Metadata for material science at the Lightsource BESSY II

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BESSY II – STORAGE RING

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

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- in user operation since 1998
- “compact”, high ratio of straight sections, ~ 38 (27) beamlines
- diverse user community
- offering short pulses

parameters	
Energy	1.7 GeV
Circumference	240 m
Horizontal emittance	5 nm rad
Beam current	300 mA
RF frequency	500 MHz
max. RF voltage	2 MV
Bunch length low-α	15 ps 2 ps
Mom. Comp. factor low-α	7.5×10^{-4} 3.5×10^{-5}

BESSY II: a 3rd generation light source optimized for soft x-ray range

courtesy of M. Ries

BESSY II – STORAGE RING

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RESEARCH FOR GRAND CHALLENGES

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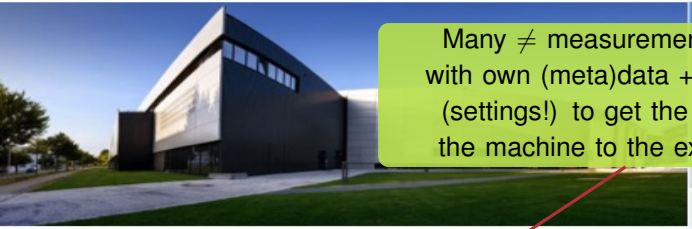

Many ≠ measurement devices with own (meta)data + beamlines (settings!) to get the light from the machine to the experiment.

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BESSY II – MULTI USER MACHINE

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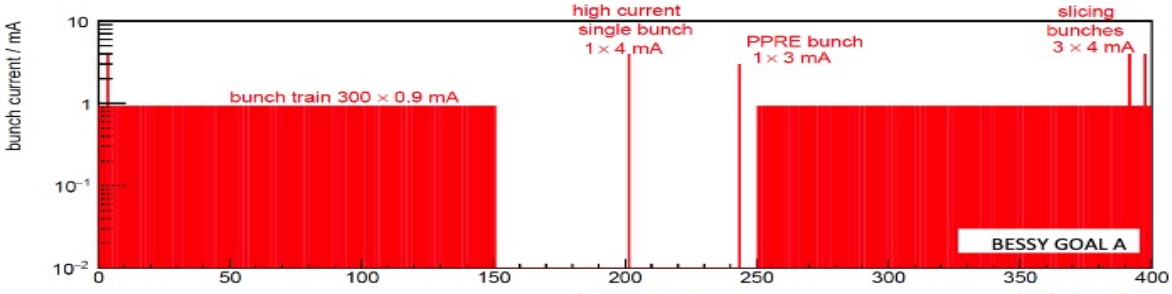
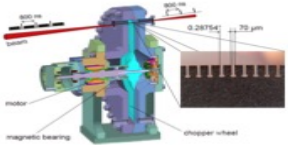
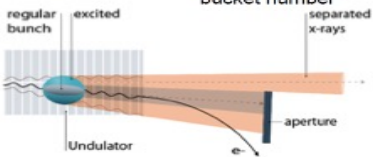




Talk P. Goslawski

Tour T. Mertens



simultaneously serving many users applying many different techniques

courtesy of M. Ries

BESSY II – OPERATION

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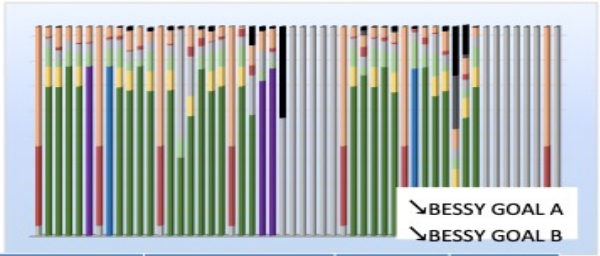
- 24/7 operation
- on average:
  4600 h / year with 96 % ± 2% availability
- positive trend trough systematic identification of root causes
- common metrics application

Tour A. Schälicke



Year	Scheduled	Downtime	# Outages	Availability	MTBF	MTTR
2013	4505 h	159.3 h	105	96.5%	42.9 h	1.52 h
2014	5408 h	384.4 h	136	92.9%	39.8 h	2.83 h
2015	3896 h	92.5 h	90	97.6%	43.3 h	1.03 h
2016	4855 h	62.9 h	69	98.7%	70.4 h	0.91 h
2017	4290 h	241.5 h	62	94.4%	69.2 h	3.90 h

BESSY II features high availability and reliability

courtesy of M. Ries

ROLLING UPGRADES – EMIL

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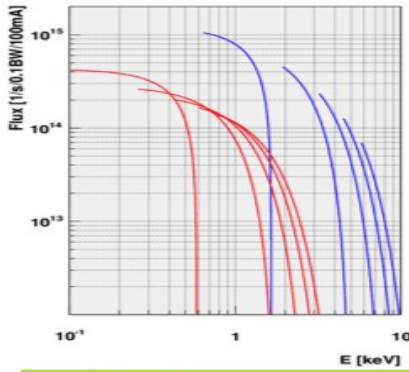
integrate a canted undulators scheme following user request

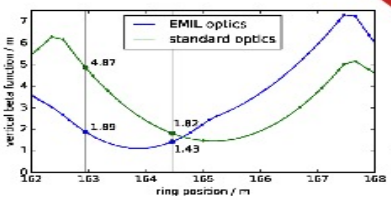
↘BESSY GOAL A
↘BESSY GOAL B

ENGERY

Tour T. Mertens

Tour C. Kuhn





Monochromator Section

PINK

SISSY-1

PEEM

flexibility: constantly evolving following the needs of the user community

courtesy of M. Ries

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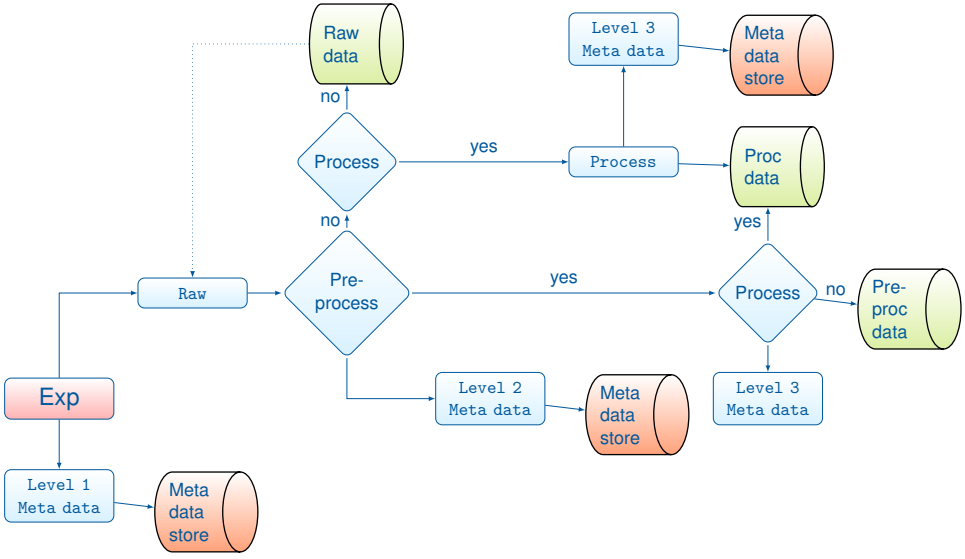
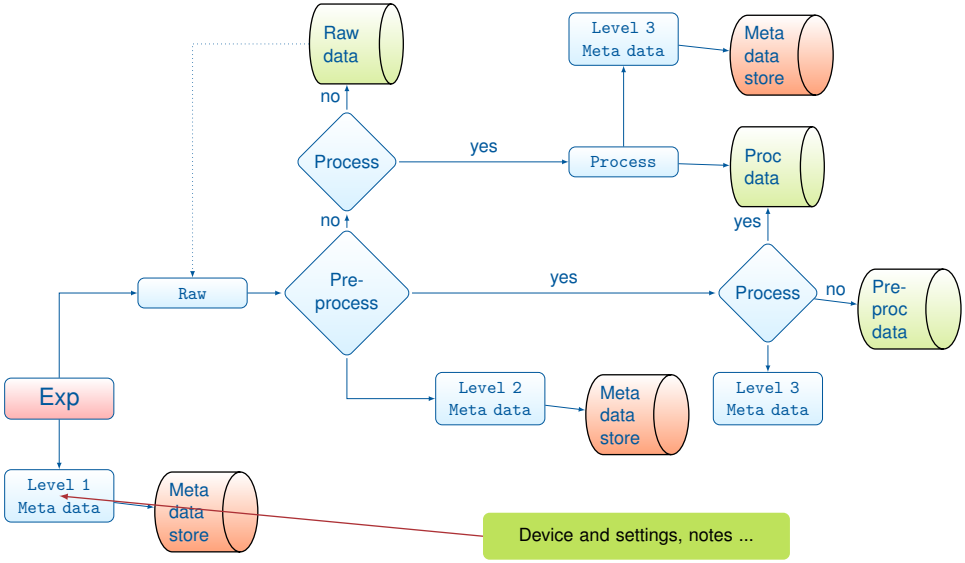
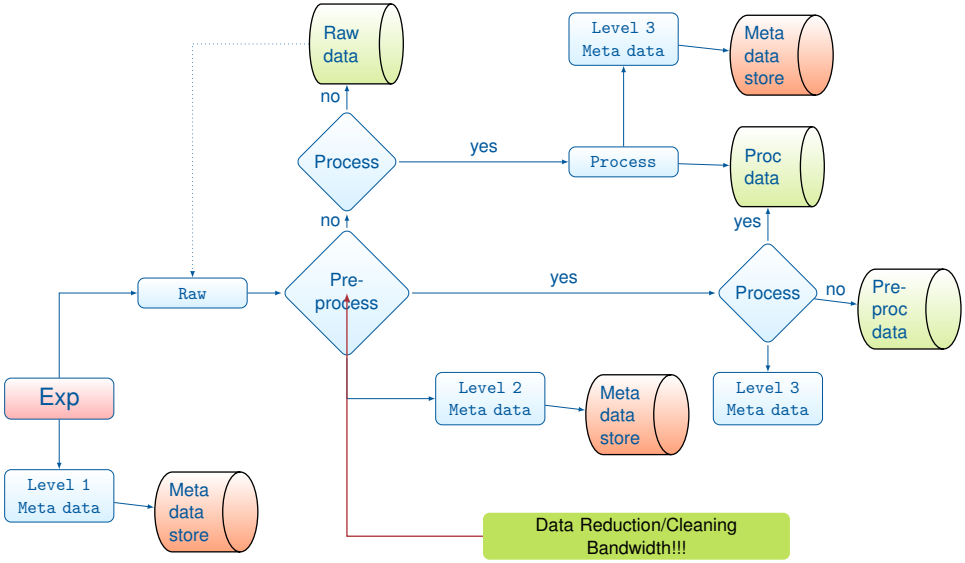
Data flow schematic



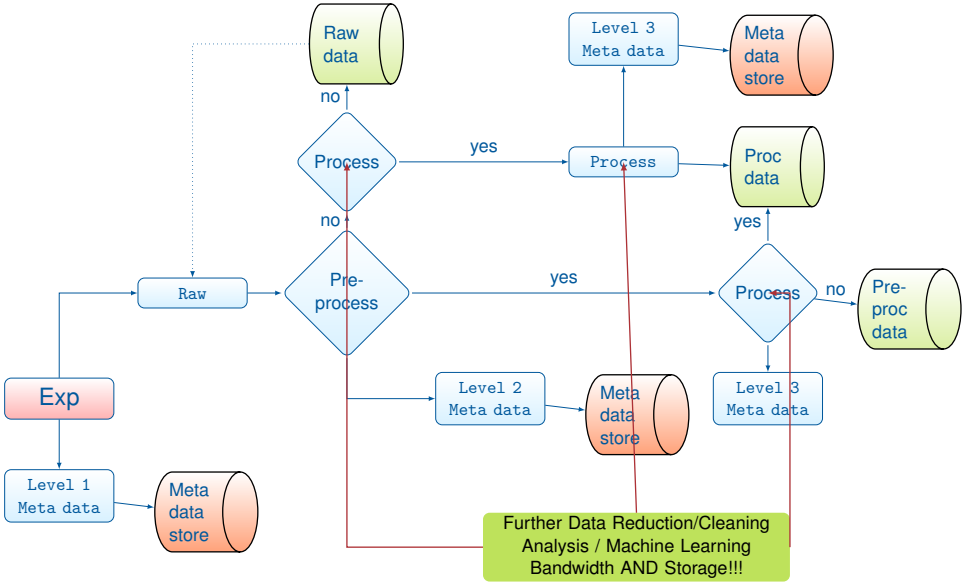
Data flow schematic



Data flow schematic



Data flow schematic



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Some (meta)data considerations

- What do we consider as metadata?
- Auto-generated? → Most
- Manual? → Some
  - Digital (elog entries)
  - Analog (handwritten)
- Data lives! → Persistent IDentification of data (unique, versioned,...)
- Logbook interface → Sometimes
- Storage: SQL/noSQL, file formats → NEXUS + mongodb + ElasticSearch
- Scalability: can we handle the future? → Elastic Stack + NEXUS?
- **Data Model?**
- Findability vs amount of metadata

Some side notes (issues acc phys):

- Accelerator Physics is experience based (an Art)

  (https://www.youtube.com/watch?v=A1L2xODZSI4)
- Trains, cell phones, cars, ...
- Running software on different systems
- Version control
- File formats
- Maintainability of packages/tools (cookiecutter, code certificates,)
- Containerization : **Singularity** with a SCIentific File System (SCIF)

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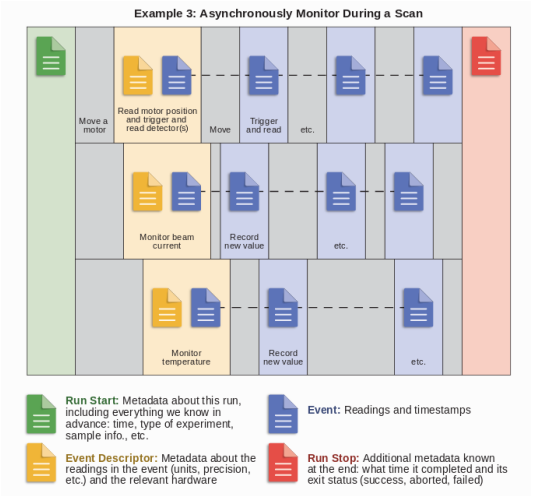
BESSY II - the machine

- Control System BESSY: Epics 3.14 (3.15 under way)
- Epics variables with unique naming convention (location, device type, etc...) **metadata**
- all channels logged in archiver
- accelerator metadata = data
- Question: which data is metadata for some exp
- **Meaning meta(data)** depends on settings (changed manually and can **NOT** be inferred from data)

- We want: Near Real Time Simulation / Analysis
- Why? Performance optimization, fast recovery, machine protection and maintenance
- Experiments: beam commissioning

Example: Bluesky and Ophyd

- Python
- Ophyd for device abstraction (epics, labview, but also extendable)
- Bluesky for experiment control and planning
- Nice data model (see right)
- Databroker available (base: sqlite and MongoDb)
- Suitcase for elasticsearch developed in house (ohters can be easily produced)
- possibility to store data in external files but keep links to data in database (adaptors can be written in straightforward way to load/save the data)
- Generates unique ID for each experiment
- Can talk to Olog
- **METADATA** and data hints
- live plotting and fitting



Example bluesky metadata


```
[{'_id': 'OPDFjmoBqZm8A59lj93a',
  '_index': 'start_run',
  '_score': 3.9233167,
  '_source': {'detectors': ['bpm'],
              'hints': {'dimensions': [[['motor2'], 'primary'],
                                       [['master_clock_frequency_readback'],
                                        'primary']]},
              'motors': ['motor2', 'master_clock_frequency'],
              'num_intervals': 49,
              'num_points': 50,
              'plan_args': {'cycler': "(cycler(MasterClockFrequency(prefix='', "
                                      "name='master_clock_frequency', "
                                      "parent='master_clock', settle_time=0.0, "
                                      "timeout=2.0, read_attrs=['setpoint', "
                                      "'readback', 'offset'], "
                                      'configuration_attrs=[], limits=(499626, '
                                      "499634), egu='kHz'), [499623.43033, "
                                      '499623.65255222225, 499623.87477444444, '
                                      '499624.0969966667, 499624.3192188889, '
                                      '499624.5414411111, 499624.7636633333, '
                                      '499624.98588555556, 499625.20810777775, '
                                      '499625.43033]) * '
                                      "cycler(SynAxis(prefix='', "
                                      "name='motor2', read_attrs=['readback', "
                                      "'setpoint'], "
                                      "configuration_attrs=['velocity', "
                                      "'acceleration']), [0, 1, 2, 3, 4]))",
                            'detectors': ["BPMStorageRing(prefix='', "
                                          "name='bpm', read_attrs=['stat', "
                                          "'stat.mean_x', 'stat.mean_y', "
                                          "'stat.rms_x', 'stat.rms_y', "
                                          "'waveform', 'waveform.packed_data', "
                                          "'waveform.counter', "
                                          "'waveform.ready', 'waveform.pos_x', "
                                          "'waveform.pos_y', "
                                          "'waveform.intensity_z', "
                                          "'waveform.intensity_s', "
                                          "'waveform.status', 'waveform.gain', "
                                          "'waveform.rms_x', "
                                          "'waveform.rms_y'], "
                                          "configuration_attrs=['stat', "
                                          "'waveform'])"],
                            'per_step': 'None'},
              'plan_name': 'scan_nd',
              'plan_type': 'generator',
              'scan_id': 1,
```

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Beamlines - Let's complain a bit.

- Different Experiment Control Softwares with different ways to control Sample Environment
- Complex software interface protocols
- Time consuming integration of new equipment with little mobility.
- No metadata standards for Sample Environments (SECoP with NEXUS?)
- Physicists programming drivers.
- Human Readable variable names?
- No generic work-/dataflow - user/beamline specific, what about authentication?
- New "workflows" (related to (meta)data) should not change users habits or create extra overhead
- Metadata database for static metadata (see further)
- Experiment controls: EPICS, Tango, Sardana $\rightarrow$ Python?
- Common Data Model Architecture vs NoMaD $\rightarrow$ **Data Model?**

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RE-USE INFORMATION, USE STANDARDS AND AUTOMATE COLLECTION

- Re-use information about data: collect static, not so static and metadata about instruments and software
- Collect and share information about standards
- Automate collection as far as possible

courtesy of H. Görzig

HOW DO WE GET THERE?

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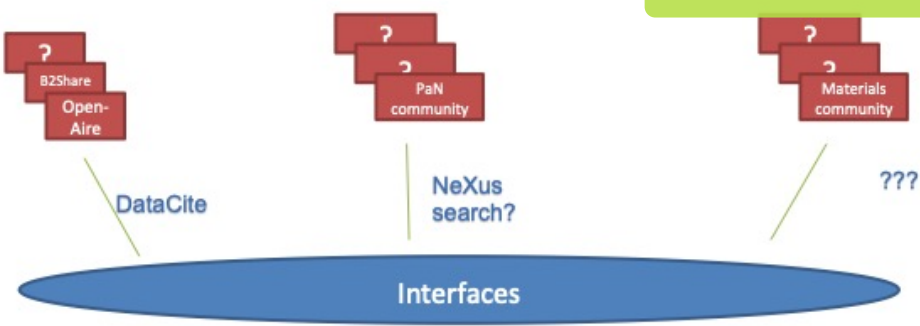
ICAT : metadata catalogue



findability

ICAT

interoperability
re-useability

courtesy of H. Görzig

WORKFLOW

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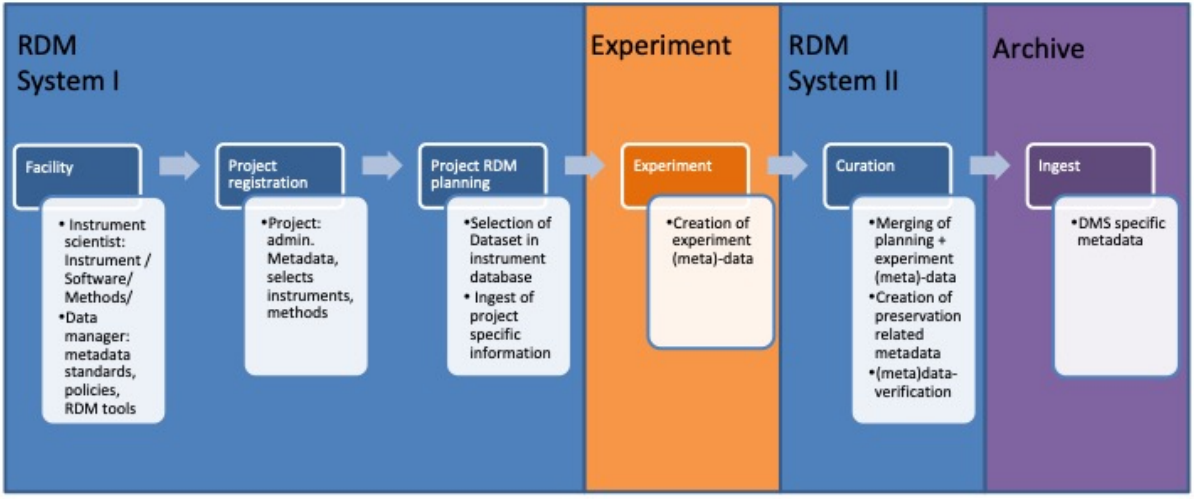

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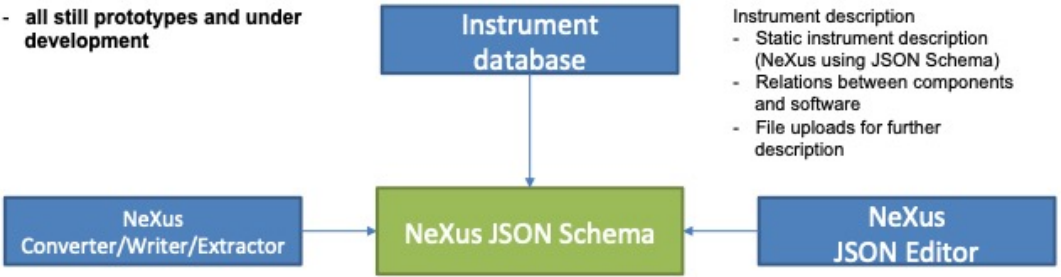
- **all still prototypes and under development**



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HOW DO WE GET THERE?

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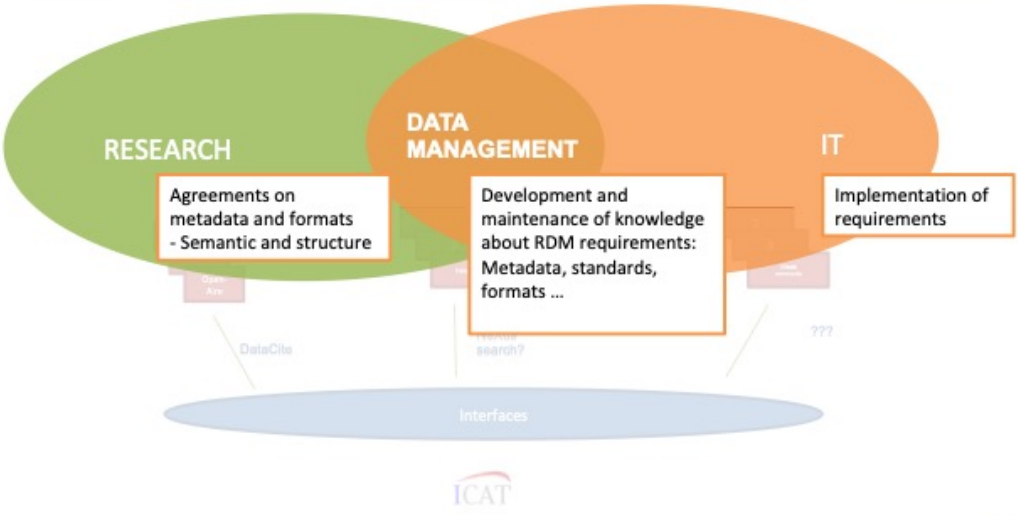

courtesy of H. Görzig

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Summary

- Many open questions.
- Initial work started both from machine side as from experiments side.
- EPICS with Bluesky (Python) + Archiver for the machine.
- ICAT database for static metadata under development.
- NEXUS interfaces for data/metadata under development.
- Some limitations can not be solved easily (bandwidth, standardization, storage, access rights,...)
- Working towards FAIR data.

Links

- Singularity :https://sylabs.io/docs/
- Bluesky, Ophyd :https://github.com/bluesky
- Scientific Filesytem :https://sci-f.github.io/