



Instrument & Facility PIDs

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CONSTRAINTS AND SOME
SUGGESTIONS


Core Facility Perspective

- Last mile problem
- Prevalent Example
- Challenges
- Ideas
- Q+A



Example: ORCID

ORCID. 2012. Adoption is widespread. Beneficial PID



User. Citation > Recognition. Accessibility > Wider Career options




Institutions. Citation > Recognition. Wider circulation > Prestige




Personal. ORCID > Institutional Career Database > Useful for my promotion > Will adopt it

Core RRID Challenge


Core RRID. Not widely adopted. Unfamiliar. PID Challenge. Early years




Core Staff. Not familiar. Usage low at Univ. settings > Lack of human resources



Links. Depend > Institutions. Disappear > Cores merge/sunset. Lack of IT Support > Web site upkeep. May lack permission to update



Repository. Institution/Core > Primary; Not permanent > So, need 2nd repository



RRID. Core: Need to promote. Staff buy-in needed. Convincing reason

Core RRID Challenge Continued


RRID. Cores not static. Dynamic. Instruments removed/added/upgraded.



Challenge: How do we reconcile RRIDs established, say 5 years apart?



Staff: What incentive staff/user have adding RRIDs? Feedback needed




Challenge: Definition. Hardware? Software? Personnel? Ownership?

Instrument RRID Challenge


Instrument RRID. Even less widely adopted. Unfamiliar. Early phase.




Staff/User. Not familiar > May not use it. Feedback for lack of use



Reference. Depend > Manufacturer. Disappear > Companies
Merge/Close > Link rot




Links. No Incentive > Old equipment; Not permanent



Companies. Incentive > New equipment; Not permanent > So, need 2nd
repository

Instrument RRID Challenge continued

RRID. Instrument: Clarification needed for usage. Hardware? Software?
Combo?



User: Use multiple instruments. How core staff handle all?



RRID. Instrument: Calibration? Add-ons/Modifications?

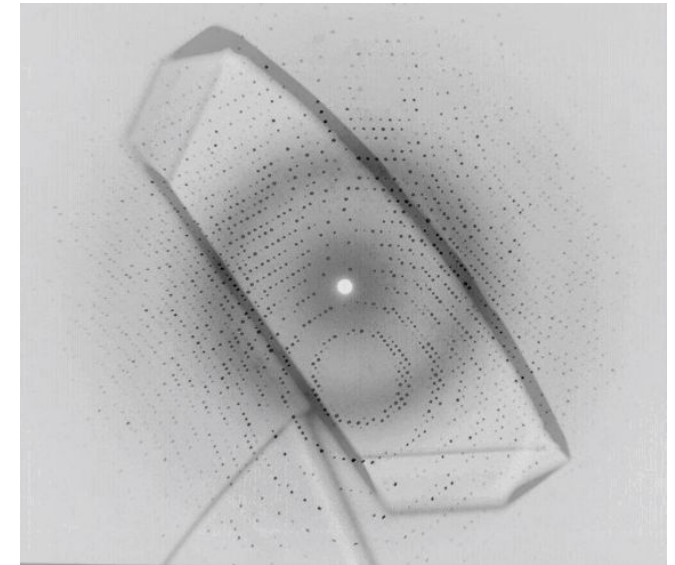


Core. Service oriented. Lack enforcement

Changing Data


Early 2000s

- ~~One structure~~ one Ph.D. student **thesis**
- **Two dozen** data sets
- Data collection lasted **days**
- Data collection was **local**
- Recollect/track most of the details
- Bulk of the data was 7MB x 60 frames **420 MB raw data**
- Processed data was 400 kB x 60 frames **24 MB**



Meta Data: User and Instrument

User Meta Data 1999

Sample#	Prep. #	Date	OD20020	Conc. (mg/ml. after dialysis)	Glycerol (%)	Mg** (mM)							
Ak_4b		n/a											
Crystallization setup	Date	Tray #	Well #	Temp (C)	Drop-PEG (%)	Glycero l (%)	Size- (μL)	Well- PEG (%)	glycerol- (%)	Size- (μL)	Growth-time (d)		
Tray1/14-24	03/23/99	B	5	4	11		2+2	22					
Crystal	Size (mm)	Appearance	Sketch										
	0.4x0.5	Small cracks, okay											
Mounting	Loop size (mm)	Date	Experimenter										
	0.5-0.7mm loop	04/15/99	Soma & Jim										
Storage	Cane #	Vial #	Change form	Cane #	Vial #								
	3	B (middle)	Transport...	3	B (middle)								
Diffraction	Date	Temp (K)	Collimator (mm)	Beam trim vertical (%)	Horizontal (%)	2-theta	Appearance on centering						
	04/22/99	97.5	0.3x0.3	N/a	N/a	0.0							
Files	Directory	Oscillation file prefix	Snapshot file prefix	Experimenters									
	/lpx/d/axjs/AK_BNL_8/AK_TD	Ak_td1		Soma									
Backup	Tape #	Date	Tape2 #	Date	Tape3 #	Date	CD1 #	date	CD2 #	date			
	3	04/22/99											
Backup format	850082007	Verified?	850082007	Verified?	850082007	Verified?	850082007	Verified?	850082007	Verified?			
(note if mirror)	8500	Yes											
Run # or Snap	Start frame	End frame	Start φ	Incl A /MPM	Exposure (sec)	Oscillation	Sample-detector (mm)	Beam position X _a	Beam position Y _a	Start current (mA)	Start counts /s	End current (mA)	End counts /s
1	001	001	-32.0	11:30	60	0.5	100	94.78	94.45	210			
	Comments: Better diffraction to 1.30A or higher, but some double spots seen; move the crystal to a new location away from growth zone.												
2	001	180	-32.0	11:45	60	0.50	100	94.78	94.45	210			
	Comments: Better diffraction and diffracts up to 1.25A; collect a complete data set												

Instrument Meta Data 2000

```

Title: Index-Quantum-04-data-from-APS-Beamline-14-BM-CF
Wavelength (Å) 1.0000
Raster size (mm) 8.16000E-02
Raster size (mm) 8.16000E-02
Film width (mm) 188.01 (default)
Film length (mm) 188.01 (default)
Record length (pixels) 2304 (default)
Number of records 2304 (default)
Top limit of useful data 0.0000 (default)
Left limit of useful data 0.0000 (default)
spots rejected when pixel overflow at value 65501.0
pixels rejected at value 0
Oscillation starts at 0.0000
Oscillation range 0.50000
Oscillation step 0.50000
Lattice type: primitive
Orientation axis 1 (vertical plane) 1*h 0*k 0*l (default)
Orientation axis 2 (spindle) 0*h 0*k 1*l (default)
Mosaicity 0.90000
Cxyz (beam) axis 0.0000 (default)
Cxyz (vertical) axis 0.0000 (default)
Cxyz (spindle) axis 0.0000 (default)
unit cell parameters not entered
Detector (mis)orientation angles:
Cassz (beam) axis 0.0000
Cassz (vertical) axis 0.0000
Cassz (spindle) axis 0.0000
Detector 2 theta 0.0000 (default)
Detector rotation 90.000 (default)
Flat detector (default)
Detector to crystal distance 120.00
X beam 93.877
Y beam 93.800
Beam polarization 0.0000 (default)
Detector absorption 100.00 (default)
Air absorption length 3450.0
Crossfire y 0.0000
Crossfire x 0.0000
Crossfire xy 0.0000
Horizontal box size 1.3872
Vertical box size 1.3872
definition of area around Bragg reflections
spot background guard area omitted area 0
    
```

Changing data

Now

- Ph.D. student thesis > **multitudes** of structures
- **Dozens** of data sets per structure
- Data collection lasts **3 hours**
- Data collection is remote at a **National lab**
- One set data is 22MB x 360 frames **7.9 GB** raw data
- Processed data is 144 MB
- Collected in **minutes**



Synchrotron Remote Data Collection

Samples in 2022 for
3 h run; one group

Number	puckName	position	sampleName
1	IMB-FSU-1	1	GBP2GD_GMPPNPdim_01
2	IMB-FSU-1	2	GBP2GD_GMPPNPdim_02
3	IMB-FSU-1	3	GBP2GD_GMPPNPdim_03
4	IMB-FSU-1	4	GBP2GD_GMPPNPdim_04
5	IMB-FSU-1	5	GBP2GD_GMPPNPdim_05
6	IMB-FSU-1	6	GBP2GD_GMPPNPdim_06
7	IMB-FSU-1	7	GBP2GD_GMPPNPdim_07
8	IMB-FSU-1	8	GBP2GD_GMPPNPdim_08
9	IMB-FSU-2	1	GBP2FLWT_GMPPNP_AmSf_01
10	IMB-FSU-2	2	GBP2FLWT_GMPPNP_SoFm_01
11	IMB-FSU-2	3	GBP2FLWT_GMPPNP_SoFm_02
12	IMB-FSU-2	4	GBP2FLWT_GMPPNP_SoFm_03
13	IMB-FSU-2	5	GBP2FLWT_GMPPNP_SoFm_04
14	IMB-FSU-2	6	GBP2FLWT_GMPPNP_SoFm_05
15	IMB-FSU-2	7	GBP2FLWT_GMPPNP_SoFm_06
16	IMB-FSU-2	8	GBP2FLWT_GMPPNP_SoFm_07
17	IMB-FSU-2	9	GBP2FLWT_GMPPNP_SoFm_08
18	IMB-FSU-2	10	GBP2FLWT_GMPPNP_SoFm_09
19	IMB-FSU-2	11	GBP2FLWT_GMPPNP_AmSf_02
20	IMB-FSU-2	12	GBP2FLWT_GMPPNP_AmSf_03
21	IMB-FSU-2	13	GBP2FLWT_GMPPNP_AmSf_04
22	IMB-FSU-2	14	GBP2FLWT_GMPPNP_SoFm_10
23	IMB-FSU-2	15	GBP2FLWT_GMPPNP_SoFm_11
24	IMB-FSU-3	1	GBP2FLWT_GMPPNP_SoFm_12
25	IMB-FSU-3	2	GBP2FLWT_GMPPNP_SoFm_13
26	IMB-FSU-3	3	GBP2FLWT_GMPPNP_SoFm_14
27	IMB-FSU-3	4	GBP2FLWT_GMPPNP_SoFm_15
28	IMB-FSU-3	5	GBP2FLWT_GMPPNP_SoFm_16
29	IMB-FSU-3	6	GBP2FLWT_GMPPNP_SdFr_ol_01
30	IMB-FSU-3	7	GBP2FLWT_GMPPNP_SdFr_ol_02
31	IMB-FSU-3	8	GBP2FLWT_GMPPNP_SdFr_ol_03
32	IMB-FSU-3	9	GBP2FLWT_GMPPNP_SdFr_ol_04
33	IMB-FSU-3	10	GBP2FLWT_GMPPNP_SdFr_ol_05
34	IMB-FSU-3	11	GBP2FLWT_GMPPNP_SdFr_01
35	IMB-FSU-3	12	GBP2FLWT_GMPPNP_SdFr_02
36	IMB-FSU-3	13	GBP2FLWT_GMPPNP_SdFr_03
37	IMB-FSU-3	14	GBP2FLWT_GMPPNP_SdFr_04
38	IMB-FSU-3	15	GBP2FLWT_GMPPNP_SdFr_05
39	IMB-FSU-3	16	GBP2FLWT_GMPPNP_SdFr_06
40	IMB-FSU-4	1	GBP2FLWT_GMPPNP_SdFr_07
41	IMB-FSU-4	2	GBP2FLWT_GMPPNP_SdFr_08
42	IMB-FSU-4	3	GBP2FLWT_GMPPNP_SdFr_09
43	IMB-FSU-4	4	GBP2FLWT_GMPPNP_SdFr_10
44	IMB-FSU-4	5	GBP2FLWT_GMPPNP_SdFr_11
45	IMB-FSU-4	6	GBP2FLWT_GMPPNP_SdFr_12
46	IMB-FSU-4	7	GBP2FLWT_GMPPNP_SdFr_13
47	IMB-FSU-4	8	GBP2FLWT_GMPPNP_SdFr_14
48	IMB-FSU-4	9	GBP2FLWT_GMPPNP_SdFr_15
49	IMB-FSU-4	10	GBP2FLWT_GMPPNP_SdFr_16
50	IMB-FSU-4	11	GBP2FLWT_GMPPNP_SdFr_17
51	IMB-FSU-4	12	GBP2GD_GMPPNPdimer_01
52	IMB-FSU-4	13	GBP2GD_GMPPNPdimer_02
53	IMB-FSU-4	14	GBP2GD_GMPPNPdimer_03
54	IMB-FSU-4	15	GBP2GD_GMPPNPdimer_04
55	IMB-FSU-4	16	GBP2GD_GMPPNPdimer_05

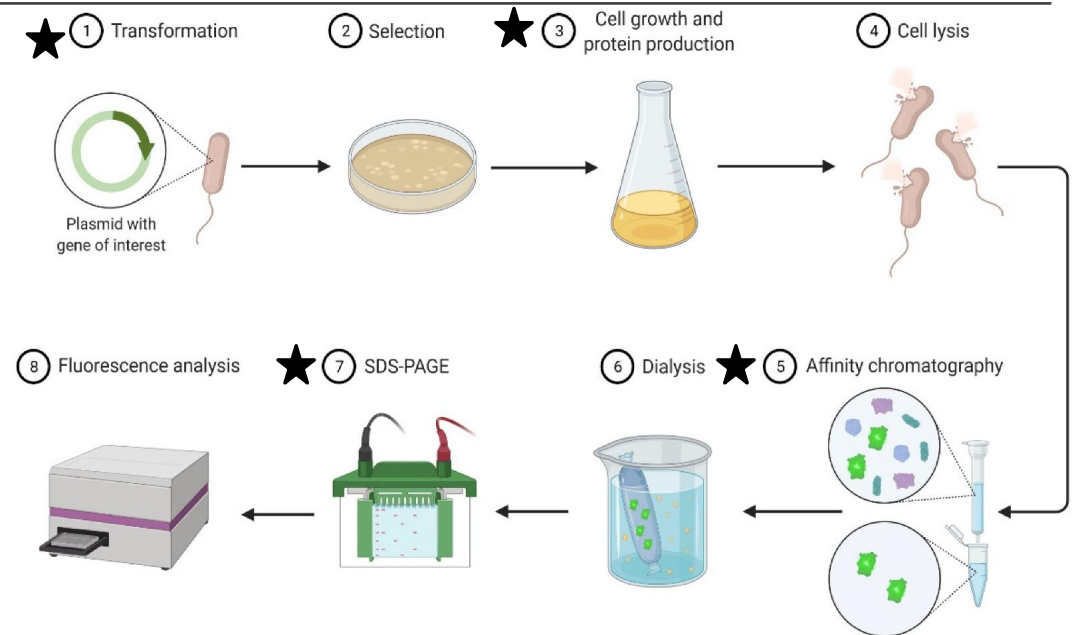


Image courtesy of: <https://doi.org/10.3390/biology11030387>

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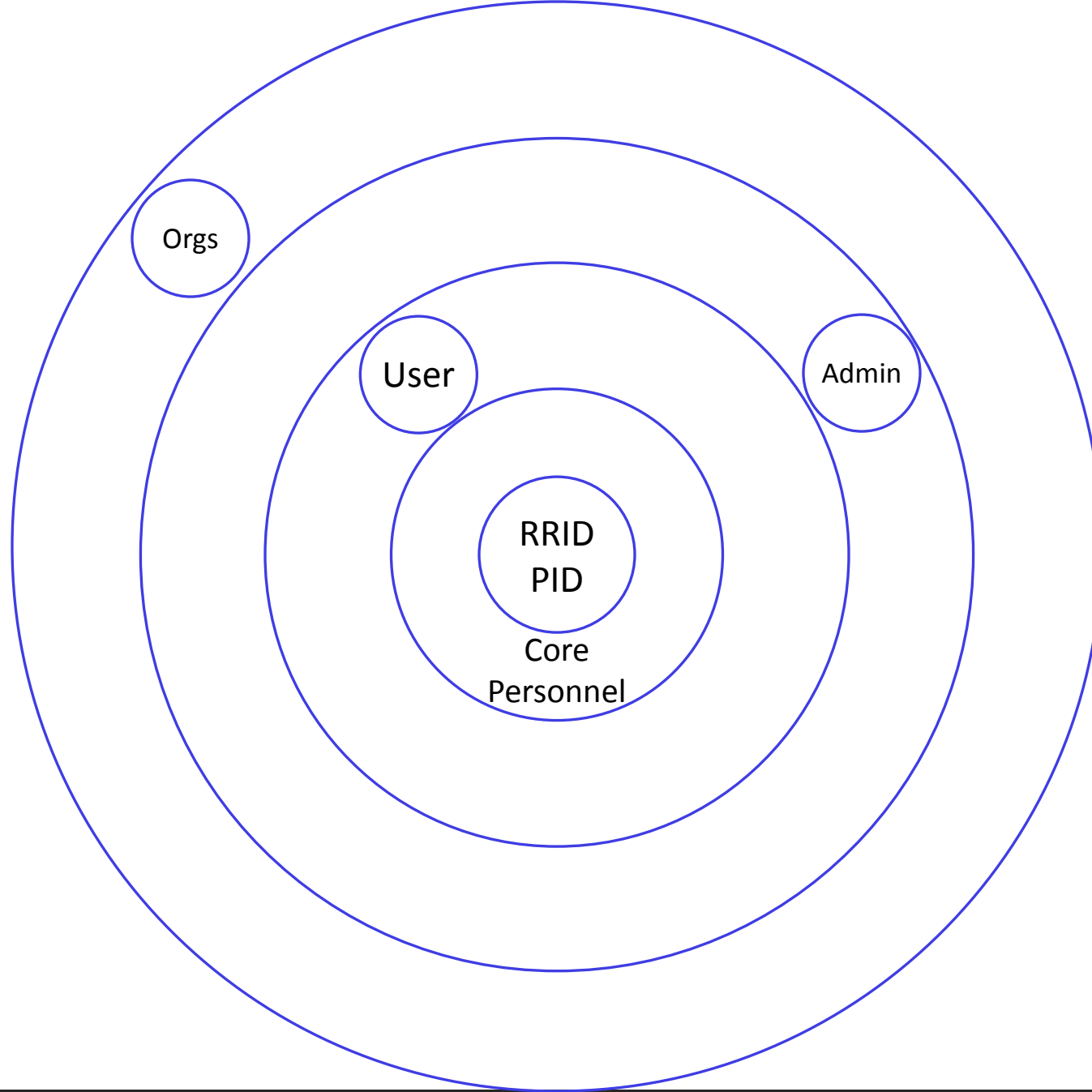
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- Clarify PID issues
- User and Staff buy-in
- Institutional Admin Incentive
- Organizational Support
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