



Northeastern Collaborative Access Team

EDNA at NE-CAT

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NE-CAT Beamlines

24ID-C

- Variable energy beamline: 6-21keV
- Focused beam flux: 10^{14} photons/s
- Focal spot: 20 microns (v) x 60 microns (h)
- MD2 micro-diffractometer with apertures down to 5 microns and SC3 Minikappa

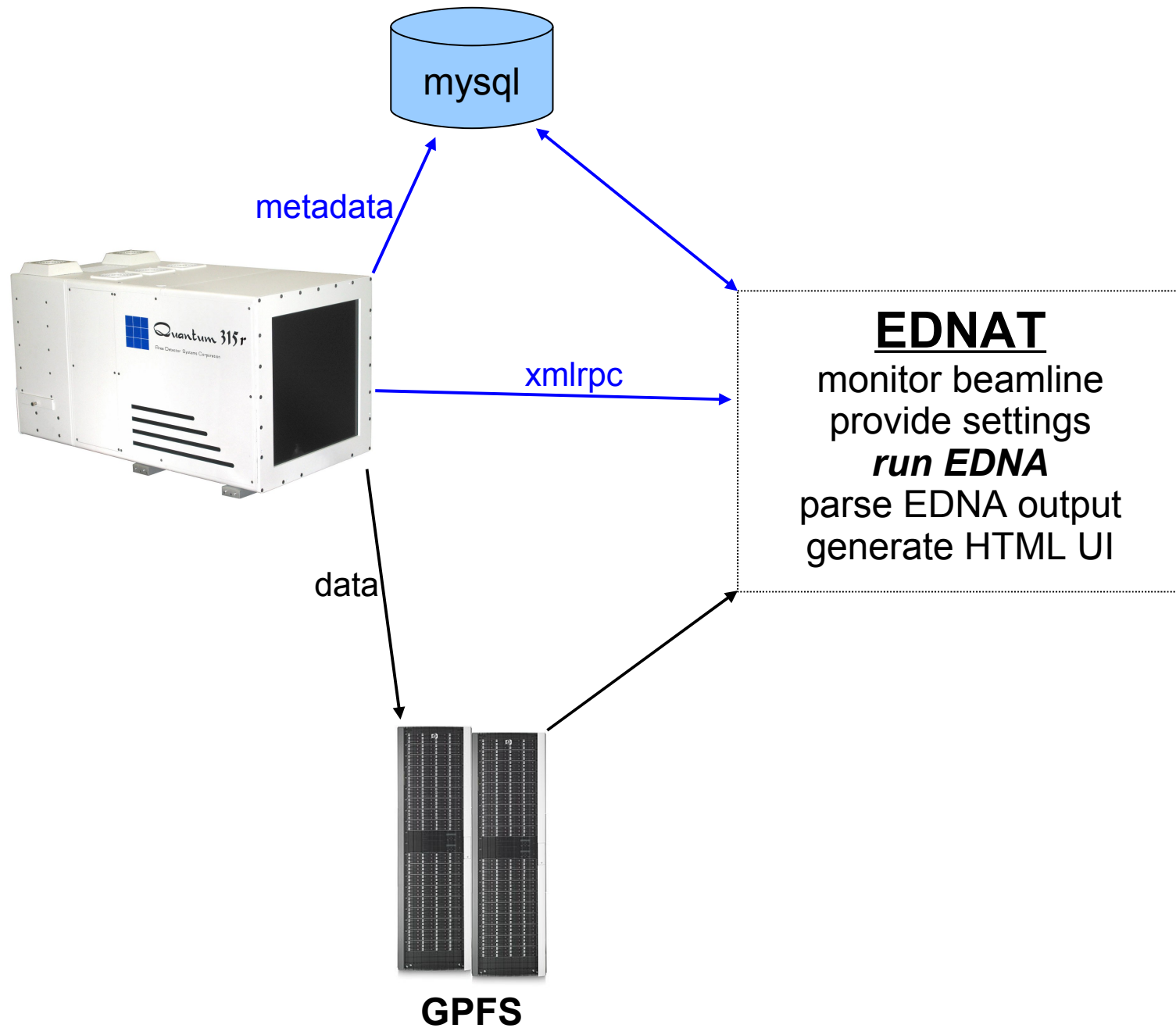
• 24ID-E

- Fixed energy beamline: 12662eV (Se Peak)
- Focused beam flux: 10^{13} photons/s
- Focal spot: 20 microns (v) x 1000 microns (h)
- MD2 micro-diffractometer with apertures down to 5 microns

How Is EDNA Used?

- Currently EDNA is the data-processing core for our automated data collection strategy generation
- Every snap that is recorded is processed.
- Each distinct “trip” has its own html GUI with all the snaps processed.
- Currently all files are on the local filesystem & copied to users' directory for transport home.

NECAT Data Flow



NECAT EDNA Control UI

Controls remote connections



EDNAT wraps EDNA and provides:

Control UI (wxPython)
Beamline monitoring
Image collection monitoring
EDNA calling & monitoring
Output parsing
Output UI (HTML)

A 'Preferences' dialog box with a blue title bar. It contains various settings for data collection. The settings are as follows:

Anomalous	False
Spacegroup Override	None
Hi Res Cutoff (A)	3.5
Transmission (%)	AUTO
Aperture Size (um)	AUTO
Crystal Size (x,y,z um)	100 100 100
Ratio crystal:beam	2.0
Sample Type	protein
Molecules in unit cell	1
Residues per Molecule	250
Susceptibility	1.0
BEST complexity	none
Max Total Exposure (s)	120
Minimum Exposure per Image (s)	1
Override user directory	False None
Override working directory	True /gpfs1/users/necat/fmurphy/

Buttons at the bottom: Cancel, OK.

Autoindexing options

From beamline

BEST options

NECAT EDNA Results UI

Snaps

- [snap_99_002.img](#)
- [snap_99_001.img](#)
- [snap_99_002.img](#)
- [snap_0_043.img](#)
- [snap_0_042.img](#)
- [snap_0_041.img](#)
- [ta_exp5_1_040.img](#)
- [ta_exp5_1_036.img](#)
- [ta_exp5_1_034.img](#)
- [ta_exp5_1_032.img](#)
- [ta_exp5_1_028.img](#)
- [ta_exp5_1_026.img](#)
- [ta_exp5_1_027.img](#)
- [ta_exp5_1_023.img](#)
- [ta_exp5_1_022.img](#)
- [ta_exp5_101_020.img](#)
- [ta_exp5_101_019.img](#)
- [ta_exp5_101_014.img](#)
- [ta_exp5_101_013.img](#)
- [ta_exp5_101_008.img](#)
- [ta_exp5_101_005.img](#)
- [ta_exp5_101_006.img](#)
- [ta_exp5_101_007.img](#)
- [ta_exp5_101_001.img](#)
- [ta_exp5_101_002.img](#)

Runs

Display full output

Mosflm Autoindexing Output

ind	pen	lat	a	b	c	alpha	beta	gamma
7	48	mC	140.38	124.75	92.81	89.92	99.79	89.93
6	40	mC	140.38	124.75	92.81	89.92	99.79	89.93
5	39	aP	92.81	93.84	93.96	83.25	97.24	97.36
4	13	hR	123.24	123.47	180.98	90.34	89.67	119.25
3	10	mC	140.38	124.75	92.81	90.08	99.79	90.07
2	1	mC	140.38	124.75	92.81	90.08	99.79	90.07
1	0	aP	92.81	93.84	93.96	83.25	82.76	82.64

Chosen spacegroup: C2 (solution number 2)
Cell refined to 140.39 124.51 93.66 90.0 99.6 90.0 (105 of 111 spots used)
Mosaicity estimated to be: 0.36 degrees

Data Collection Strategy

Phi start 164.00 deg
Phi range 112.0 deg

With mosflm predictions

Ad nauseam

Parsed log

Continuously updated

Presently unworkable

Done

EDNA Implementation

- GUI is actually parsed logfile, xml was explored, but parsing logfile was easier
- RADDDOSE is calibrated to a test crystal experimentally
- Modules, input.xml and command line modified to take a range of keywords

Additional Keywords

- crystal size x, y, z
- beam size x, y, gauss
- susceptibility
- # monomers, residues, heavy atoms, copies in ASU
- shape
- anomalous
- indexing high resolution
- changed default solvent content 47% -> 55%

Problems in Implementing

- Program versions mismatching – mosflm, Best
- Prototype fails due to results being too precise – if result off by 0.0001 = Failure
- Default settings are too buried – being in one top level module would make more accessible
- Running time dependent on directory tree size – seems to be a python module search issue

EDNA Weaknesses

(an end user's view)

No GUI

Not enough “intelligence” at decision points

e.g. autoindexing resolution setting

Logging and directory structure is overly burdensome

Integration does not work

Defaults are inaccessible