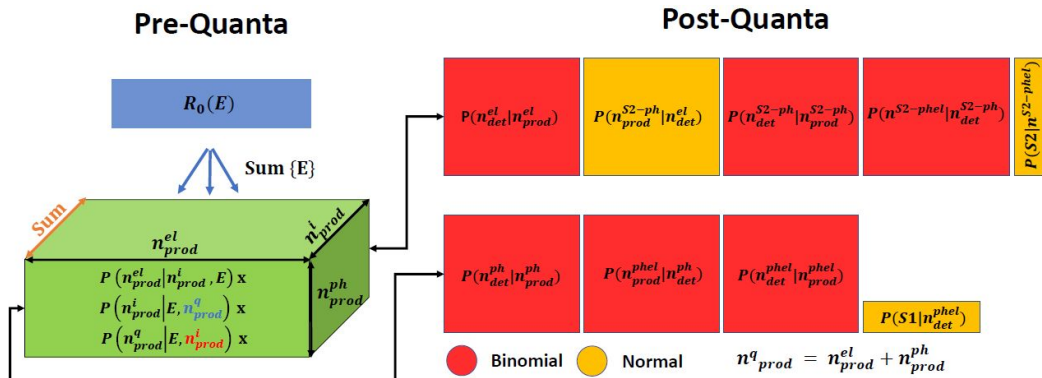
# Likelihood evaluation with templates

$$\ln(L) = \underbrace{-\nu(\vec{\theta})}_{\text{easy}} + \underbrace{\sum_e \ln \left( \sum_j R_j(\vec{d}_e; \vec{\theta}) \right)}_{\text{difficult}} + \underbrace{\sum_k C_k(\vec{\theta})}_{\text{easy}}$$

- 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  $\rightarrow$  gradients + Hessian  $\rightarrow$  vastly improved likelihood maximisation
- No scaling with 2D  $\rightarrow$  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 -  $\rightarrow$  S1  
detector response

energy -  $\rightarrow$   
electron/photon yields

electron yield -  $\rightarrow$  S2  
detector response

$\sum$

$$P(S1|i)P(i|j)P(j|\dots)P(k|\gamma)P(e, \gamma|E)R^j(E)P(l|e)\dots P(m|\dots)P(n|m)P(S2|n),$$

$E, e, \gamma, i, j, k, l, m, n, \dots$

# 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
- 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

**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](https://github.com/FlamTeam/flamedisx)

# Part II

## Applications to LZ

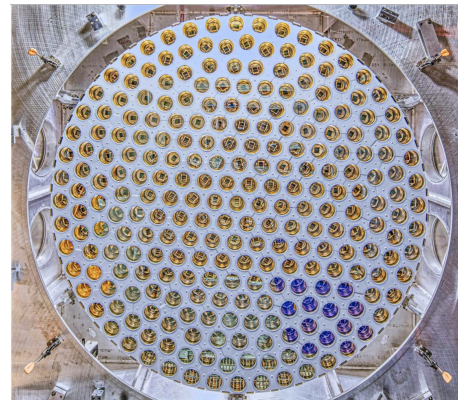
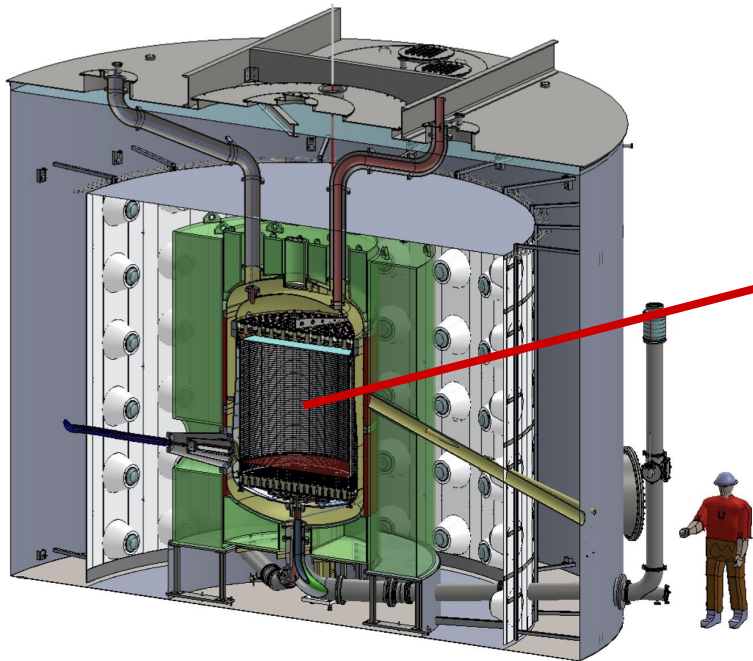


# The LUX-ZEPLIN experiment

- 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

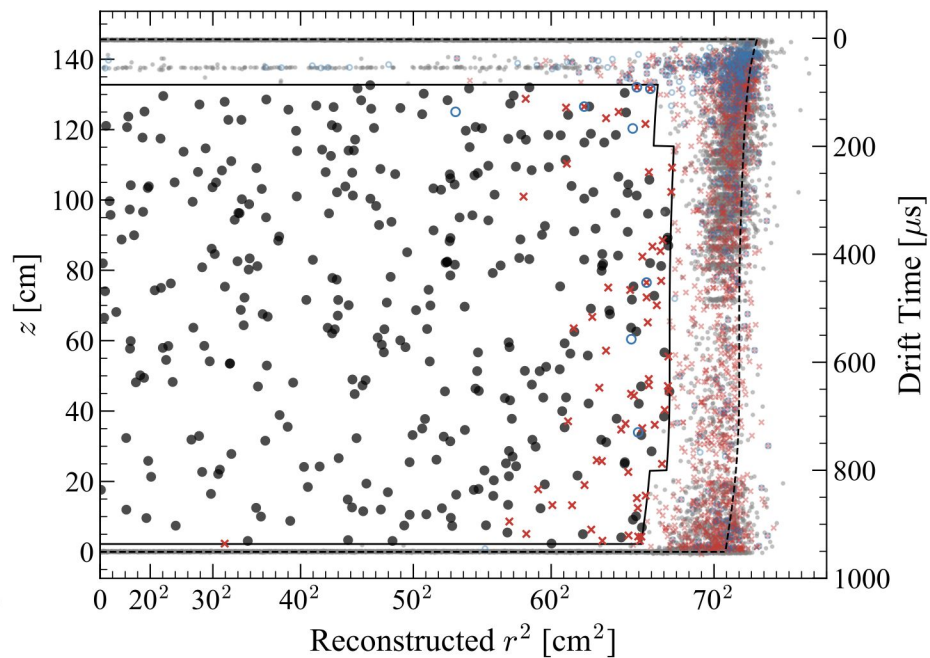
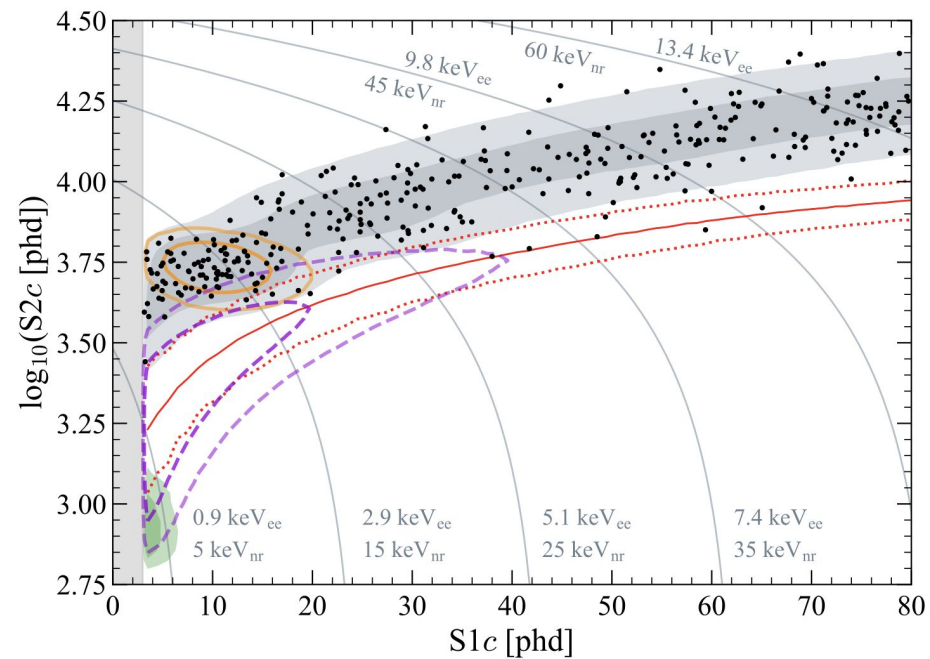


# SR1: run parameters

- 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

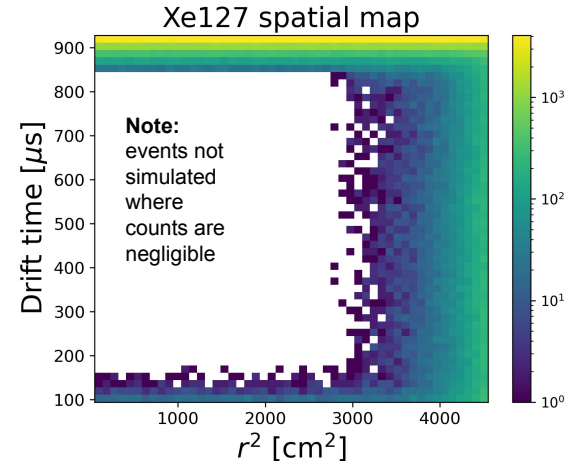
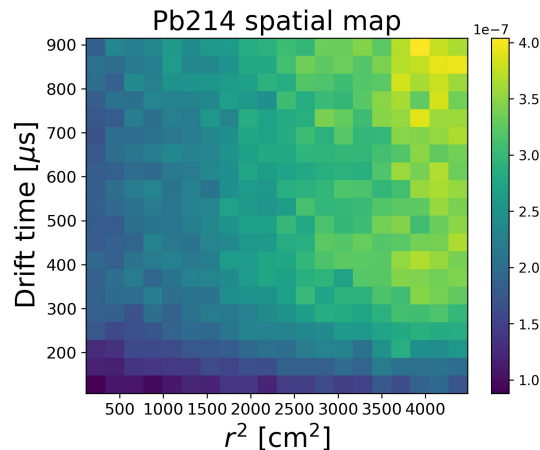
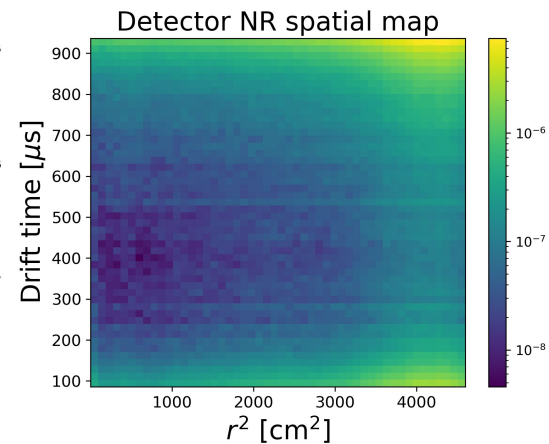
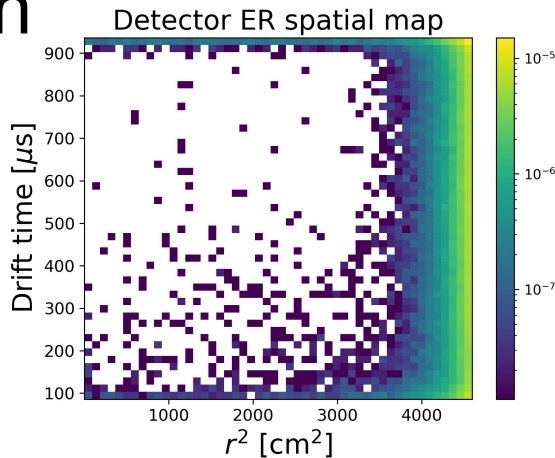


# LZ SR1 WIMP search data



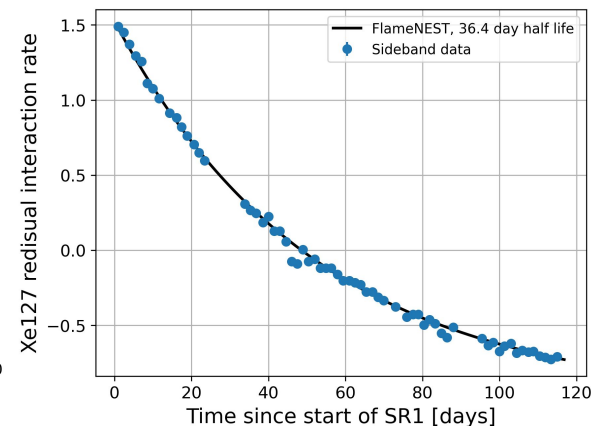
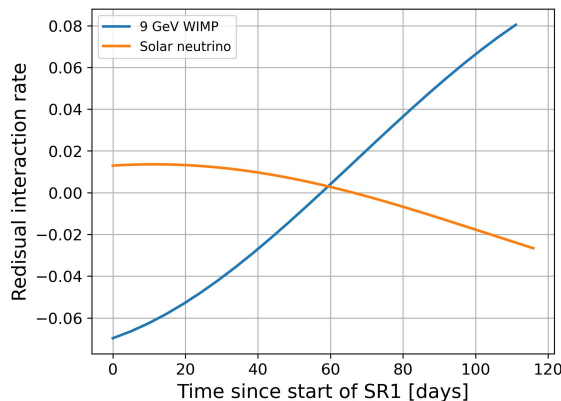
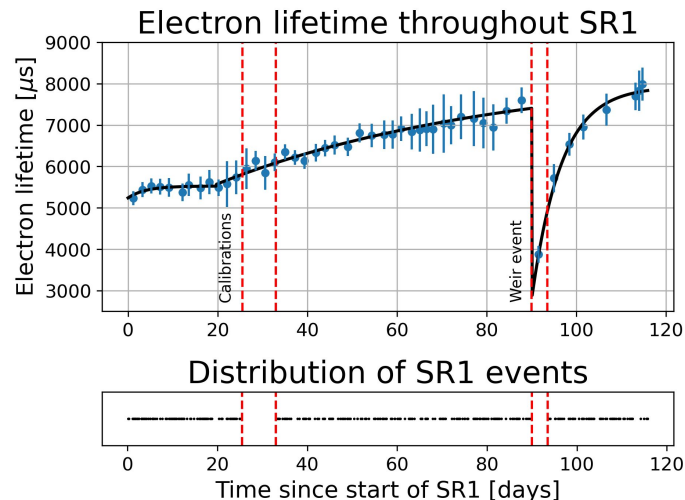
# SR1: spatial variation

- Key backgrounds present with spatial non-uniformities throughout the detector
- Including this information in the inference improves discrimination
- Relevant for the primary ER background ( $^{214}\text{Pb}$ ) 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



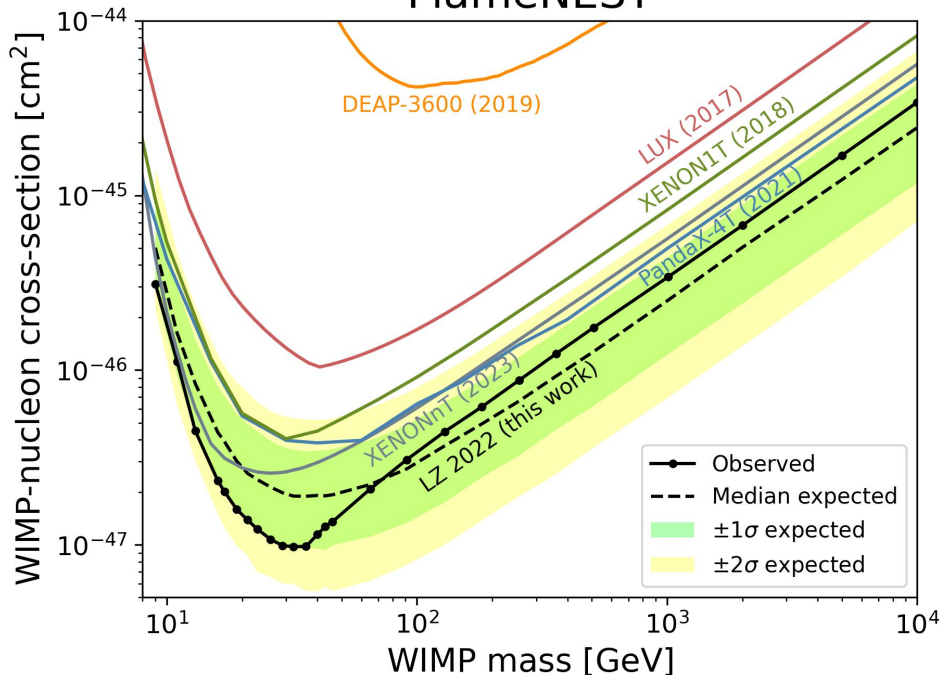
# SR1: temporal variation

- 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 limit curve with FlameNEST

SI WIMP upper limit, LZ SR1,  
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

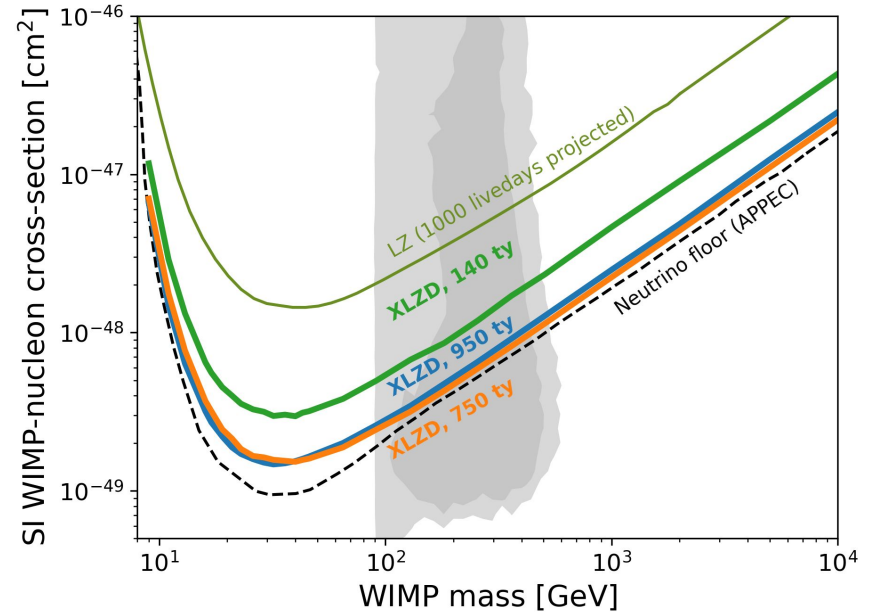
# The XLZD consortium

- 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



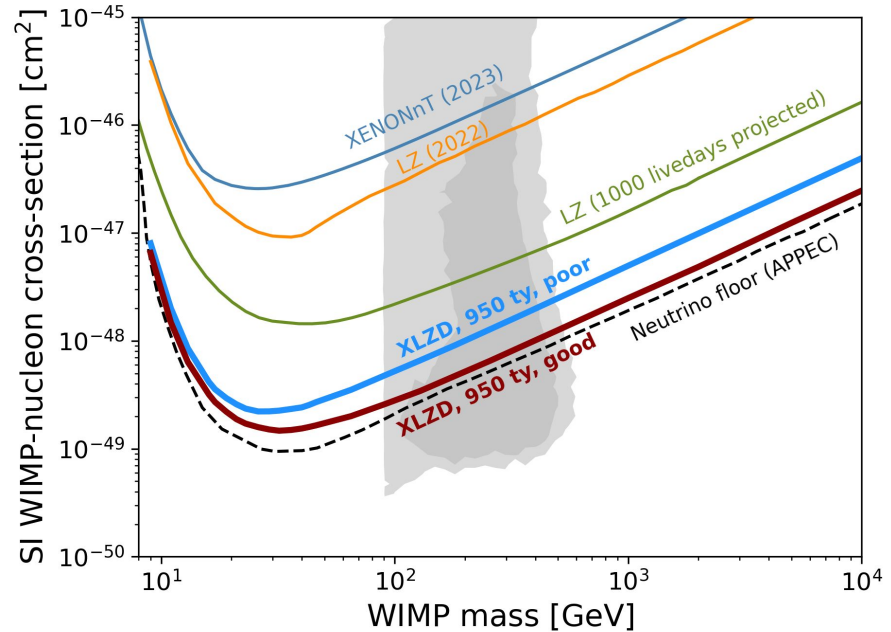
# WIMP sensitivity: exposure

- **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



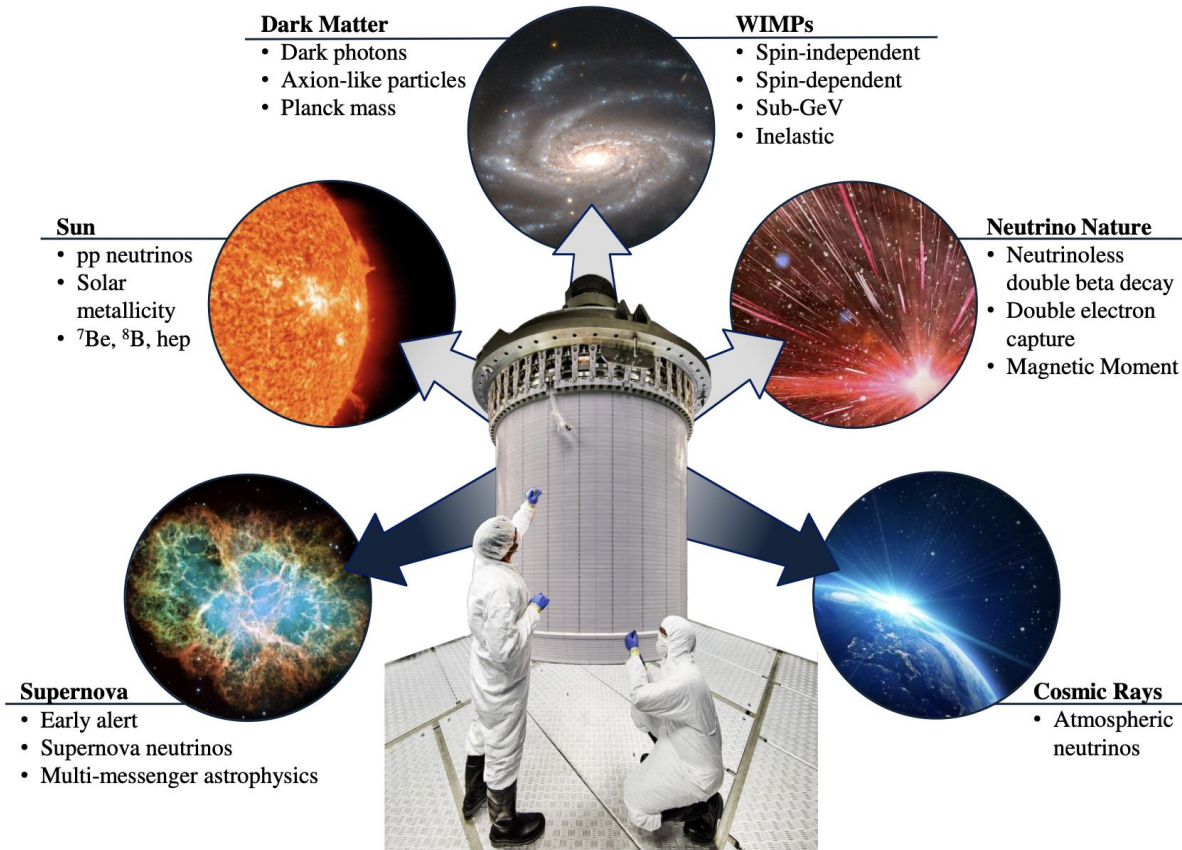
# WIMP sensitivity: conditions

- **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

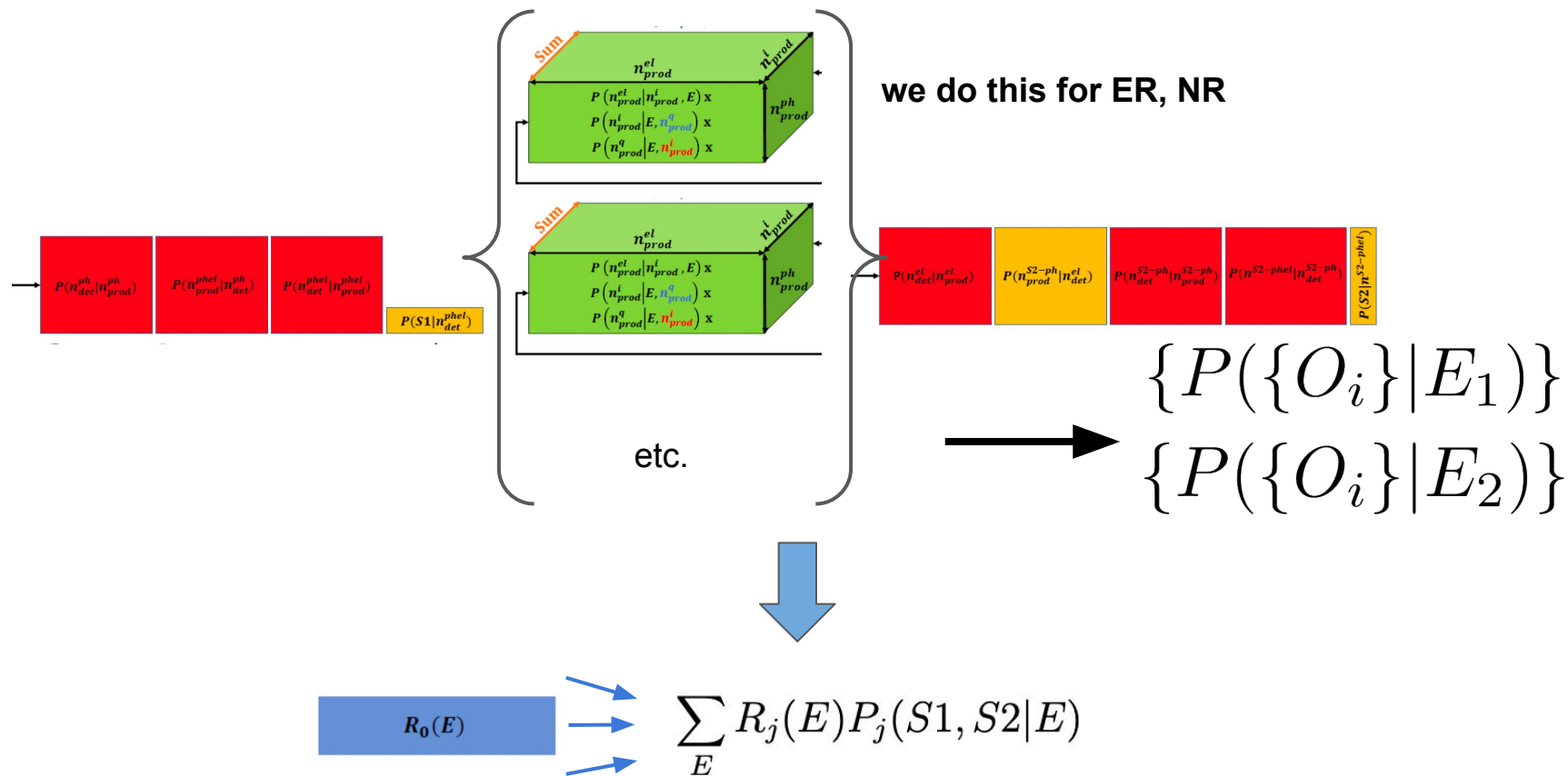




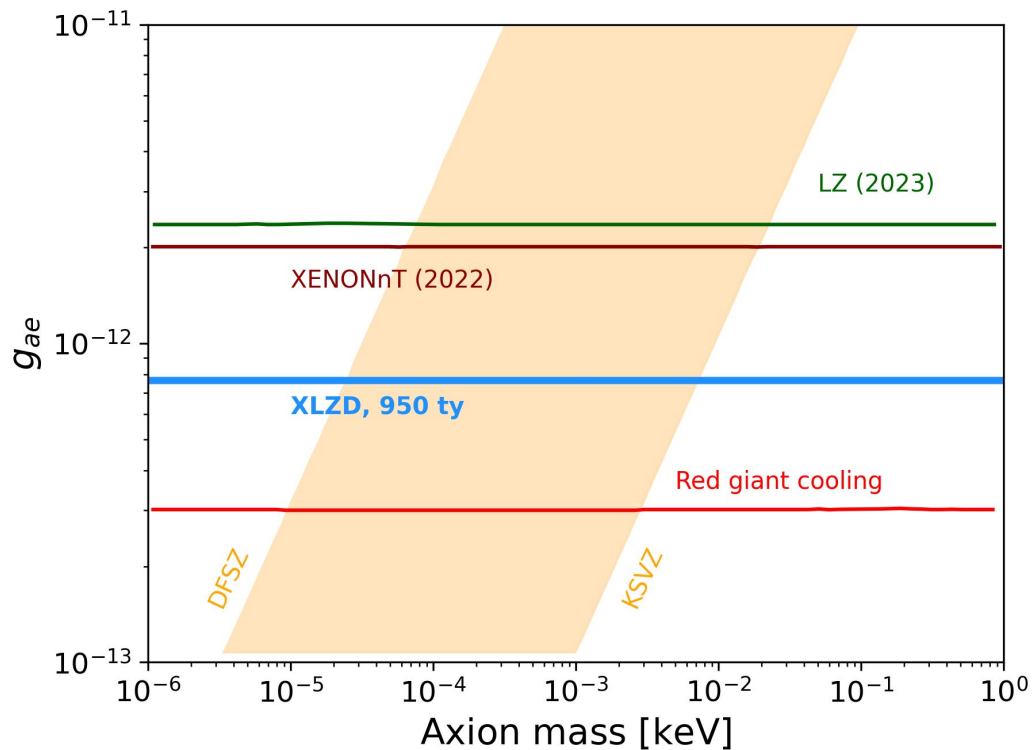
# A broad science programme



# Enabling rapid sensitivity scans

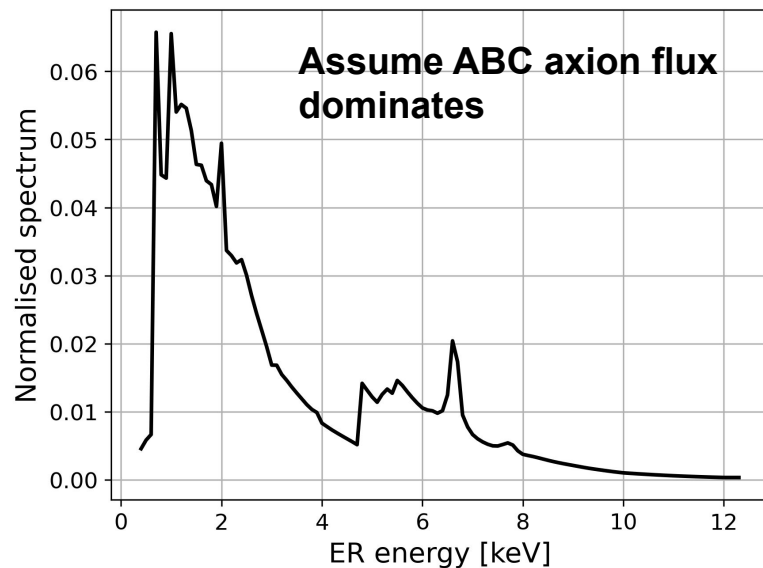


# Example: solar axions



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

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



# XLZD in Australia

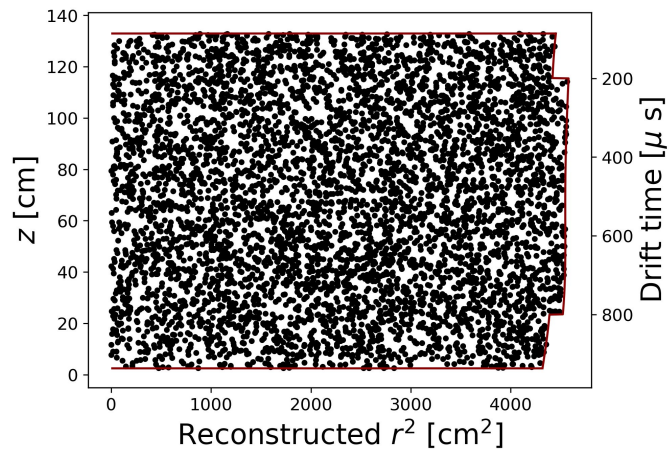
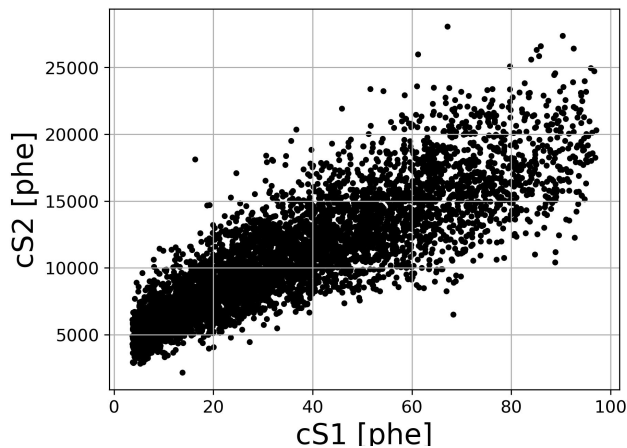
- University of Melbourne:
  - Myself, Phillip Urquijo, Elisabetta Barberio, Owen Stanley, Nicole Bell, Jayden Newstead, Yajing Xing (next year)
- University of Sydney
  - Theresa Fruth, Ciaran O'Hare, Celine Boehm
- Collaboration with Subatech, France
  - Sara Diglio, Marina Bazyk, Lorenzo Principe
- 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

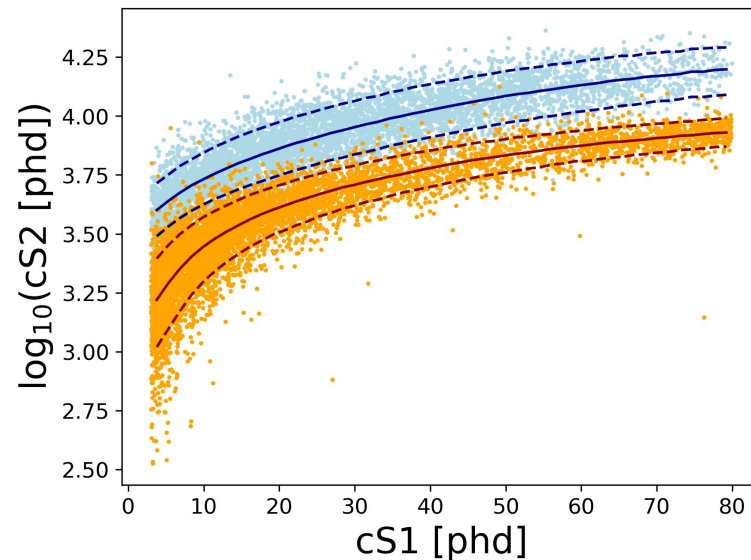
- FlameNEST allows for likelihood evaluation that negates the need for Monte Carlo simulation: higher dimensional observable space, good scaling with additional shape-varying nuisance parameters
- Enhanced discrimination power and robustness of inference
- State-of-the-art NEST models used, enabling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

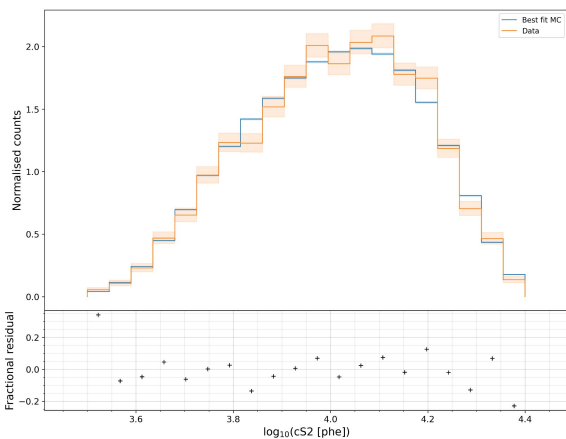
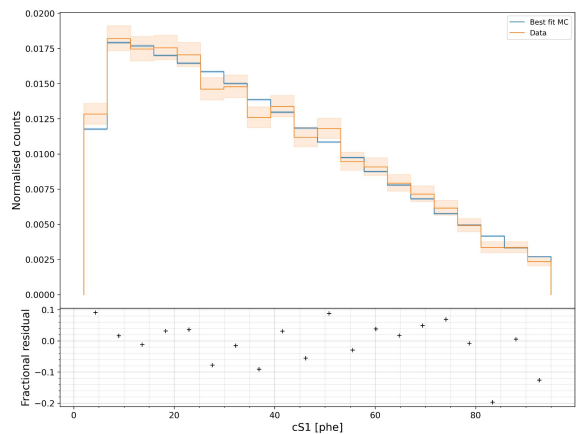
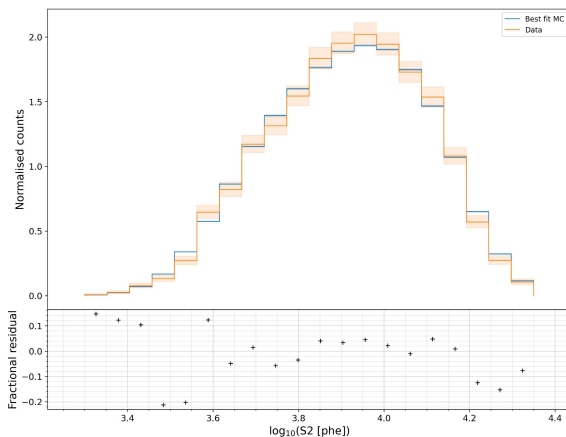
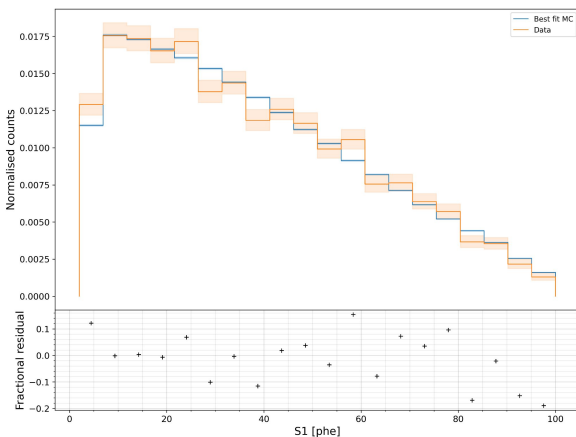
# Detector parameter fitting with FlameNEST



Parameter	Fit result
$g1$	$0.114 \pm 0.001$
$g1_{\text{gas}}$	$0.0929 \pm 0.0005$



# Goodness of fit results: calibrations

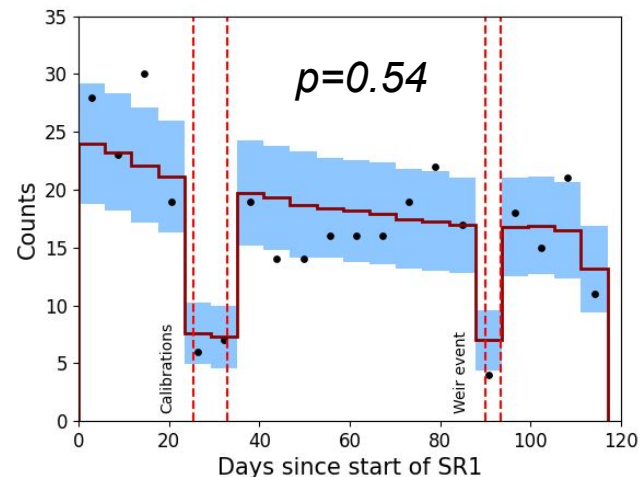
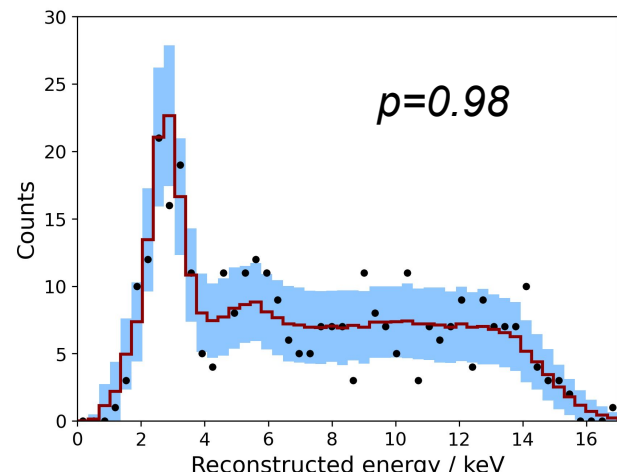


Variable	p-value (KS)	p-value (Anderson-Darling)
S1	0.36	0.17
$\log_{10}(S2)$	0.45	0.24
cS1	0.4	0.24
$\log_{10}(cS2)$	0.41	0.25

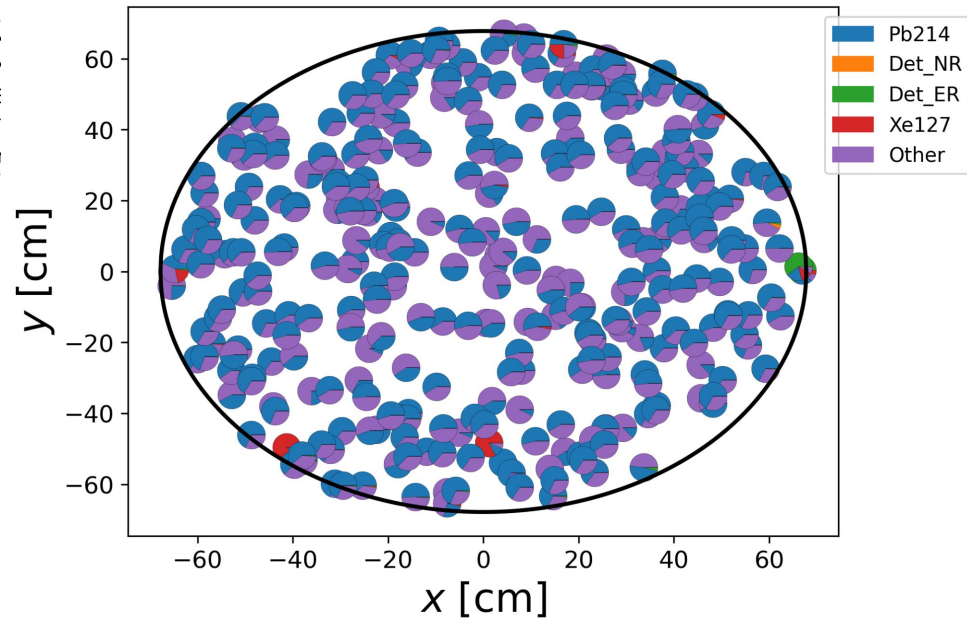
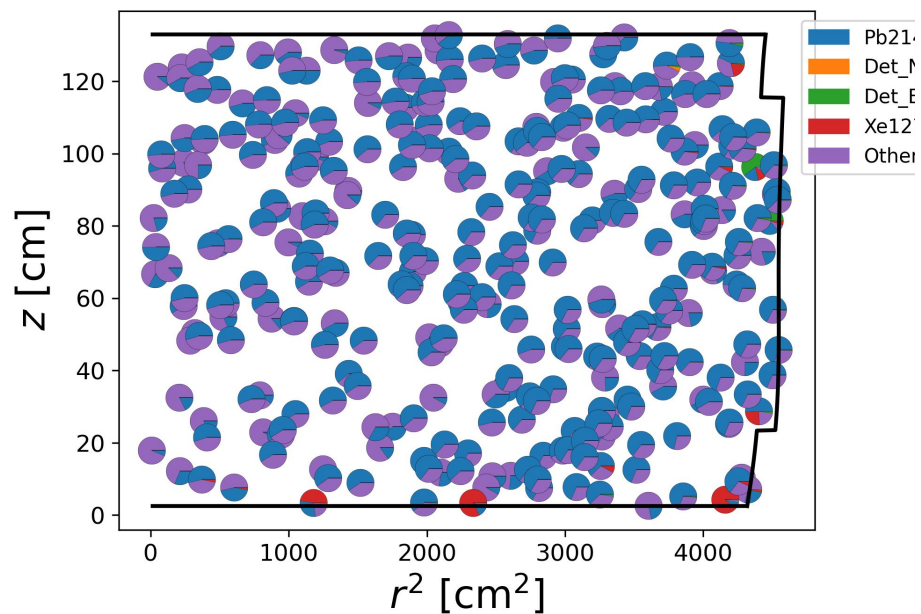


# SR1 fit results with FlameNEST

Source	Counts	Uncertainty
$\nu$ ER (pp+CNO+ $^7\text{Be}$ )	27.4	1.6
$\nu$ NR ( $^8\text{B}$ )	0.143	0.009
$^{214}\text{Pb}$	168	17
Detector ER	1.24	0.32
$\beta$	52.9	6.9
$^{124}\text{Xe}$	5.34	1.39
$^{136}\text{Xe}$	15.5	2.4
$^{127}\text{Xe}$	8.77	0.82
$^{37}\text{Ar}$	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

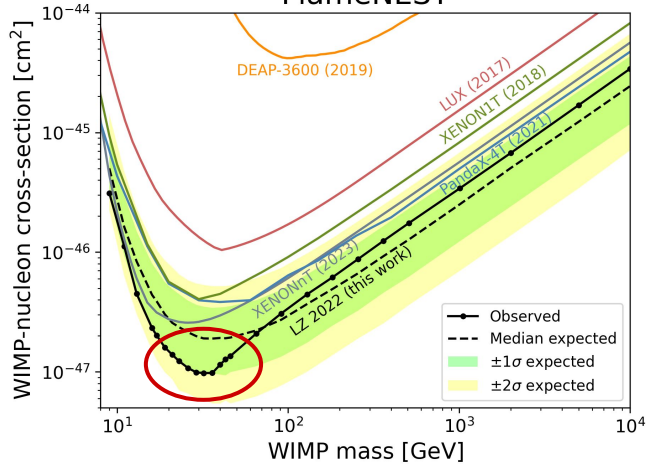


# Spatial event probability distributions

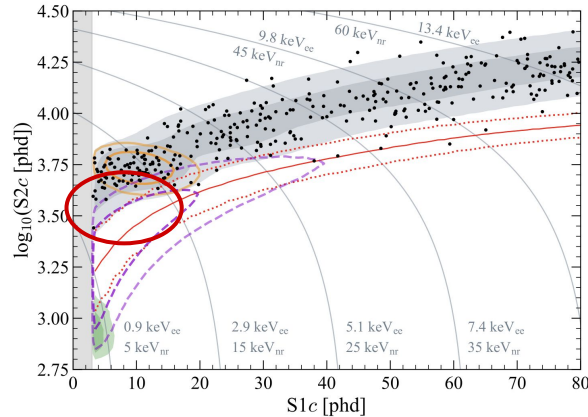


# Power constraint and under-fluctuation

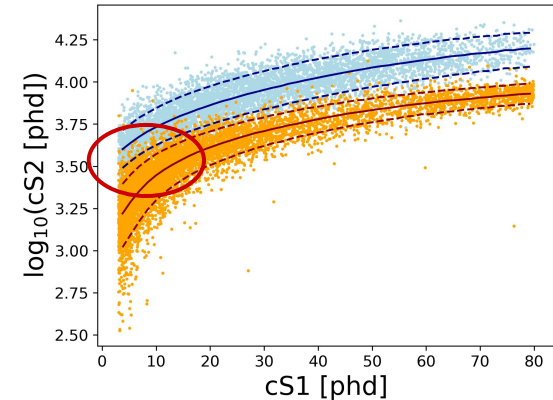
SI WIMP upper limit, LZ SR1, FlameNEST



Limit curve here falls below  $-1\sigma$  band (power constraint applied)...



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

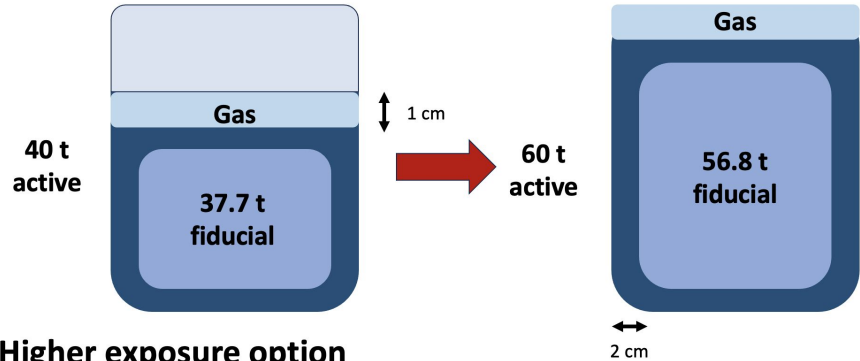


...consistent with the fact that modelling here agrees very well with calibration data.

# 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?

Lower exposure option



Higher exposure option

