

Monte Carlo Simulations in CUORE

Michinari Sakai on behalf of the CUORE collaboration

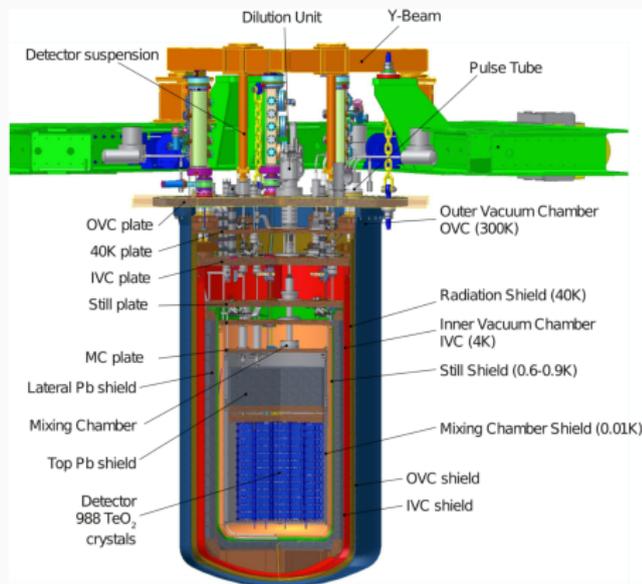
Monte Carlo Tools for Beyond the Standard Model Physics 2018
Institute for Particle Physics Phenomenology - Durham University
April 18, 2018

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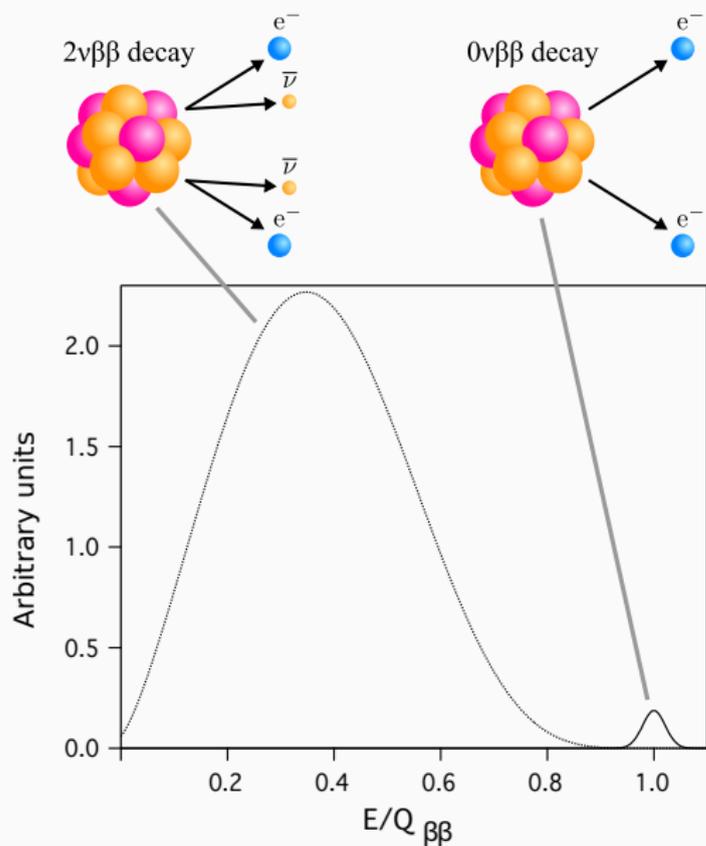


CUORE (Cryogenic Underground Observatory for Rare Events)

- Objective:
Search for Majorana neutrino ($\nu = \bar{\nu}$) through neutrinoless double beta ($0\nu\beta\beta$) decay of ^{130}Te
- Detector:
Array of 988 TeO_2 bolometers
- Mass:
742 kg of TeO_2
206 kg of ^{130}Te (34.2 % natural abundance in Te)
- Operating temperature:
 ~ 15 mK
- Energy resolution goal:
5 keV FWHM @ 2615 keV
- $T_{1/2}$ sensitivity goal:
 $\sim 9 \times 10^{25}$ yr (90 % C.L.) in 5 years of data taking
- Background goal:
0.01 counts/(keV · kg · yr) in energy region of interest

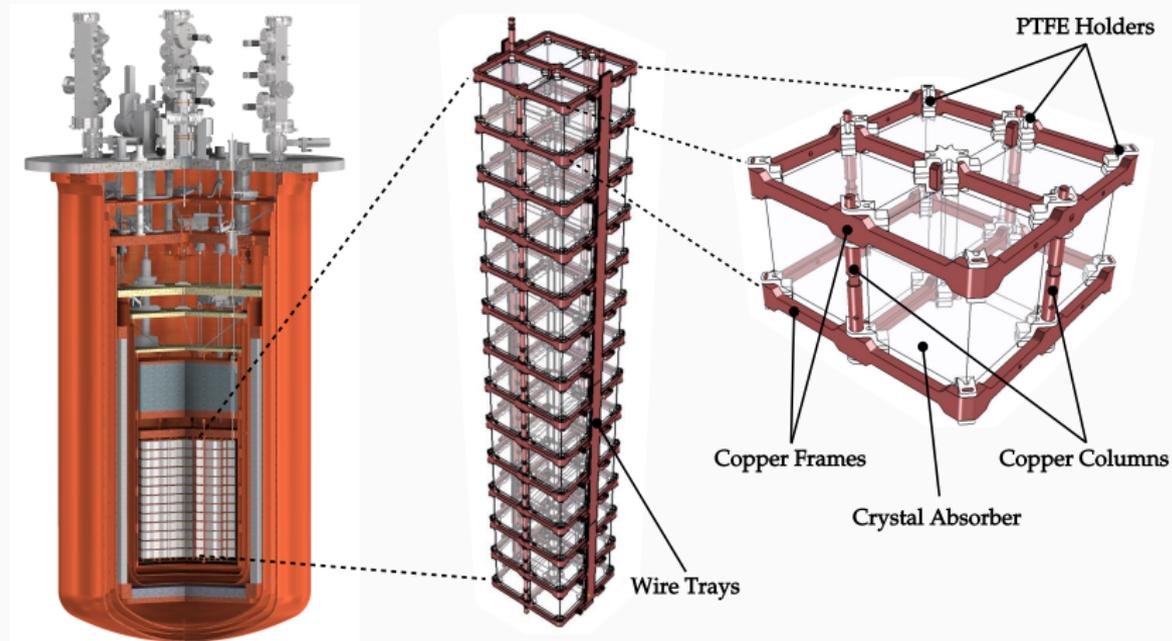


DOUBLE BETA ($\beta\beta$) DECAY SIGNATURE



- $^{130}\text{Te} \rightarrow ^{130}\text{Xe} + 2\beta^-$ decay
Q value = 2528 keV
- Region of Interest (ROI)
 $\approx [2470, 2570]\text{keV}$
- $0\nu\beta\beta$ decay signature: Faint mono-energetic decay peak at Q value smeared only by detector resolution if β s deposit full energy in detector
- $2\nu\beta\beta$ decay signature: Broad peaked continuum up to decay Q value with neutrinos carrying away energy across phase space

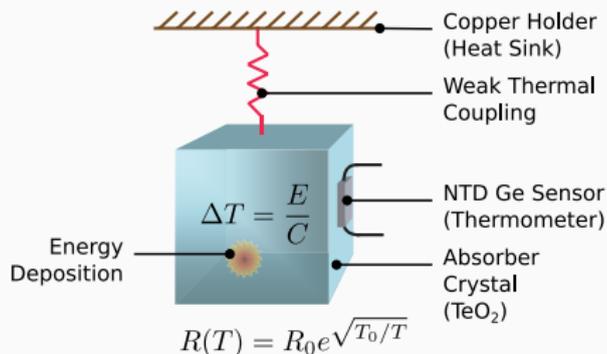
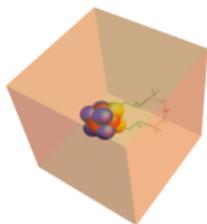
DETECTOR GEOMETRY



- Closely packed array of 988 TeO_2 thermal detectors are housed in 19 towers
- Each tower holds 13 floors with 4 detectors on each floor
- Detector: $5 \times 5 \times 5 \text{ cm}^3$, 0.75 kg each
- Detectors are mechanically held in place only by polytetrafluoroethylene (PTFE) holders
- Entire structure is held together by copper frames

DETECTOR PRINCIPLE

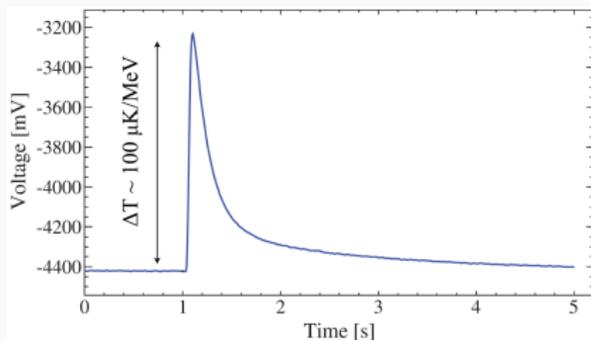
Source = Detector

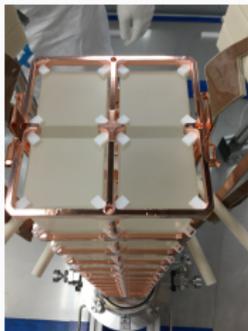


$$C(T) \propto T^3$$

- Electron events from $\beta\beta$ decay mostly contained in bulk (88.4% containment efficiency)
 - ⇒ Anti-coincidence cuts backgrounds
- Detector only sensitive to temperature change
 - ⇒ No active background rejection

Slow (~ 1 s) signal pulse
suitable for rare event searches





Sources Near Detectors

- ^{238}U , ^{232}Th and decay products on surface and in bulk of TeO_2 crystals and nearby materials
- Multi-Compton events from 2615 keV γ from ^{208}Tl (from ^{232}Th chain)*
- Both bulk and surface contaminations are significant and unique backgrounds

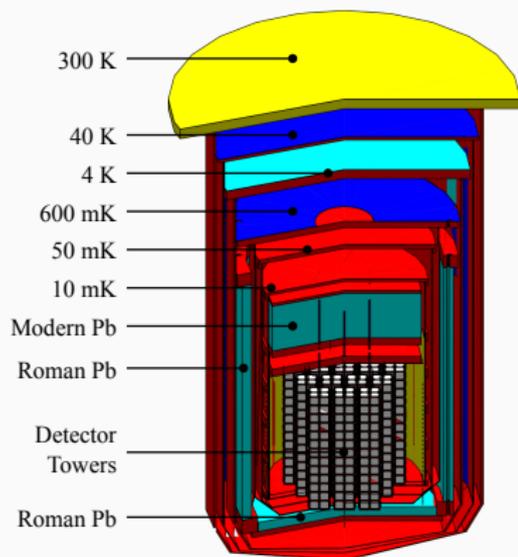
Sources Far from Detectors

- Cu and Pb shields
- Background contribution from bulk/surface contaminations degenerate \implies only simulate bulk

Modeling backgrounds is important part of CUORE!

*This is the only environmental γ line with B.R. $> 1\%$ with energy $> Q_{\beta\beta}$

DETECTOR SIMULATION



Based on GEANT4 with geometries:

- Array of 988 TeO_2 crystals
- PTFE supports, NTD Ge thermistors
- Cu frame structure holding crystals, wire trays
- Thermal shields
- Pb shields, steel rods supporting Pb shields
- Calibration source guiding tubes
- External Pb and polyethylene shields

2 step detector simulation

1. Propagate particles from nuclear decay chains down to \sim keV energies and record energy depositions in TeO_2 thermal detectors
2. Important observables are saved and further processed applying detector response and readout features mimicking real data

GEOMETRY ELEMENTS[†]

Region	Element	Mass (g)	Surface Area (cm ²)
Near TeO ₂ detectors	TeO ₂ crystals	7.42×10^5	148 200
	Si heaters	6.8	158
	NTD Ge thermistors	42	228
	PEN-Cu cables	389	1200
	Cu wire pads	57	1140
	PTFE crystal supports	5500	29 800
	NOSV Cu parts	9.4×10^5	278 900
Far from TeO ₂ detectors	OFE Cu parts	7.0×10^6	—
	Superinsulation layers	17×10^3	—
	Roman Pb shield	4.5×10^6	—
	Modern Pb shield	2.1×10^6	—
	Stainless steel rods	15.2×10^3	—
	300 K steel flange	1.9×10^6	—

- Surface contamination is simulated only for parts near TeO₂ detectors*

*The projected background for the CUORE experiment, Eur.Phys.J. C77 (2017) no.8, 543

[†]Elements are geometrical volumes made of the same material with similar production history and contamination levels.

Physics

- Variable physics list that defaults to Livermore for accurate low energy (0–10 TeV) physics relevant in underground applications

Sources

- Arbitrary sub-chains of decaying isotopes
 - ⇒ Useful for studying breaks in secular equilibrium within one chain
- $\beta\beta$ decays with/without ν s from the ground or excited states of ^{130}Te

Source Positions

- Bulk of detector parts
- Surface of detector parts (uniform distribution up to some depth into surface, or exponential profile)

Detector Response

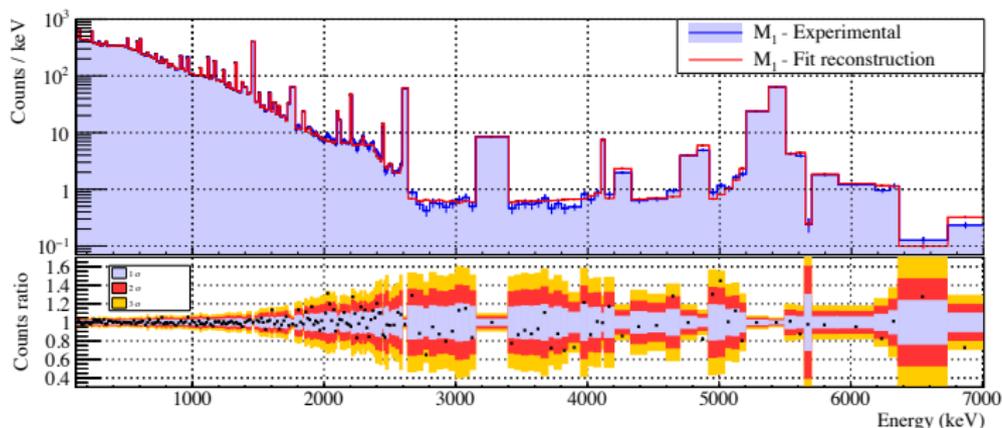
- Timing resolution:
Sum energy depositions occurring in same crystal in time window of ± 5 ms
- Energy resolution:
$$FWHM(E) = a + b \cdot E(\text{keV})$$
- Define coincidences:
Events between multiple bolometers within ± 5 ms window

Accidental Coincidences

- In real data, particles from different decay chains can hit multiple detectors simultaneously in time (e.g. during calibration using high activity sources)
 \implies Decay rate of progenitor nucleus of decay chain can be set retroactively

Particle Quenching

- E.g. α s exhibit negative quenching factor ($\sim 1\%$) that can be modeled

M_1 Spectrum JAGS Reconstruction (Simulation vs Data)

- Fit residuals have a Gaussian-like distribution compatible with mean = 0 and standard deviation = 1σ
- Reconstruction of similar quality also obtained with M_2 , Σ_2 spectra

*arXiv:1610.04518v1 [nucl-ex]

CUORE-0 BULK CONTAMINATION MODEL

Bulk Contamination of TeO₂ and Cu Frame (90 % C.L.)*

Material	Source	Activity (Bq/kg)
TeO ₂	²¹⁰ Po	$(2.39 \pm 0.11) \times 10^{-6}$
	²¹⁰ Pb	$(1.37 \pm 0.19) \times 10^{-6}$
	²³⁰ Th only	$(2.8 \pm 0.3) \times 10^{-7}$
	²³² Th only	$(7 \pm 3) \times 10^{-8}$
	²²⁸ Ra to ²⁰⁸ Pb	$< 3.5 \times 10^{-8}$
	²³⁸ U to ²³⁰ Th	$< 7.5 \times 10^{-9}$
	²²⁶ Ra to ²¹⁰ Pb	$< 7 \times 10^{-9}$
Cu frame [†]	²³⁸ U	$< 1.2 \times 10^{-5}$
	²³² Th	$< 2.1 \times 10^{-6}$

* Alduino, C., Alfonso, K., Artusa, D.R. et al. Eur. Phys. J. C (2017) 77: 543

[†] Cu frame includes all other small detector parts that have degenerate spectral contribution

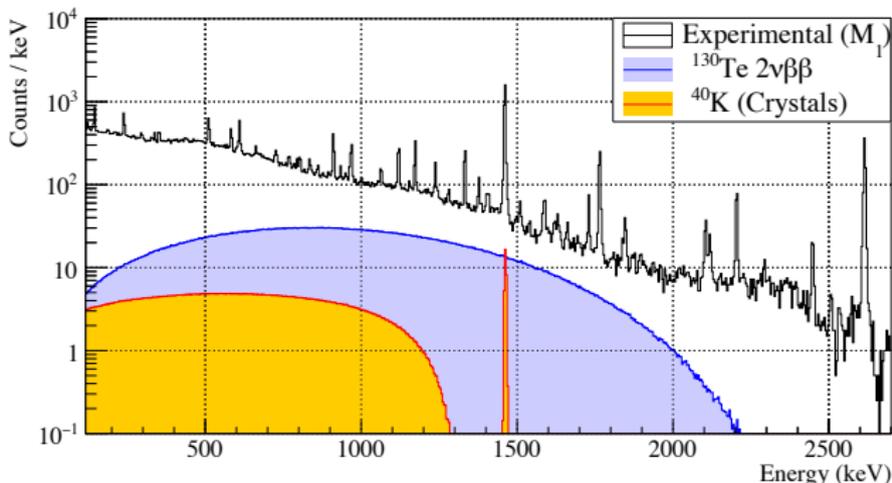
CUORE-0 SURFACE CONTAMINATION MODEL

Surface Contamination of TeO₂ and Cu Frame (90 % C.L.)*

Material	Contamination	Depth (μm)	Activity (Bq/cm ²)
TeO ₂	²¹⁰ Pb	0.001	$(6.02 \pm 0.08) \times 10^{-8}$
	²¹⁰ Pb	1	$(8.6 \pm 0.8) \times 10^{-9}$
	²²⁶ Ra to ²¹⁰ Pb	0.01	$(3.14 \pm 0.10) \times 10^{-9}$
	²²⁸ Ra to ²⁰⁸ Pb	0.01	$(2.32 \pm 0.12) \times 10^{-9}$
	²³⁸ U to ²³⁰ Th	0.01	$(2.07 \pm 0.11) \times 10^{-9}$
	²³⁰ Th only	0.01	$(1.15 \pm 0.14) \times 10^{-9}$
	²¹⁰ Pb	10	$< 2.7 \times 10^{-9}$
	²³² Th	10	$(7.8 \pm 1.4) \times 10^{-10}$
	²³² Th only	0.01	$(3 \pm 1) \times 10^{-10}$
Cu frame [†]	²³⁸ U	10	$< 3.3 \times 10^{-11}$
	²¹⁰ Pb	0.1	$(4.3 \pm 0.5) \times 10^{-8}$
	²¹⁰ Pb	0.01	$(2.9 \pm 0.4) \times 10^{-8}$
	²³⁸ U	10	$(1.38 \pm 0.16) \times 10^{-8}$
	²¹⁰ Pb	10	$< 1.9 \times 10^{-8}$
	²³² Th	10	$(5.0 \pm 1.7) \times 10^{-9}$

*Alduino, C., Alfonso, K., Artusa, D.R. et al. Eur. Phys. J. C (2017) 77: 543

†Cu frame includes all other small detector parts that have degenerate spectral contribution

Fitted Contribution of $2\nu\beta\beta$ and ^{40}K Background
 in Crystals (Simulation) to M_1 Spectrum (Data)


- $2\nu\beta\beta$ decay of ^{130}Te produce $\sim 10\%$ of events in γ region [118, 2700]keV
- $\Gamma_{2\nu} = (3.43 \pm 0.09) \times 10^5 \text{ Bq/kg}$
 $\Rightarrow T_{1/2}^{2\nu} = [8.2 \pm 0.2 \text{ (stat.)} \pm 0.6 \text{ (syst.)}] \times 10^{20} \text{ yr}$

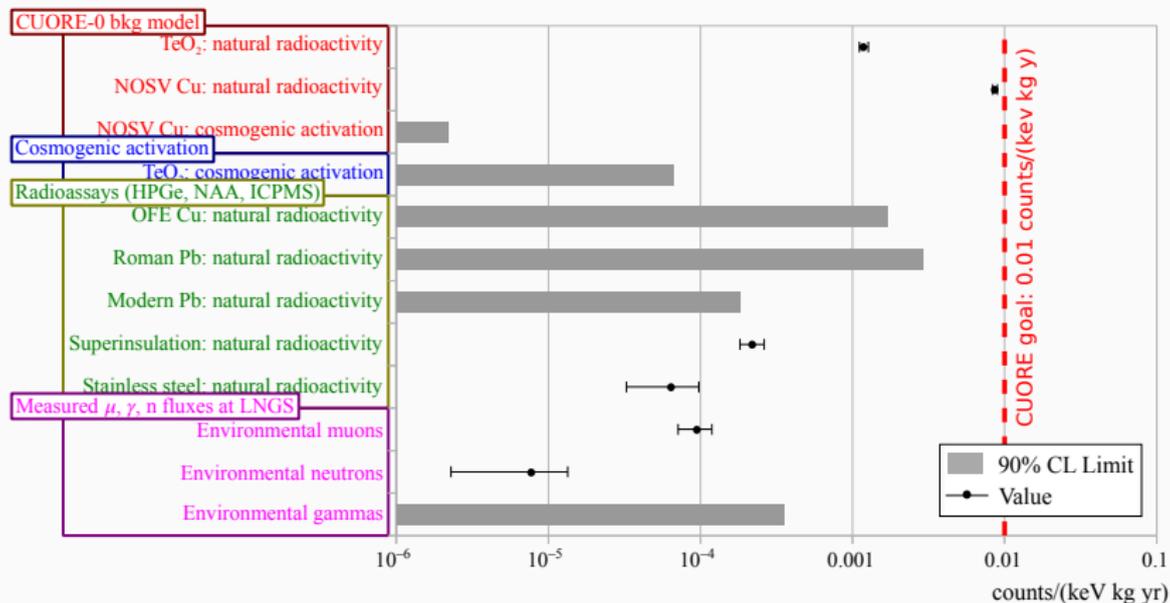
*arXiv:1610.04518v1 [nucl-ex]

CUORE-0 BACKGROUND FIT PROCESS

- Energy spectra for 57 contamination sources and distribution profiles created
- The activities of the sources are fitted to the experimental M_1 , M_2 , and Σ_2 spectra through a linear combination of the simulated spectra
- Fits are done using a Bayesian approach using JAGS* exploiting Markov Chain Monte Carlo simulations to sample the joint posterior PDF of source activities
- Priors:
 - Gaussian (or half-Gaussian) priors used when activity of source (or upper limits) known
 - Otherwise, uniform non-informative priors from 0 to upper limits compatible with data
- Fit allows for disentangling of contamination sources and study of secular equilibrium violations in radioactive decay chains

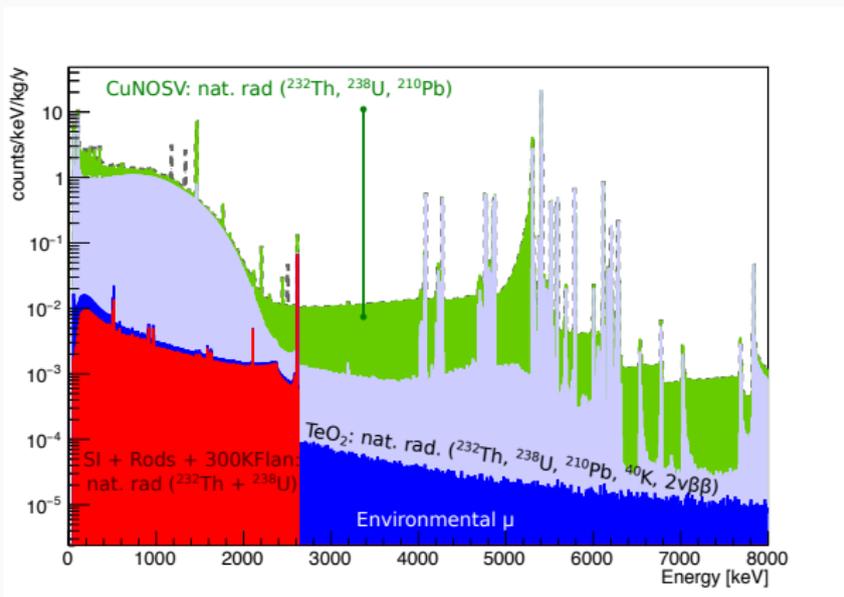
*Just Another Gibbs Sampler (JAGS), <http://mcmc-jags.sourceforge.net/>

CUORE BACKGROUND EXPECTATION*



*The projected background for the CUORE experiment, Eur. Phys. J. C (2017) 77:543

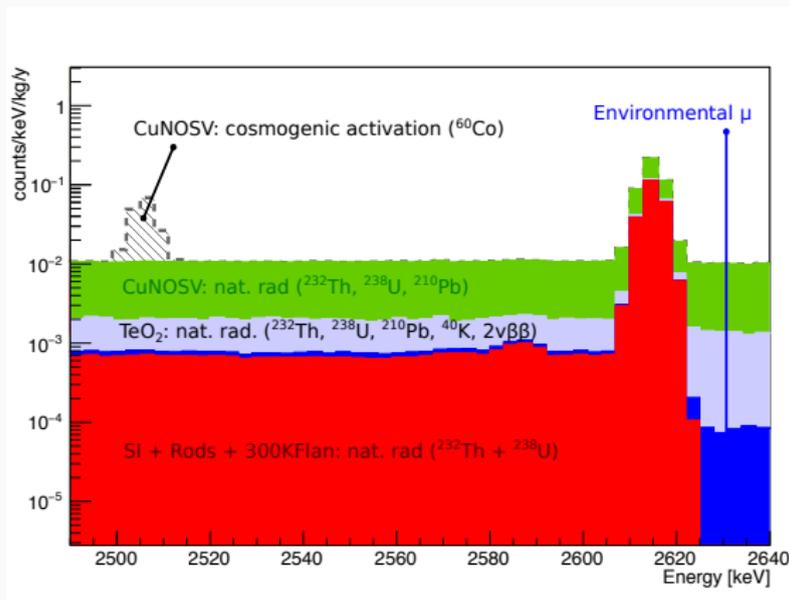
Full Spectrum [0, 8000]keV



- Anti-coincidence spectrum recorded by the 988 bolometer array
- ^{60}Co contamination in CuNOSV set at 90 % C.L. upper limit
- Additional sources set at values from CUORE-0 ($2\nu\beta\beta$, ^{40}K)

*The projected background for the CUORE experiment, Eur. Phys. J. C (2017) 77:543

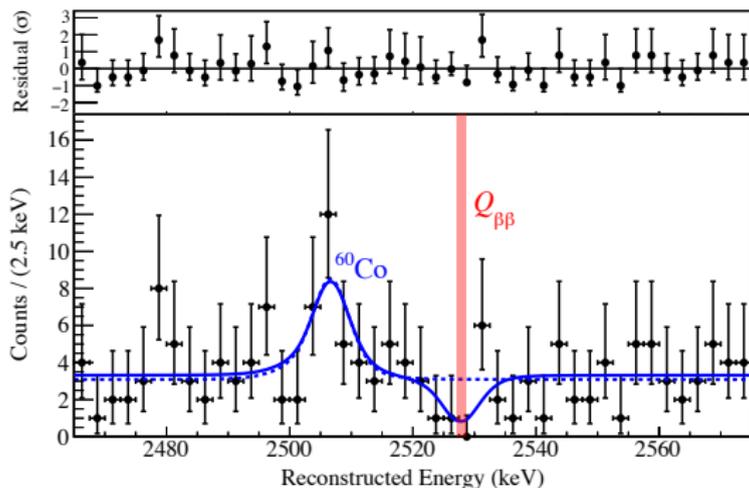
Region of Interest [2490, 2640]keV



- Anti-coincidence spectrum recorded by the 988 bolometer array
- ^{60}Co contamination in CuNOSV set at 90 % C.L. upper limit
- Additional sources set at values from CUORE-0 ($2\nu\beta\beta$, ^{40}K)

*The projected background for the CUORE experiment, Eur. Phys. J. C (2017) 77:543

$0\nu\beta\beta$ Peak Fit in ROI [2465, 2575]keV around ^{130}Te $Q_{\beta\beta} = 2528$ keV

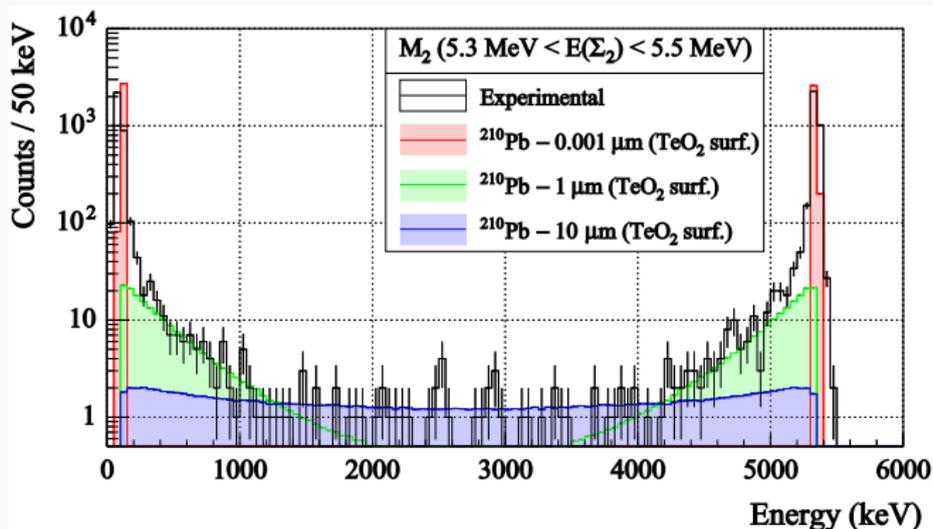


Best fit from unbinned extended maximum likelihood fit:

- Flat background in ROI = (0.014 ± 0.002) counts/(keV · kg · yr)
- Peak at $Q_{\beta\beta} = 2528$ keV fitted with variable rate
- Best fit decay rate (90 % C.L.): $\Gamma_{0\nu} < 0.52 \times 10^{-25} \text{ yr}^{-1} \implies T_{1/2}^{0\nu} > 1.3 \times 10^{25} \text{ yr}$

* First Results from CUORE: A Search for Lepton Number Violation via $0\nu\beta\beta$ Decay of ^{130}Te , CUORE Collaboration, Phys.Rev.Lett. 120 (2018) no.13, 132501

CUORE-0 ^{210}Po α decay*



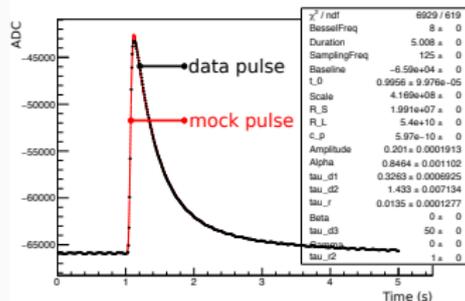
- Comparison between the experimental and the Monte Carlo M_2 spectra with Σ_2 energy equal to the Q value of ^{210}Po α decay.
- MC spectra with different TeO_2 surface contamination average depths 0.001, 1, 10 μm can be combined to fit shape of data

* Measurement of the two-neutrino double-beta decay half-life of ^{130}Te with the CUORE-0 experiment, Eur. Phys. J. C (2017) 77:13

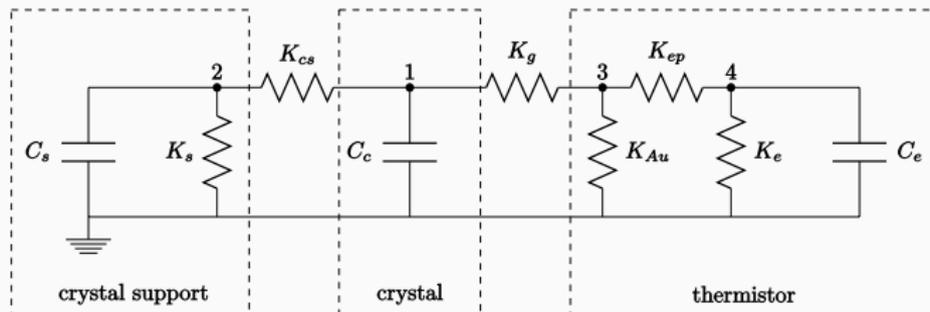
SIGNAL PULSE MODEL

- Rise time ~ 0.05 s
- 2 decay times: $\tau_1 \sim 0.2$ s, $\tau_2 \sim 1.5$ s
- Mock signal pulses can be reverse engineered from data based on thermal model circuit of bolometers
- Can be useful to test/optimize analysis steps or for pulse shape analysis by using “realistic” data

Real/Simulated Bolometer Pulse



Thermal model circuit*

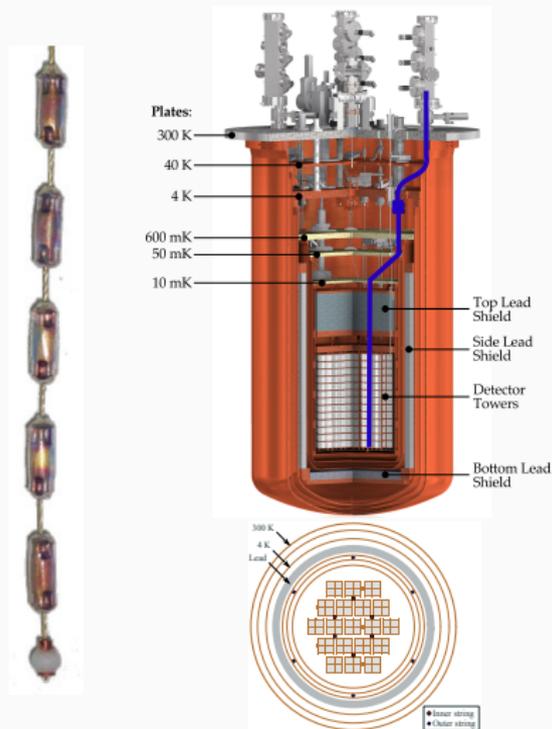


* M. Carrettoni and M. Vignati, 2011 JINST 6 P08007

- Detector simulations and background modeling were successfully demonstrated in pilot experiment CUORE-0
- Framework was updated to model backgrounds in CUORE and first analysis results further confirm accuracy of software
- Additional R&D efforts are underway to better understand backgrounds and improve our understanding of the detector

Backup Slides

DETECTOR CALIBRATION (IN-SITU)*



- Sources are put on 12 Kevlar strings and lowered under their own weight; a series of tubes in the cryostat guide the strings
- ^{232}Th γ sources (thoriated tungsten) are outside cryostat during physics data-taking and lowered into cryostat and cooled to base temperature for calibration
- Heat from sources is removed with:
 - A pair of copper blocks that mechanically squeezes on the sources at 4 K
 - Contact between the sources and their guide tubes, which are thermalized to different cryostat stages
- Temperature stabilization of the Mixing Chamber is able to compensate for the power dissipated during the deployment
- 6 inner strings: ~ 4 Bq
- 6 outer strings: ~ 20 Bq

CUORE BACKGROUNDS IN REGION OF INTEREST (ROI) (BACKUP)

Most Common Background Sources

- Long-lived radioactive nuclei: ^{40}K , ^{238}U , ^{232}Th
- Anthropogenic radioactive isotopes: ^{60}Co , ^{137}Cs , ^{134}Cs
- Cosmogenically-produced radioactive isotopes by n activation in Cu/Te



- Environmental n , μ , γ

Main Background Contributors to ROI

- multi-Compton events from 2615 keV γ from ^{208}Tl (from ^{238}U chain)*
- ^{238}U , ^{232}Th and decay products on surface of TeO_2 crystals
- ^{238}U , ^{232}Th and decay products on surface of materials close to TeO_2 crystals

Modeling backgrounds is important part of CUORE!

*This is the only environmental γ line with B.R. > 1% with energy > $Q_{\beta\beta}$

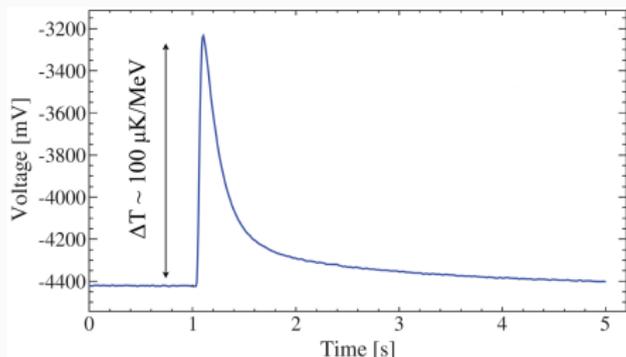
PARTICLE PROPAGATION (BACKUP)

- Program interface uses the standard UNIX command line options convention (e.g. `<executable> -<option> [argument]`) instead of using messenger classes derived from `G4UIMessenger` with macro files
 - ⇒ Easy storage of simulation settings in output data files for future reference
- Variable physics list that defaults to Livermore for accurate low energy (0–10 TeV) physics relevant in underground applications
- Variable material dependent tracking cuts used to balance simulation detail and speed, e.g.
 - 1 mm in TeO_2/Cu close to bolometers
 - 1 cm for high Z Pb and outer shields
- Particle sources:
 - Single particles: $e^\mp, \mu^\mp, \gamma, \alpha, \mathbf{n}$
 - Arbitrary sub-chains of decaying isotopes
 - ⇒ Useful for studying breaks in secular equilibrium within one chain
 - $\beta\beta$ decays with/without ν s from the ground or excited states of ^{130}Te
 - Thermal neutrons
 - Cosmic ray μ with zenith angle dependent flux
- Source positions:
 - Geometrically shaped distributions
 - Bulk of detector parts
 - Surface of detector parts (uniform distribution up to some depth into surface, or exponential profile)

DETECTOR PRINCIPLE (BACKUP)

Ultra-cold TeO_2 crystals function as very sensitive bolometer

- Energy response calibrated using known γ source
- Slow (~ 1 s) pulses suitable for rare event searches



OUTPUT SAVED FROM PARTICLE PROPAGATION (BACKUP)

Save important simulation output in 2 Trees

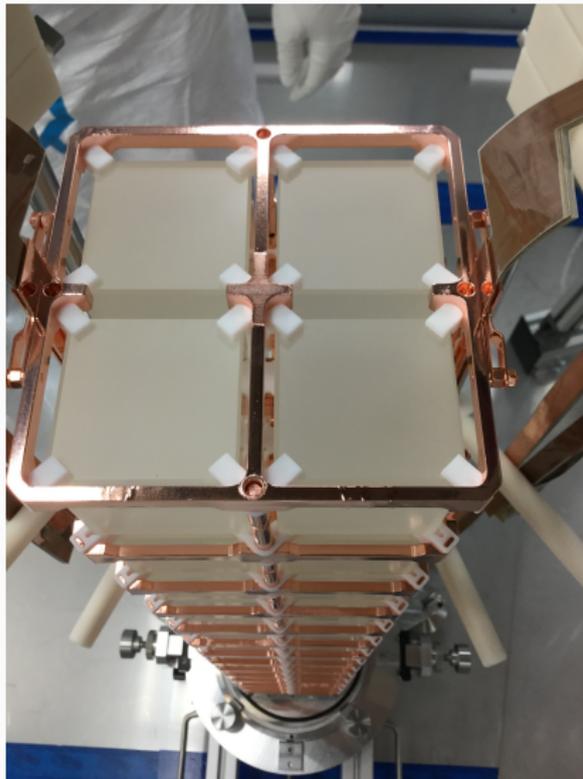
Tree 1

- Command line used to run simulation (with all options)
- Number of simulated events
- Number of simulated decay chains

Tree 2

- Channel number of TeO₂ bolometer
- Decay chain number
- Time of energy deposition
- Deposited energy (total)
- Deposited energy by particle (γ , e^{\pm} , \bar{p} , \bar{n} , α , ion, μ^{\mp})
- Energy deposited in surrounding copper material
- Parent ion of event
- Initial energy of parent ion
- Topological information of parent ion
 - x-position
 - y-position
 - z-position
 - x-direction
 - y-direction

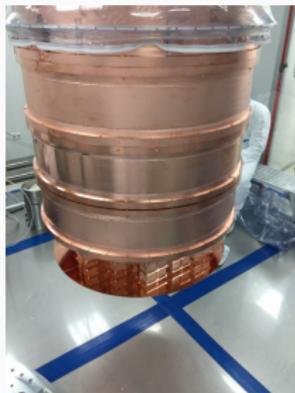
BACKGROUND FROM SOURCES NEAR TeO_2 DETECTORS (BACKUP)



- Both bulk and surface contaminations are significant and unique backgrounds from near sources
 - \therefore Closest to TeO_2 detectors, so radiation is not hindered
 - ^{40}K contamination significantly affects energy region of $2\nu\beta\beta$ spectrum
- Measured in CUORE-0
 - Single CUORE-like tower in Cuoricino cryostat
 - Saw reductions in α backgrounds due to improvements in construction process compared to predecessors

BACKGROUND FROM SOURCES FAR FROM TeO_2 DETECTORS (BACKUP)

10 mK Shield



Roman Pb Shield



4 K Insulation Foil



300 K Shield

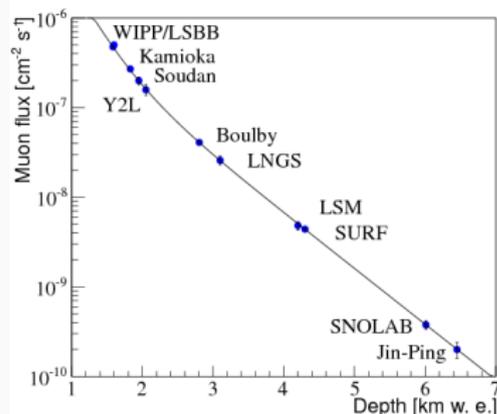


- Background contribution from bulk/surface contaminations degenerate
- Contaminations in shields act as background sources
- 4.5 t Roman lead
- 2.1 t modern lead
- Largest contributor: Roman Pb extracted from ancient shipwreck
 - $T_{1/2} = 22.3 \text{ yr}$

BACKGROUND FROM EXTERNAL SOURCES (BACKUP)

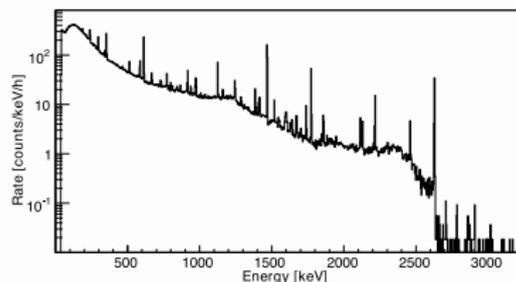
- Cosmic ray muons
 - Overburden 3600 m.w.e.
 - Flux $\sim 3 \times 10^{-8}$ /s/cm²
 - Average Energy ≈ 270 GeV

Underground Lab Depths



γ Spectrum in CUORE Hall*

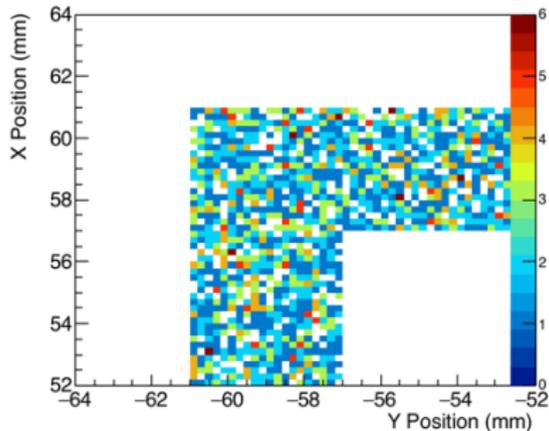
- Natural rock radioactivity
 - Gamma: ~ 0.73 /s/cm², energy $\lesssim 3$ MeV
 - Neutron: $\sim 4 \times 10^{-6}$ /s · cm², energy $\lesssim 10$ MeV



* Bellini, F., et al. Monte Carlo evaluation of the external gamma, neutron and muon induced background sources in the CUORE experiment. *Astroparticle Physics* 33.3 (2010): 169-174.

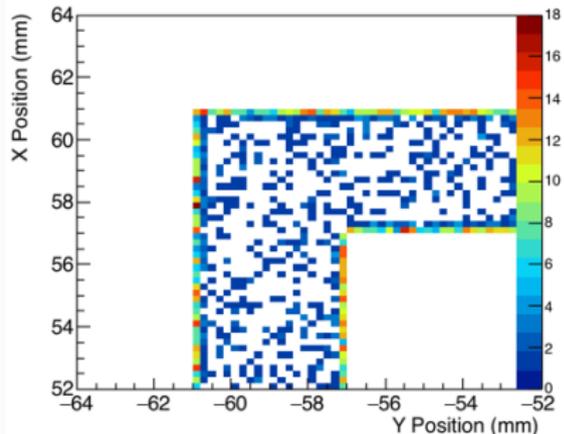
CONTAMINATION PROFILE (BACKUP)

Bulk Contamination^{*}



- Bulk contamination is assumed to be spatially uniform

Surface Contamination[†]



- Surface contamination is modeled with exponential density profile
- $\rho = \rho_0 \times \exp(-x/\lambda)$, where
 - x = penetration depth into surface
 - ρ_0 = impurity density
 - λ = mean depth, 0.001–30 μm

^{*}K. Alfonso

[†]K. Alfonso

SIMULATED BULK CONTAMINATION PARTS

TeO2-pt190	CuNOSV-u238	mu-R5m
TeO2-ra226-pb210	CuNOSV-co60	SteelRods-th232
TeO2-ra228-pb208	CuNOSV-th232	300K-2615
TeO2-sb125	CuNOSV-k40	300KFlan-2615
TeO2-2nu	CuNOSV-mn54	40K-2615
TeO2-2nu	PTFE-th232	4K-th232
TeO2-ag110m	PTFE-u238	4KTot-co60
TeO2-co60	PbRCu-th232	600mK-bi210
TeO2-th230only	PbRCu-u238	600mK-co60
TeO2-k40	PbR-ag108m	600mKFlan-th232
TeO2-th232only	PbR-bi210	600mKFlan-u238
TeO2-pb210	PbR-th232	600mK-th232
TeO2-u238-th230	PbR-u238	600mK-u238
TeO2-po210	CuUpStdPbPlug-th232	50mK-th232
NTD-th232	CuUpStdPbPlug-u238	50mK-u238
NTD-u238	TopPb5cm_210Bi	
	ExtPb5cm_210Bi	
	StdPbPlug-th232	
	StdPbPlug-u238	
	SI-2615	
	SI-2615	
	SI-tl208	

SIMULATED SURFACE CONTAMINATION PARTS

TeO2Sx-pb210-.001

TeO2Sx-pb210-10

TeO2Sx-pb210-1

TeO2Sx-ra226-pb210-.01

TeO2Sx-ra228-pb208-.01

TeO2Sx-th230only-.01

TeO2Sx-th232-10

TeO2Sx-th232only-.01

TeO2Sx-u238-10

TeO2Sx-u238-th230-.01

PTFESx-pb210-5

PTFESx-th232-5

PTFESx-u238-5

CuNOSVSx-pb210-.01

CuNOSVSx-pb210-10

CuNOSVSx-pb210-.1

CuNOSVSx-th232-.01

CuNOSVSx-th232-10

CuNOSVSx-u238-.01

CuNOSVSx-u238-10

CuNOSVTowerSx-pb210-1

CuNOSVTowerSx-th232-.01

CuNOSVTowerSx-th232-10

CuNOSVTowerSx-u238-.01

CuNOSVTowerSx-u238-10

CuNOSVTowerSx-pb210-.01

CuNOSVTowerSx-pb210-10

CuNOSVTowerSx-pb210-1

CuNOSVOthersSx-u238-10

CuNOSVOthersSx-u238-.01

CuNOSVOthersSx-th232-10

CuNOSVOthersSx-th232-.01

CuNOSVOthersSx-pb210-1

CuNOSVOthersSx-pb210-.1

CuNOSVOthersSx-pb210-10

CuNOSVOthersSx-pb210-.01

600mKSx-pb210-.01