(One Scientist's Perspectives on)

Radiopurity Databases for Detector Development

Douglas Leonard
IBS, Center for Underground Physics
05/24/2017

The (obvious) Need for Assay Databases

Published data:

Clearly there is much related published assay data. Some "random" examples:

D. Leonard, et al. (EXO-200 Colab.), Nucl. Inst. Meth. A 591 (2008) 490. **225 measurements**

D. Leonard, et al (EXO-200 Colab.), Nucl. Inst. Meth (2017) in press **91 measurements**

https://doi.org/10.1016/j.nima.2017.04.049

.. And many others (some referenced therein)

But no one paper contains all the world's copper measurements for example.

Conceptual Experiment Design:

- Need library of known realistically obtainable materials to design and show proof of principle of initial detector concept.
- Radiopurity.org serves well for surveying the published data to find realistic assumptions about obtainable material. (I look up my own data there often).
- But then must source and measure new items.
- Logs are born from materials or parts received.
  - Multiple samples and/or measurements come later.
  - History naturally fits hiearchical data structure well.
  - Radiopurity.org top level entry is a measurement.
  - Logbooks can link to measurement ID, but it's not as cohesive and ID's don't obtain conversational meaning.

Some History: Birth of a database

We've all sat in design meetings that went like this:

Joe: "What's the background if we use the new aluminum?"
Sue: "The new aluminum from last year."
Joe: "Yeah"
Matt: "40 uBq/kg… converting to ppt, I mean ppb."
Sue: "You forgot the branching ratio."
Jack: "Wait, wait, that's with *old-new* aluminum, not the *new-new* aluminum."
Joe: "Some grad student figure this out for next week."

Next week
Joe: "What's the background if we use the new aluminum?"
Sue: "The new aluminum from last year…."

Random Post doc (that was me): "**Hey, let's use our e-log and write this stuff down!**"

This costs real time and productivity.

More than just numbers

A real experiment needs to track complex and in-house information.

- Invoices
- Quoted text from email conversations with suppliers.
- Information on batches, quantities, locations, handling, cleaning.
- Preliminary (not always publishable) analysis results, still under discussion.
- Measurements of “trade secret” parts and materials, sometimes under active development with corporations, even with NDA’s. (non-disclosure agreements).
- How material connects to internal design decisions/applications.

These things sound like experimental log books, not public data summaries.

The simple solution: PSI E-log

- In EXO-200 we gave a material or part a numbered e-log entry.
- Sub id's like 34.a and 34.b assigned by hand (text). For batches, varieties, etc.
- Extensive notes about dates, batches, handling methods etc.
- Summarized and attached analysis reports.
- Sometimes attached related MC background reports as well.
- Related entries were "linked" simply by writing about them.

Pros:

-Very easy to setup when it was needed yesterday.

-Encouraged communication with complete thoughts and stories.

-Real log-booking like scientists should do.

-Helps avoid tunnel vision, missing details.

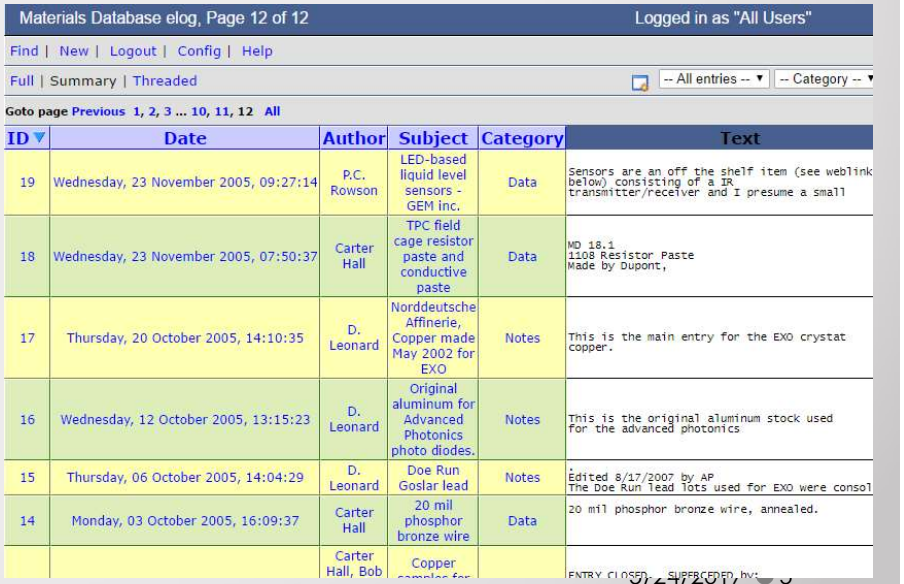
Cons:

-No structured data

-No automated overview of assay results

-Overview summaries were made by hand in excel.

-No revision history or dates => updates to summaries required diligent oversight or reviewing EVERY entry for changes.



Materials Database elog, Page 12 of 12 — Logged in as "All Users"

Find | New | Logout | Config | Help

Full | Summary | Threaded — -- All entries -- — -- Category --

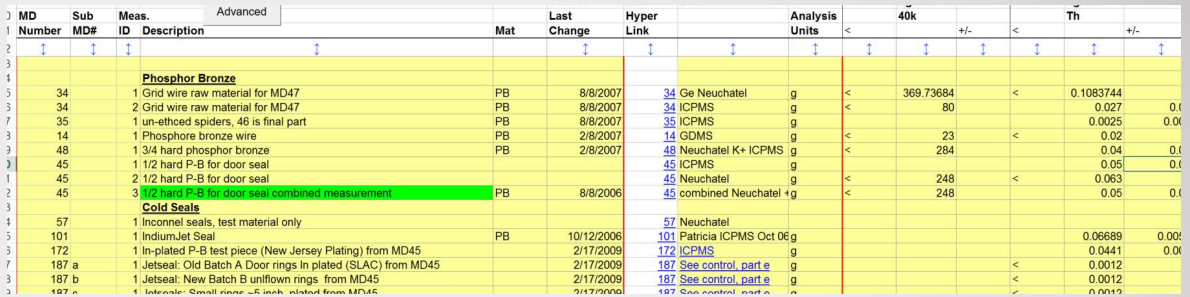
Goto page Previous 1, 2, 3 ... 10, 11, 12 All

ID	Date	Author	Subject	Category	Text
19	Wednesday, 23 November 2005, 09:27:14	P.C. Rowson	LED-based liquid level sensors - GEM inc.	Data	Sensors are an off the shelf item (see weblink below) consisting of a IR transmitter/receiver and I presume a small
18	Wednesday, 23 November 2005, 07:50:37	Carter Hall	TPC field cage resistor paste and conductive paste	Data	MD 18.1 1108 Resistor Paste Made by Dupont,
17	Thursday, 20 October 2005, 14:10:35	D. Leonard	Norddeutsche Affinerie, Copper made May 2002 for EXO	Notes	This is the main entry for the EXO crystat copper.
16	Wednesday, 12 October 2005, 13:15:23	D. Leonard	Original aluminum for Advanced Photonics photo diodes.	Notes	This is the original aluminum stock used for the advanced photonics
15	Thursday, 06 October 2005, 14:04:29	D. Leonard	Doe Run Goslar lead	Notes	. Edited 8/17/2007 by AP The Doe Run lead lots used for EXO were consol
14	Monday, 03 October 2005, 16:09:37	Carter Hall	20 mil phosphor bronze wire	Data	20 mil phosphor bronze wire, annealed.
		Carter Hall, Bob	Copper		ENTRY CLOSED - SUPERCEDED by:

Beyond logging: Bkgd Estimations

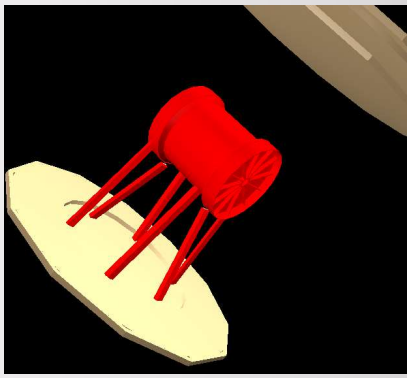
Programmatic spreadsheet to summarize :

1) Materials assay (auto-linked to elog)
2) Monte Carlo efficiencies.



MD Number	Sub MD#	Meas. ID	Description	Mat	Last Change	Hyper Link		Analysis Units	<	40k	+/-	<	Th	+/-
			Phosphor Bronze											
34		1	Grid wire raw material for MD47	PB	8/8/2007	34	Ge Neuchatel	g	<	369.73684		<	0.1083744	
34		2	Grid wire raw material for MD47	PB	8/8/2007	34	ICPMS	g	<	80			0.027	0.0
35		1	un-ethced spiders, 46 is final part	PB	8/8/2007	35	ICPMS	g					0.0025	0.00
14		1	Phosphore bronze wire	PB	2/8/2007	14	GDMS	g	<	23		<	0.02	
48		1	3/4 hard phosphor bronze	PB	2/8/2007	48	Neuchatel K+ ICPMS	g	<	284			0.04	0.0
45		1	1/2 hard P-B for door seal			45	ICPMS	g					0.05	0.0
45		2	1/2 hard P-B for door seal			45	Neuchatel	g	<	248		<	0.063	
45		3	1/2 hard P-B for door seal combined measurement	PB	8/8/2006	45	combined Neuchatel +	g	<	248			0.05	0.0
			Cold Seals											
57		1	Inconnel seals, test material only			57	Neuchatel							
101		1	IndiumJet Seal	PB	10/12/2006	101	Patricia ICPMS Oct 06	g					0.06689	0.005
172		1	In-plated P-B test piece (New Jersey Plating) from MD45		2/17/2009	172	ICPMS	g					0.0441	0.0
187 a		1	Jetseal: Old Batch A Door rings In plated (SLAC) from MD45		2/17/2009	187	See control, part e	g				<	0.0012	
187 b		1	Jetseal: New Batch B unlflown rings from MD45		2/17/2009	187	See control, part e	g				<	0.0012	

3) Parts. Could create parts on-the-fly (during meetings) to estimate backgrounds
   - Select material
   - Enter mass/quantity
   - Choose closest existing MC (guess) efficiencies.
   - Estimates background impact.
   - For quick decisions, MUCH faster than waiting for a new MC, and often good enough.



- Includes functions to standardize Bayesian limit calculations and prepare latex table for publication, but it wasn't very friendly to most users.

Material Description	URL	Sort	Update	Log	/use/location/notes	mat.	MD#	MD#	ID	IDX	[fraction]	Used	Status	Assigned to	items	per item	unit	units	Match	qu
Combined Shiva+INMS unaltered spectator	13	1	10/6/2009		Cryostat		13	2	2	2	1	1	Choose right material		1	5901000	g	g	yes	
Flat cable, 25um, kapton layer	1	2	9/1/2006	34	OV feedthrough		1	1-kapt	1	2	1	1	Final: installed		1	20	cm^2	cm^2	yes	
Flat cable, 25um, kapton layer	1	3	8/9/2006	13	Used as cover in Vac region		1	1-kapt	1	2	1	1	Final: installed		1	323	cm^2	cm^2	yes	
Flat cable, 40um, kapton layer	1	4	8/9/2006	13	Used as cover in Vac region		1	2-kapt	1	2	1	1	Final: installed		1	1084	cm^2	cm^2	yes	
APD combined worst case limit	98	5	9/13/2006			170&98	98		3	1	1	1	Final		518	1	APD	APD	yes	
Paint for Lead bricks, Doe Run Goslar	29	6	8/8/2006		Lead brick paint		29		1	4	1	1	Final		1	300	g	g	yes	
Goslar Lead MD25-28, worst case limits.	25-28	7	8/8/2006		Lead Rear plus main		25-28		1	6	1	1	Final		1	43819000	g	g	yes	4
SNO Acrylic	59	8	8/26/2006		ring supports??		59		1	1	1	1	needs info, see also MD 180	Pocar	1	1000	g	g	yes	
vaccum grease	213	9	8/14/2008		outside OV		213		1	4	1	1	Quantities can't be known		1	5	g	g	yes	
Simolex translucent Si crown o-ring, 7mm	165	10	1/22/2007		crown ring		165	1	1	4	1	1	Final		1	233	g	g	yes	
Simolex translucent Si door o-ring, 8mm	165	11	1/22/2007		door ring		165	2	1	4	1	1	Final		1	201.6	g	g	yes	
Phosphor bronze bolts for IV teflon support	108	12	8/24/2006	18	vacuum region		108		1	2	1	1	nuts&bolts need checking	Pocar	4	80	g	g	yes	
Phosphor bronze bolts for IV teflon support	108	13	1/24/2007	18	vacuum region		108		2	2	1	1	nuts&bolts need checking	Pocar	4	80	g	g	yes	
5/8"-11 x 2" Si-bronze screws	75	14	8/31/2006		outside OV		75		1	4	1	1	nuts&bolts need checking	Pocar	96	53.6	g	g	yes	
5/8" flat washers (copper color)	76	15	8/31/2006		outside OV		76		1	4	1	1	nuts&bolts need checking	Pocar	96	15	g	g	yes	
5/8" Si-bronze lock washers	77	16	8/31/2006		outside OV		77		1	4	1	1	nuts&bolts need checking	Pocar	96	11.4	g	g	yes	

Incremental advance: Present CUP Materials Database

- Motivation again dominated by deployment speed (and learning curve/resistance).
- Reimplementation (by me) of e-log in Twiki environment.
- Does about everything E-log does (except maybe threaded replies).
- But with power of Twiki (now FosWiki):relative links, advanced search, formatting, tables, etc.

Big Advantage: Revision History

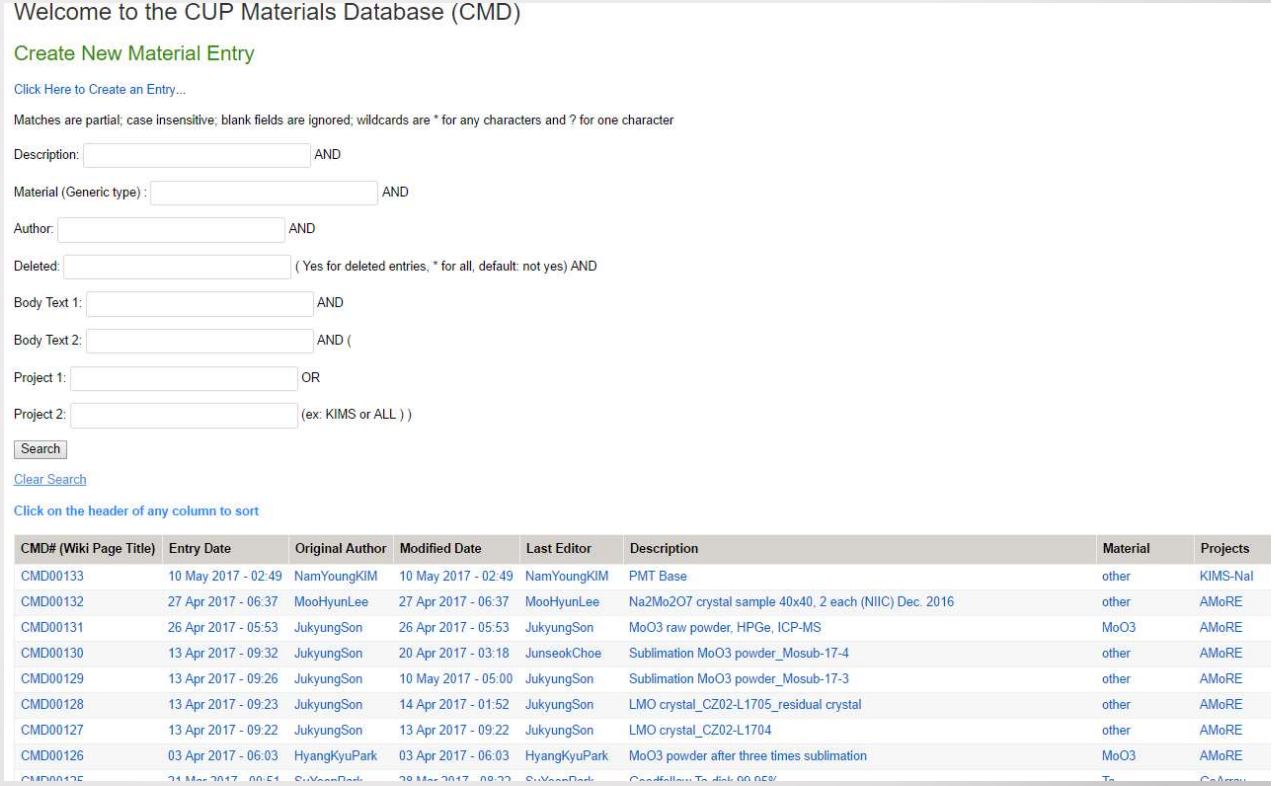
-Can sort entries to find recent changes.

-Can show differences and old versions, (mostly meets no-erasure logging requirements).

- Integrated with/auto-linked-from CUP assay request queues.

Cons:

Still just log entries at its core.



Welcome to the CUP Materials Database (CMD)

Create New Material Entry

Click Here to Create an Entry...

Matches are partial; case insensitive; blank fields are ignored; wildcards are * for any characters and ? for one character

Description: AND

Material (Generic type) : AND

Author: AND

Deleted: (Yes for deleted entries, * for all, default: not yes) AND

Body Text 1: AND

Body Text 2: AND (

Project 1: OR

Project 2: (ex: KIMS or ALL))

Search

Clear Search

Click on the header of any column to sort

CMD# (Wiki Page Title)	Entry Date	Original Author	Modified Date	Last Editor	Description	Material	Projects
CMD00133	10 May 2017 - 02:49	NamYoungKIM	10 May 2017 - 02:49	NamYoungKIM	PMT Base	other	KIMS-NaI
CMD00132	27 Apr 2017 - 06:37	MooHyunLee	27 Apr 2017 - 06:37	MooHyunLee	Na2Mo2O7 crystal sample 40x40, 2 each (NIIC) Dec. 2016	other	AMoRE
CMD00131	26 Apr 2017 - 05:53	JukyungSon	26 Apr 2017 - 05:53	JukyungSon	MoO3 raw powder, HPGe, ICP-MS	MoO3	AMoRE
CMD00130	13 Apr 2017 - 09:32	JukyungSon	20 Apr 2017 - 03:18	JunseokChoe	Sublimation MoO3 powder_Mosub-17-4	other	AMoRE
CMD00129	13 Apr 2017 - 09:26	JukyungSon	10 May 2017 - 05:00	JukyungSon	Sublimation MoO3 powder_Mosub-17-3	other	AMoRE
CMD00128	13 Apr 2017 - 09:23	JukyungSon	14 Apr 2017 - 01:52	JukyungSon	LMO crystal_CZ02-L1705_residual crystal	other	AMoRE
CMD00127	13 Apr 2017 - 09:22	JukyungSon	13 Apr 2017 - 09:22	JukyungSon	LMO crystal_CZ02-L1704	other	AMoRE
CMD00126	03 Apr 2017 - 06:03	HyangKyuPark	03 Apr 2017 - 06:03	HyangKyuPark	MoO3 powder after three times sublimation	MoO3	AMoRE

(Brief) Outline of a Gen 2 Database

4 Parts of an advanced Database (based on EXO-200 experience, outlined for nEXO)

1) "Material" Entries:

- Track materials and/or parts having potential bkgd impacts to experiments.
- Track samples, assays, and quantitative results.

2) Monte Carlo:

- Database for MC efficiencies in re-normalizable units: ex: hits per decay in ROI.
- Better yet, root file of full MC output, or both.

3) Detector Models,

- Multiple detectors definable for development/hypotheticals
- Consists of parts defined by:
  - Material
  - MC
  - Mass or extent (cm^2 of reflector, cm of cable, ea PMT etc) and count. …

4) Background Impact Estimation

- Estimate backgrounds from detector models and parts.
- Depending on level of detail stored in MC database, can be simple bkgd ROI estimates, or full virtual experiment sensitivity estimations.

Of course include revision date and history.

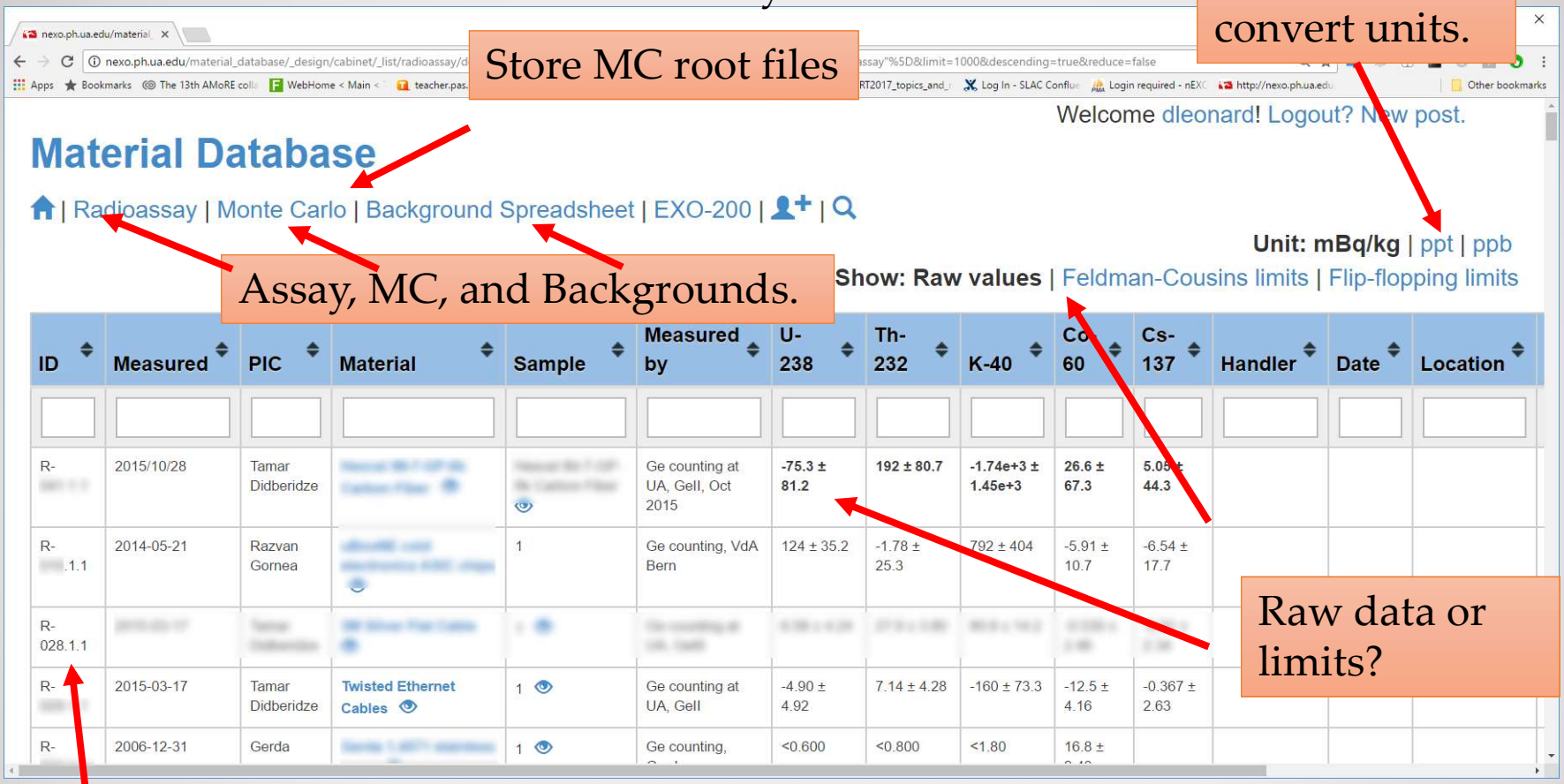
Full design defined efforts and interfaces in detail. Forethought is required.

More detail of original concept provided in backup slides.

nEXO "Cabinet" Database ("Gen 2" design)

- Programmed by R. Tsang, inspired by concept above.

Summary view:



Software:

- Couchdb database engine
- Json document format
- Elasticsearch searching

Cons:

Attachments, formatting, linking etc.. less advanced than Twiki (for now).

Cabinet Assay Entry

- **Title**: Twisted Ethernet Cables
- **ID**: R-029
- **Material Name**: Cinch cat ethernet cable
- **Original Author**: Tamar Didberidze
- **Intended use**: Cables
- **Actual use**:
- **Real or MC**: Real
- **Descriptions**: Received from Ralph DeVoe at the University of Alabama on ~ 02/24/2015.
  Twisted pair: 2 25 foot lengths of Cinch cat 6 ethernet cable, part # 73-8891-25. Ordered from Mouser
  Related counting and analysis information on UA Elog: http://130.160.100.75/Gell/64 .
- **Remarks**: Technical Drawing: EthernetCabledr-73-8891-25.pdf
- **Tags**:

Remarks fields replaces elog text. (poor example)

R-029.1
1

Sample 1

- **Sample ID**: 1
- **Supplier**: Mouser(Ralph DeVoe)
- **Product**: Cinch cat ethernet cable
- **Part number**: 73-8891-25
- **Lot number**:
- **Normalized by (e.g. mass, area, length)**: -
- **Mass/Area/Length (without unit)**: 312.1
- **Unit (of mass/area/length)**: g
- **Sample descriptions**: Twisted pair: 2 25 foot lengths of Cinch cat 6 ethernet cable, part # 73-8891-25. Ordered from Mouser.
- **Remaining quantity**:
- **Unit (for 'Remaining quantity')**:
- **Location**:
- **Date (yyyy-mm-dd)**:
- **Mother sample (leave blank if from vendor)**:
- **Sample remarks**:

Measurement 1

R-029.1.1
Ge counting at UA, Gell

- **Label (e.g. 'UA, NAA, 2015-09-01')**: Ge counting at UA, Gell
- **Detector**: Gell at University of Alabama
- **Measured by**: Tamar Didberidze
- **Date of measurement (yyyy-mm-dd)**: 2015-03-17
- **Counted from (yyyy-mm-dd)**: 2015-02-26
- **Counted to (yyyy-mm-dd)**: 2015-03-17
- **Livetime [s]**: 1537398.6
- **Normalized by (e.g. mass, area, length)**: -
- **Mass/Area/Length (without unit)**: 312.1
- **Unit (of mass/area/length)**: g

Analysis 1

R-029.1.1.1
Tamar Didberidze

- **Analyzer**: Tamar Didberidze
- **Analysis quality**: -
- **Measurement type**: Regular measuremer
- **U-238**:
  - **Specific Activity**:
  - **Error type**: Symmetric error (68% C
  - **Error**: 4.92
  - **Alternate limit**:
  - **Systematic error**:
  - **Lower error (for asym. err.)**:
  - **Unit of measurement**: mBq/kg
- **Th-232**:
  - **Specific Activity**

Attachments

Attachments
TwistedCablesIntheGellDetector_UA.jpg
TwitedCablesIntheGellDetector_UA.jpg
GellBackground_vs_nEXOTwistedCable_UniversityofAlabama_Gell.pdf
EthernetCabledr-73-8891-25.pdf
SimulationofTwistedEthernetCables_Gell_UniversityofAlabama.pdf
TwistedEthernetCables_UniversityofAlabama_Gell_Analysis.xlsx
TwistedEthernetCable_UniversityofAlabama_Gell_Fits.pdf
Internal ID: #75250f269e3ebe9e66512ef1512611a1

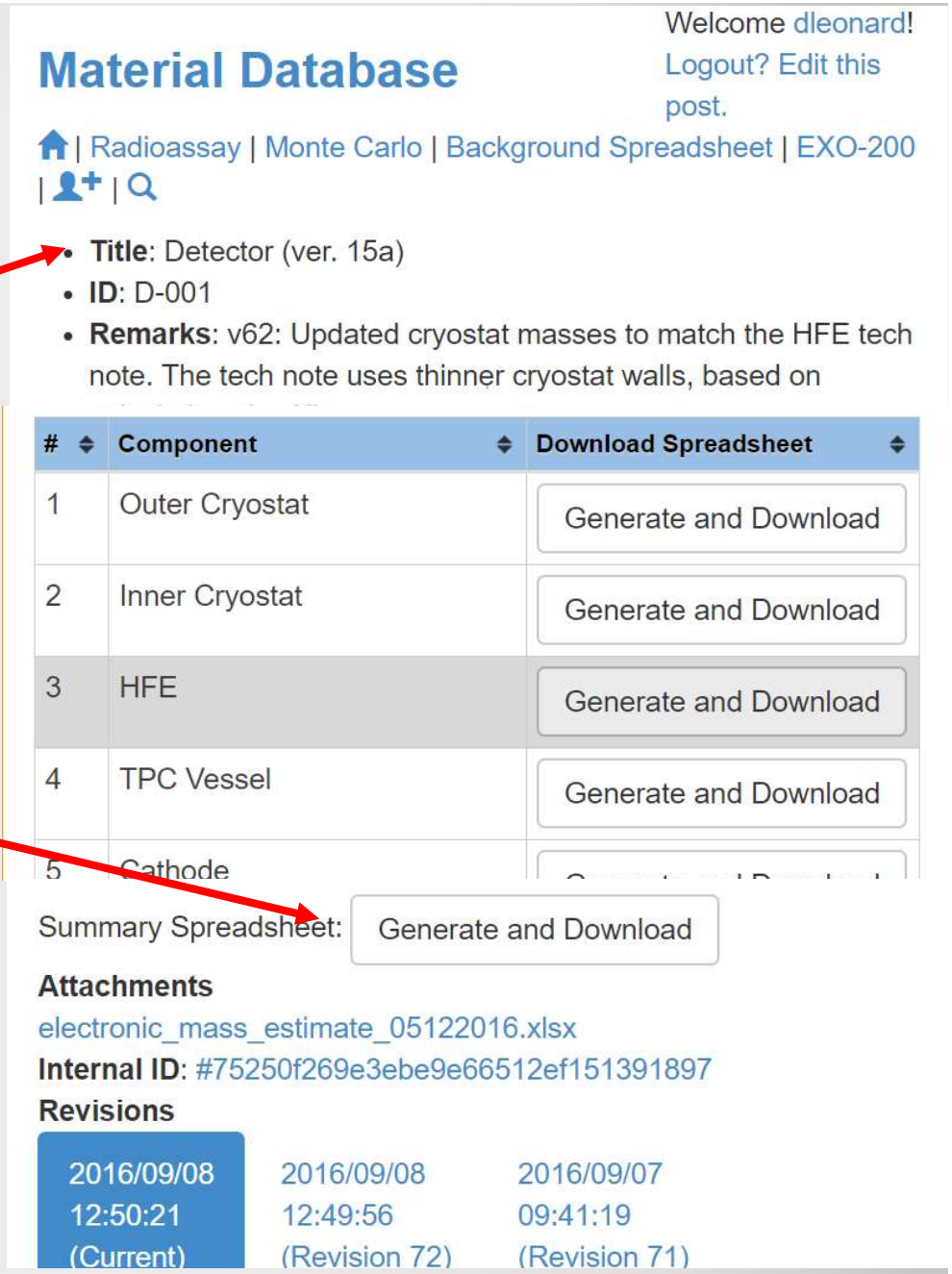
Revisions

Revisions

2017/05/18 14:42:11	2015/03/27 11:28:24	2015/03/26 18:36:53	2015/03/26 18:20:42	2015/03/26 18:17:40	2015/03/26 18:17:17	Show More

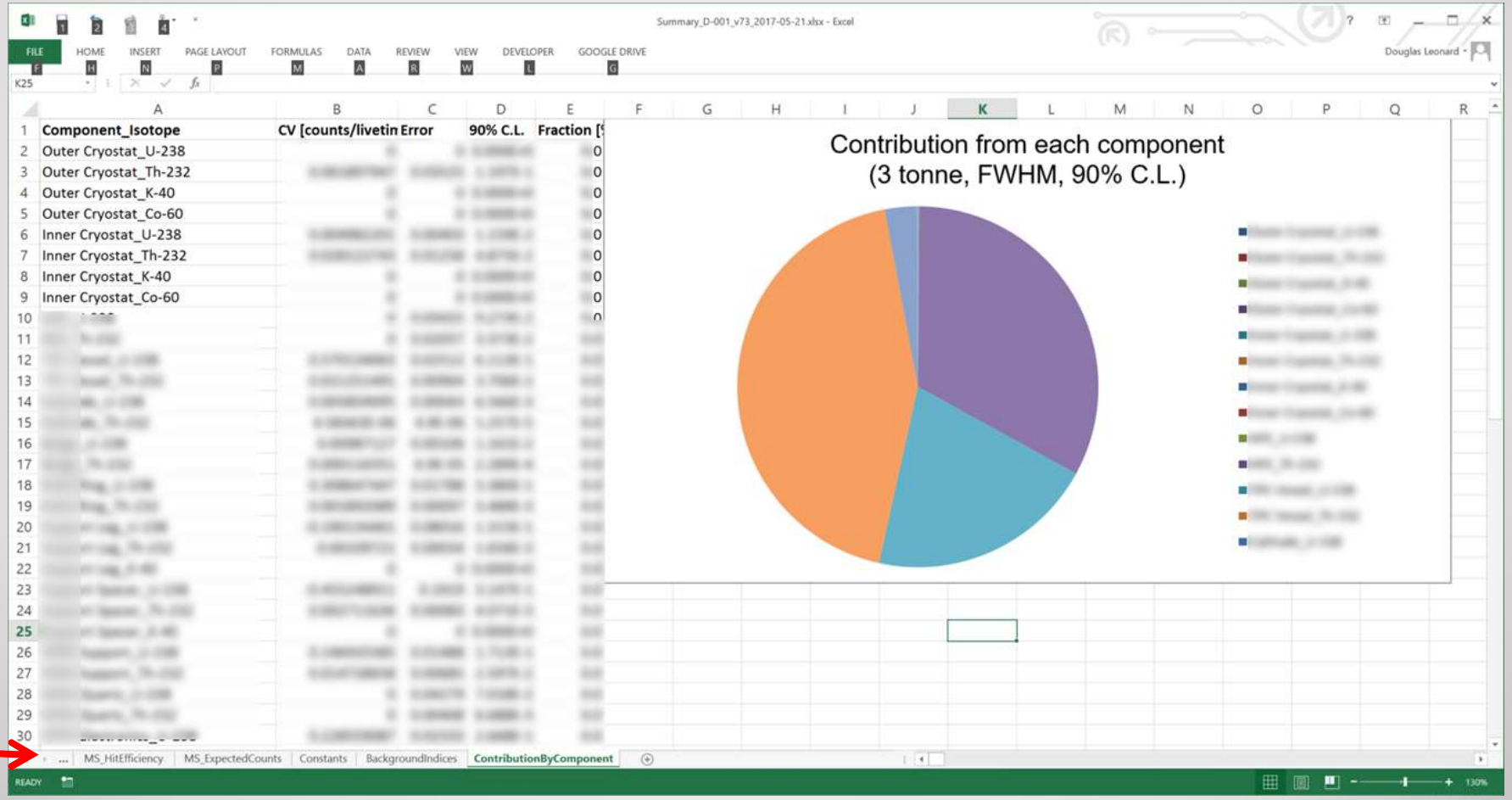
Cabinet Detector Model

- Detector models
- Built from parts.
  (defined by material, MC, etc)
- Generates background spreadsheet.



Cabinet Background Summaries

- Many, many, tables and views provided to assess bkgd contributions.
- What-if analysis can be done at spreadsheet level or starting in database.
- Limits using Bayeseian/FC/truncated-gaussian.



Component_Isotope	CV [counts/livetin	Error	90% C.L.	Fraction [%
Outer Cryostat_U-238				0
Outer Cryostat_Th-232				0
Outer Cryostat_K-40				0
Outer Cryostat_Co-60				0
Inner Cryostat_U-238				0
Inner Cryostat_Th-232				0
Inner Cryostat_K-40				0
Inner Cryostat_Co-60				0

(Some) Other Databases

- Radiopurity.org (previous talk)

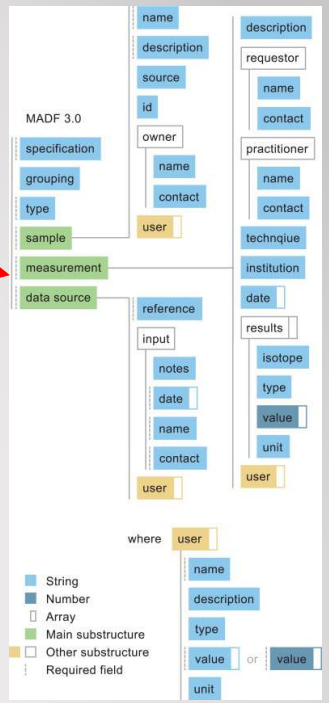
J.C Loach, J. Cooley, G.A. Cox, Z. Li, K.D. Nguyen, A.W. P. Poon, Nucl. Instrum. Meth. A 839 (2016) 6-11

nEXO database developed independently, but ultimately very similar.

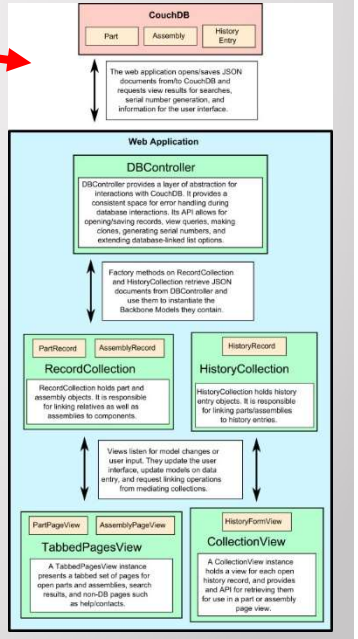
nEXO data structure more hiearchical.

-radiopurity.org one document per measurement, very suitable for published data.

-nEXO document vaguely defines a "material" with many "samples", "measurements" and "analyses"



- Majoranna : N. Abgrall et. al. Nucl. Instrum. Meth. A 779 (2015) 52-62.
  - Also couchdb, json, (and I think elasticsearch from discussion with Robert Varner)
  - Parts tracking database, NOT an assay database.
    - Three record types: parts, assemblies, histories.
    - In my experience, this is important, difficult, and potentially lacking in other solutions.
    - But also difficult to structure.
  - Paper notes the flexibility of json documents (and difficulty of generic queries).



- Kamioka: Next talk.

(Some) Other Databases contd..

- LZ:

LZ Information Repository

Database:	Screening	Cleanliness Controls	Analytics	Parts
eLog:	Screening	Cleanliness Controls	Materials	Parts
Tools:	Custom QR generator	Calculators	Geo-location	Apply account
Auxiliary:	WindChill	PMT test@Brown	LZ Twiki	Help

- Maintained by Joseph Hor and Jerry Busenitz. University of Alabama.

Similarly includes tools for:

  - Assay measurements
  - Cleaning protocols and related docs
  - Parts tracking
  - Background calculations, with what-if scenarios.
  - Uses QR labels to find web entry.
  - Based on MongoDB (like couchdb, holds json documents)

- **Others? Probably far from exhaustive list.**

Final Thoughts

- Real experiments complicate software and data structure demands.
- Json is flexible (extensible), difficult to query, but unanimous favorite.
- Hiearchy may limit compatibility though.
- Can databases be similar enough to easily transfer data to a world database?
  Probably yes, but will it anyone spend time on automated translation?
- Published data needs review of details anyway.

- Now considering Cabinet (nEXO) database for future of CUP experiments (and elsewhere?)
  - May use professional development support.
  - Other similar efforts ongoing, let's keep in touch when possible.

- Is too much structure bad?
  - Do people still pause to write down what happened?
  - Do they see a logbook?
    … Or a computer system with check boxes?
  - Do they just ask (ok, ok, but which boxes do you want me to tick?)
  - Is e-log (or the Twiki replacement) still the best?
  - Can we ever know all the data structure we'll need?
  - Is json flexibility enough to overcome that (does nothing without human work)?

- Fast estimates from existing MC and assay are crucial to efficient design cycle.
- **Decisions** are facilitated by structured databases providing the latest answers and summaries.