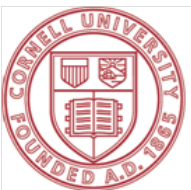




RAPD - Rapid Automated Processing of Data

Jonathan P. Schuermann
Cornell University / NE-CAT



RAPD

- RAPD (Rapid Automated Processing of Data)
- Software Suite for Automated Macromolecular Crystallographic Data Analysis in Real Time
- Initial goal: Quickly provide automatic autoindexing and data collection strategies
- Morphed into much larger suite with additional pipelines for data processing and structure determination
- PI can monitor progress from home
- Results stored in database for improving RAPD or database mining



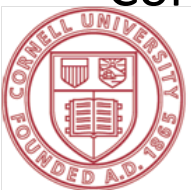
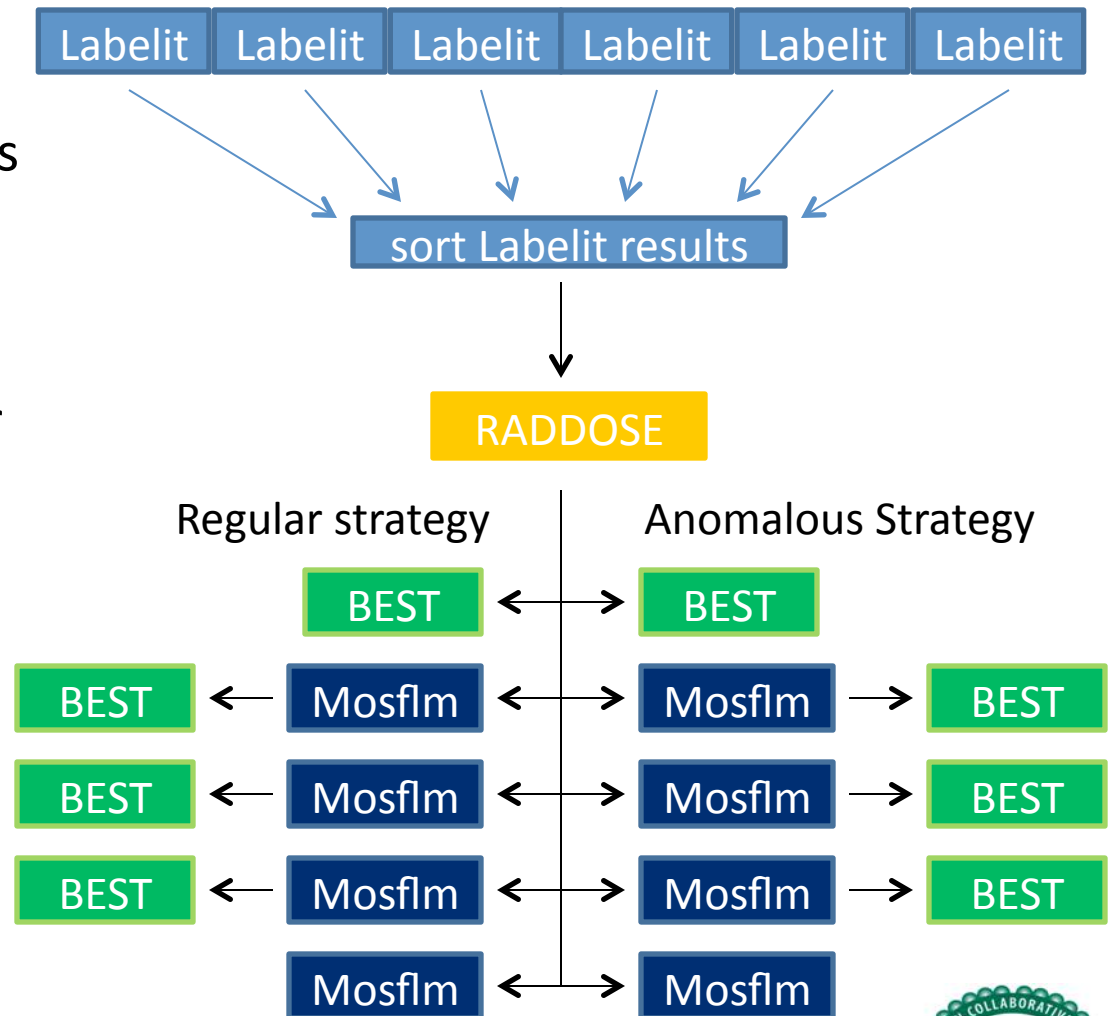
RAPD Pipelines

- **Autoindexing and strategy**
- STAC
- Data (re)processing and merging (David Neau)
- Data analysis
- SAD
- Molecular replacement



RAPD Autoindex/Strategy

- Multiple Labelit runs with different peak picking settings for Distl
- Sort by highest symmetry
- Raddose
- BEST strategies calculated for regular and anomalous data collections
- If BEST fails, Mosflm strategy calculated
- Highly parallelized code with several layers of error detection/correction
- Run time: ~25s on an Intel Core i7



Distl Settings

ADSC Q315

Labelit run number	1	2	3	4	5	6
distl.minimum_spot_area (10)		6		7	8	6
distl.minimum_spot_height (3.5)			6			
distl.minimum_signal_height (1.5)		4.3		1.2		
distl_highres_limit						5

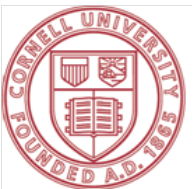
Dectris Pilatus

Labelit run number	1	2	3	4	5	6
distl.minimum_spot_area (5)		3		2	3	2
distl.minimum_spot_height (3.5)			6			
distl.minimum_signal_height (2.5)		4		2.3		
distl_highres_limit						5



Labelit Error Checking

- The code will attempt to fix common autoindexing errors and rerun Labelit
 - If too few spots, resets min # of spots required
 - If unit cell/SG (specified by user) fails, resets without cell/SG restraints
 - If Mosflm step fails, lowers resolution limit
 - And any combination of the previous errors



RAPD Autoindex and Strategy

The screenshot shows the RAPD Autoindex and Strategy web application running in a Mozilla Firefox browser. The browser's address bar displays the URL `https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php`. The application interface includes a top navigation bar with tabs for 'Data' and 'Structure'. The 'Data' tab is active, showing a list of image files on the left and a summary of the Labelit autoindexing process on the right. The summary includes a table of image files, a table of data collection strategy from BEST, and a table of anomalous data collection strategy from BEST.

Labelit autoindexing summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

Space Group	a	b	c	α	β	γ	mosaicity	resolution
P4	57.70	57.70	150.10	90.00	90.00	90.00	0.125000	3.28

Data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	2.00	57.0	55.0	55	1.00	1.00	200.0	2.0

ANOMALOUS data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	96.00	178.0	82.0	82	1.00	1.00	200.0	2.0

RAPD Autoindex and Strategy

The screenshot shows the RAPD Autoindex and Strategy web application running in a Mozilla Firefox browser. The browser's address bar displays the URL `https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php`. The application interface is divided into several sections:

- Left Panel:** Contains a list of image files under the "Snaps" tab. A context menu is open over the file `sample1_PAIR_0_1+2.img`, showing options like "View", "Reindex", "MiniKappa", "Alignment", and "Hide/Show".
- Top Panel:** Includes tabs for "Data" and "Structure". Below these are sub-tabs for "Summary", "Detail", "Images", "Plots", "Snaps", "Runs", and "Samples".
- Right Panel:** Features a "Controls" section with buttons for "Main", "Trips", "Settings", and "Pucks".
- Main Content Area:** Displays the "Labelit autoindexing summary for:" section, which includes image paths and a table of space group parameters.

Labelit autoindexing summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

Space Group	a	b	c	α	β	γ	mosaicity	resolution
P4	57.70	57.70	150.10	90.00	90.00	90.00	0.125000	3.28

Data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	2.00	57.0	55.0	55	1.00	1.00	200.0	2.0

ANOMALOUS data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	96.00	178.0	82.0	82	1.00	1.00	200.0	2.0

RAPD Autoindex and Strategy

The screenshot shows the RAPD Autoindex and Strategy web application running in a Mozilla Firefox browser. The browser's address bar displays the URL `https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php`. The application interface is divided into several sections:

- Left Panel:** Contains a list of image files under the "Snaps" tab. The files are organized into groups, with "sample1_PAIR_0_1+2.img" and "junk_PAIR_0_002.img" being prominent.
- Top Panel:** Features a "Summary" tab, which is currently selected. Other tabs include "Detail", "Images", "Plots", "Snaps", "Runs", and "Samples".
- Right Panel:** Contains a "Controls" section with buttons for "Main", "Trips", "Settings", and "Pucks".
- Main Content Area:** Displays the "Labelit autoindexing summary for:" section. It includes a table for "User chose space group as P422" and two tables for "Data collection strategy from BEST" and "ANOMALOUS data collection strategy from BEST".

Labelit autoindexing summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

User chose space group as P422

Space Group	a	b	c	α	β	γ	mosaicity	resolution
P422	57.70	57.70	150.10	90.00	90.00	90.00	0.125000	3.28

Data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	4.00	44.5	40.5	30	1.35	1.00	200.0	2.0

ANOMALOUS data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	2.00	46.55	44.55	33	1.35	1.00	200.0	2.0

RAPD Pipelines

- Autoindexing and strategy
- **STAC**
- Data (re)processing and merging (David Neau)
- Data analysis
- SAD
- Molecular replacement



RAPD Autoindex and Strategy

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- Left Panel:** Contains a list of image files under the "Snaps" tab. A context menu is open over the file `sample1_PAIR_0_1+2.img`, showing options like "View", "Reindex", "MiniKappa", "Alignment", and "Hide/Show".
- Top Panel:** Includes tabs for "Data" and "Structure". Below these are sub-tabs for "Summary", "Detail", "Images", "Plots", "Snaps", "Runs", and "Samples".
- Right Panel:** Labeled "Controls", it contains buttons for "Main", "Trips", "Settings", and "Pucks".
- Main Content Area:** Displays the "Labelit autoindexing summary for:" section, which includes image paths and a table of space group parameters.

Labelit autoindexing summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

Space Group	a	b	c	α	β	γ	mosaicity	resolution
P4	57.70	57.70	150.10	90.00	90.00	90.00	0.125000	3.28

Data collection strategy from BEST

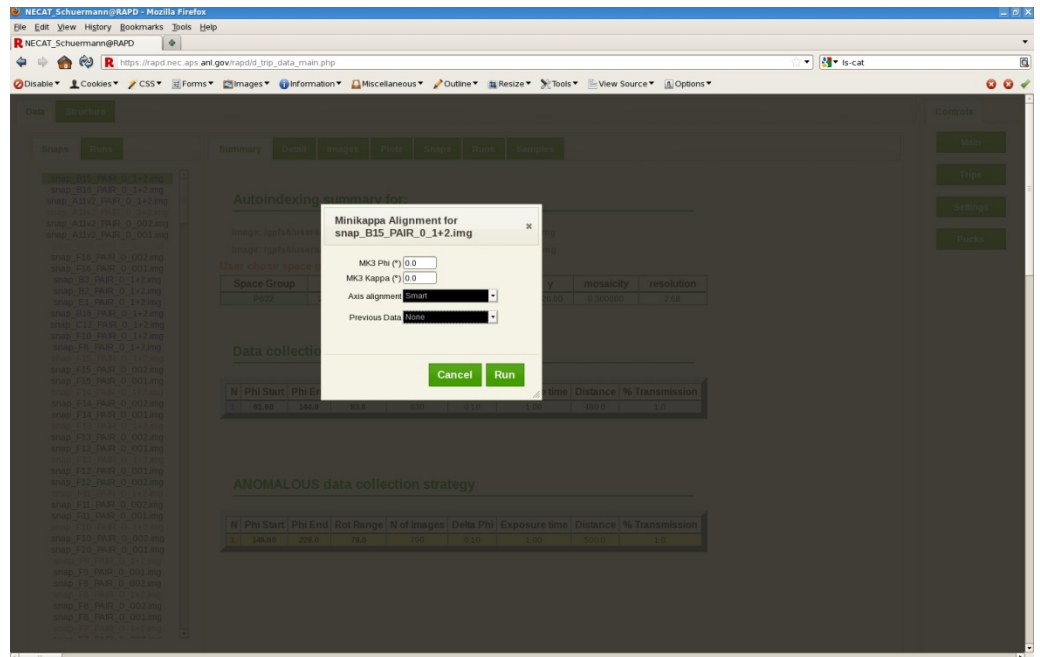
N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	2.00	57.0	55.0	55	1.00	1.00	200.0	2.0

ANOMALOUS data collection strategy from BEST

N	Phi Start	Phi End	Rot Range	N of Images	Delta Phi	Exposure time	Distance	% Transmission
1	96.00	178.0	82.0	82	1.00	1.00	200.0	2.0

STAC Options

- Alignment options:
 - smart, long, anomalous, a^*, b^*, c^* , split a^*b^* , split a^*c^* , split b^*c^* , all
 - Can align crystal to previously collected crystal



STAC Alignment Results

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NECAT_Schuermann@RAPD

anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php

WHT002795

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Data Structure

Snapshots Runs

sample1_PAIR_0_1+2.img
sample1_PAIR_0_1+2.img
sample1_PAIR_0_1+2.img
junk_PAIR_0_002.img
junk_PAIR_0_003.img
junk_PAIR_0_2+3.img
junk_PAIR_0_1+2.img
junk_PAIR_0_001.img
sample1_PAIR_0_1+2.img
sample1_PAIR_0_002.img
sample1_PAIR_0_001.img
a10_PAIR_0_002.img
a9_PAIR_0_002.img
a8_PAIR_0_006.img
a6_PAIR_0_5+6.img
a8_PAIR_0_4+5.img
a8_PAIR_0_005.img
a8_PAIR_0_3+4.img
a8_PAIR_0_004.img
a8_PAIR_0_2+3.img
a8_PAIR_0_003.img
a8_PAIR_0_002.img
a6_0_004.img
a6_0_003.img
a6_PAIR_0_002.img
a4_PAIR_0_1+2.img
a4_PAIR_0_002.img
a4_PAIR_0_001.img
ghhgd_a2_PAIR_0_3+4.img
ghhgd_a2_PAIR_0_004.img
ghhgd_a2_PAIR_0_2+3.img
ghhgd_a2_PAIR_0_003.img
ghhgd_a2_PAIR_0_002.img
ghhgd_PAIR_0_002.img
ghhgd_PAIR_0_001.img
ghhgd_PAIR_0_1+2.img

MiniKappa Snapshots Runs Samples

STAC summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

Space Group	a	b	c	α	β	γ
P422	57.70	57.70	150.10	90.00	90.00	90.00

STAC Alignment Results

Aligning each axis parallel to the spindle axis.

ID	V1	V2	Omega	Kappa	Phi
1	(0.819;-0.497;0.287)	b*	299.29	147.33	61.45
2	(0.819;-0.497;0.287)	b*	266.01	208.37	28.14
3	(0.819;-0.497;0.287)	b*	119.29	147.33	61.45
4	(0.819;-0.497;0.287)	b*	86.01	208.37	28.14
5	(0.819;-0.497;0.287)	c*	213.26	147.33	61.45
6	(0.819;-0.497;0.287)	c*	179.98	208.37	28.14
7	(0.819;-0.497;0.287)	c*	33.26	147.33	61.45
8	(0.819;-0.497;0.287)	c*	359.98	208.37	28.14
9	b*	a*	72.15	112.44	171.19
10	b*	a*	252.15	112.44	171.19
11	b*	c*	342.15	112.44	171.19
12	b*	c*	162.15	112.44	171.19
13	(-0.044;-0.075;0.996)	a*	107.49	146.25	288.89
14	(-0.044;-0.075;0.996)	a*	73.05	209.45	254.42
15	(-0.044;-0.075;0.996)	a*	287.49	146.25	288.89
16	(-0.044;-0.075;0.996)	a*	253.05	209.45	254.42
17	(-0.044;-0.075;0.996)	b*	16.24	146.25	288.89
18	(-0.044;-0.075;0.996)	b*	341.80	209.45	254.42
19	(-0.044;-0.075;0.996)	b*	196.24	146.25	288.89
20	(-0.044;-0.075;0.996)	b*	161.80	209.45	254.42

STAC Loofile

Controls

Main

Trips

Settings

Pucks

Send STAC Alignment to Beamline

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anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php WHT002795

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Data Structure

Snaps Runs

sample1_PAIR_0_1+2.img
sample1_PAIR_0_1+2.img
sample1_PAIR_0_1+2.img
junk_PAIR_0_002.img
junk_PAIR_0_003.img
junk_PAIR_0_2+3.img
junk_PAIR_0_1+2.img
junk_PAIR_0_001.img
sample1_PAIR_0_1+2.img
sample1_PAIR_0_002.img
sample1_PAIR_0_001.img
a10_PAIR_0_002.img
a9_PAIR_0_002.img
a8_PAIR_0_006.img
a6_PAIR_0_5+6.img
a8_PAIR_0_4+5.img
a8_PAIR_0_005.img
a8_PAIR_0_3+4.img
a8_PAIR_0_004.img
a8_PAIR_0_2+3.img
a8_PAIR_0_003.img
a8_PAIR_0_002.img
a6_0_004.img
a6_0_003.img
a6_PAIR_0_002.img
a4_PAIR_0_1+2.img
a4_PAIR_0_002.img
a4_PAIR_0_001.img
ghhgd_a2_PAIR_0_3+4.img
ghhgd_a2_PAIR_0_004.img
ghhgd_a2_PAIR_0_2+3.img
ghhgd_a2_PAIR_0_003.img
ghhgd_a2_PAIR_0_002.img
ghhgd_PAIR_0_002.img
ghhgd_PAIR_0_001.img
ghhgd_PAIR_0_1+2.img

MiniKappa Snaps Runs Samples

STAC summary for:

Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_001.img
Image: /gpfs6/users/necat/NECAT_E_26/images/Frank/thaum/snaps/sample1_PAIR_0_002.img

Space Group	a	b	c	α	β	γ
P422	57.70	57.70	150.10	90.00	90.00	90.00

STAC Alignment Results

Aligning each axis parallel to the spindle

ID	V1	Phi
1	(0.819;-0.497;0.287)	61.45
2	(0.819;-0.497;0.287)	28.14
3	(0.819;-0.497;0.287)	61.45
4	(0.819;-0.497;0.287)	28.14
5	(0.819;-0.497;0.287)	61.45
6	(0.819;-0.497;0.287)	28.14
7	(0.819;-0.497;0.287)	61.45
8	(0.819;-0.497;0.287)	28.14
9	b*	171.19
10	b*	171.19
11	b*	171.19
12	b*	171.19
13	(-0.044;-0.075;0.996)	288.89
14	(-0.044;-0.075;0.996)	254.42
15	(-0.044;-0.075;0.996)	288.89
16	(-0.044;-0.075;0.996)	254.42
17	(-0.044;-0.075;0.996)	288.89
18	(-0.044;-0.075;0.996)	254.42
19	(-0.044;-0.075;0.996)	288.89
20	(-0.044;-0.075;0.996)	254.42

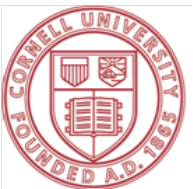
Success

Minikappa settings sent to beamline

STAC Loofile

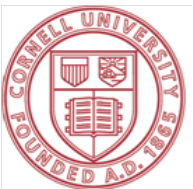
RAPD Pipelines

- Autoindexing and strategy
- STAC
- Data (re)processing and merging (David Neau)
- **Data analysis**
- SAD
- Molecular replacement



Data Analysis Pipeline

- Unit cell analysis
- Xtriage
- Xtriage plots
- Molrep self-rotation function
- labelit.precession_photo



Unit Cell Analysis

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anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php# mysql

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Data Structure

Snapshots Runs

thau1_4
thau1_2
thau1_3
thau1_1
thau1_3H_distance_down_10
thau1_3H_distance_down_9
thau1_3H_distance_down_8
thau1_3H_distance_down_7
thau1_3H_distance_down_6
thau1_3H_distance_down_5
thau1_3H_distance_down_4
C12_1
B9_1
B7_2
B7_1
B3_1
A9_1
A8_2+A8_1
A8_2
A8_1
perozo_D10_225C_Hg_2
perozo_D10_225C_Hg_1

Summary Detail Plots Analysis Snapshots Runs Samples

Cell Summary Xtriage Plots Self Rotation Precessions

Unit Cell Analysis

a	b	c	α	β	γ
57.9070	57.9070	150.8040	90.0000	90.0000	90.0000

Structures with unit cell dimensions within +/- 2.0%

PDB ID	Description	Phaser Statistics			
		LL-Gain	RF Z-score	TF Z-score	# of Clashes
1T0O	alpha-galactosidase	No solution	No solution	No solution	No solution
1RQW	Thaumatococcus	3101	7.0	14.4	0
1LXZ	Thaumatococcus	3019	7.1	13.8	0
1TFK	Colicin D	No solution	No solution	No solution	No solution
1KWN	Thaumatococcus	2974	6.8	13.9	0
1LY0	Thaumatococcus	2987	7.4	13.5	0
1THW	THAUMATOCOC	2921	6.9	14.4	0
1LR3	Thaumatococcus	3062	7.1	13.8	0
1LR2	Thaumatococcus	3035	6.7	14.1	0
1OEK	HYPOTHETICAL PROTEIN YODA	No solution	No solution	No solution	No solution

RAPD Logfile

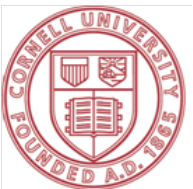
Click to view log of top solution

Controls

Main
Trips
Settings
Pucks

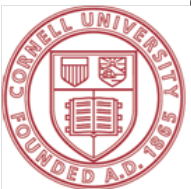
RAPD Pipelines

- Autoindexing and strategy
- STAC
- Data (re)processing and merging (David Neau)
- Data analysis
- **SAD**
- Molecular replacement



SAD Pipeline

- SHELX(CDE)
- Run all possible space groups and cell permutations simultaneously
- Code written to parallelize SHELXD similar to SGXPro and new code written by Sheldrick to parallelize further
- Results: 960 trials in all SG ~1 minute
- SHELXE autotrace
- SHELX sites given to AutoSol for another autotrace
- 'Hand' and SG determined automatically
- User can rerun changing the resolution cutoff, number of sites, or number of SHELXD trials
- All results and plots presented on RAPD GUI and are downloadable



SAD Pipeline

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File Edit View History Bookmarks Tools Help

NECAT_Schuermann@RAPD x file:///gpfs6/u...mary_long.html x file:///gpfs6/u...ary_short.html x file:///gpfs6/us...best_plots.html x Spotfinder Command Line O... x

anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php# WHT002795

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Data Structure

SAD MR

zf2_30-75

p19_12_4

p19_5_1

p19_6_1

p19_4_2

p19_1_1-90

p19_1_1

Summary Plots Autobuild

SHELXC Results

Resolution	8.0	6.0	5.0	4.5	4.3	4.1	3.9	3.7	3.5	3.3	3.09
N(data)	793	1007	1221	1087	582	690	846	1029	1244	1591	2093
Mean I/sig	73.7	52.8	42.7	37.0	30.4	23.9	19.8	11.8	6.8	4.0	1.7
% Complete	94.9	99.3	97.4	99.8	99.8	99.9	99.8	99.6	97.3	99.7	99.6
Mean d"/sig	4.96	3.70	2.37	1.71	1.46	1.35	1.07	0.96	0.87	0.83	0.73

SHELXD Results

Space Group	Max CCall	Max CCweak	Max PATFOM
P4232	28.25	11.74	17.29
P432	22.15	9.78	103.4
P4332 (P4132)	55.00	34.49	10.6

SHELXE Results

SHELXE may have found a solution in P4132

Site	x	y	z	occ*Z	density
1	0.1888	0.0602	0.9119	34.0000	38.51
2	0.2995	0.0457	0.8885	32.2456	38.24
3	0.0682	-0.0601	0.9437	4.8722	4.13
4	0.1124	-0.1181	0.8174	3.5972	1.20
5	0.1114	-0.1438	0.9082	2.4650	2.05
6	0.1397	-0.1624	0.7045	2.4412	1.61
7	0.0942	-0.1498	0.8154	2.1454	1.38
8	0.2758	0.0225	0.9361	0.5134	1.57

SHELXE FOM 0.664

SHELXE Pseudo-free CC 68.73

SHELXE autotraced # of residues 79

SHELXE autotraced CC (>25 is good) 11.14

Phenix AutoSol completed successfully.

Controls

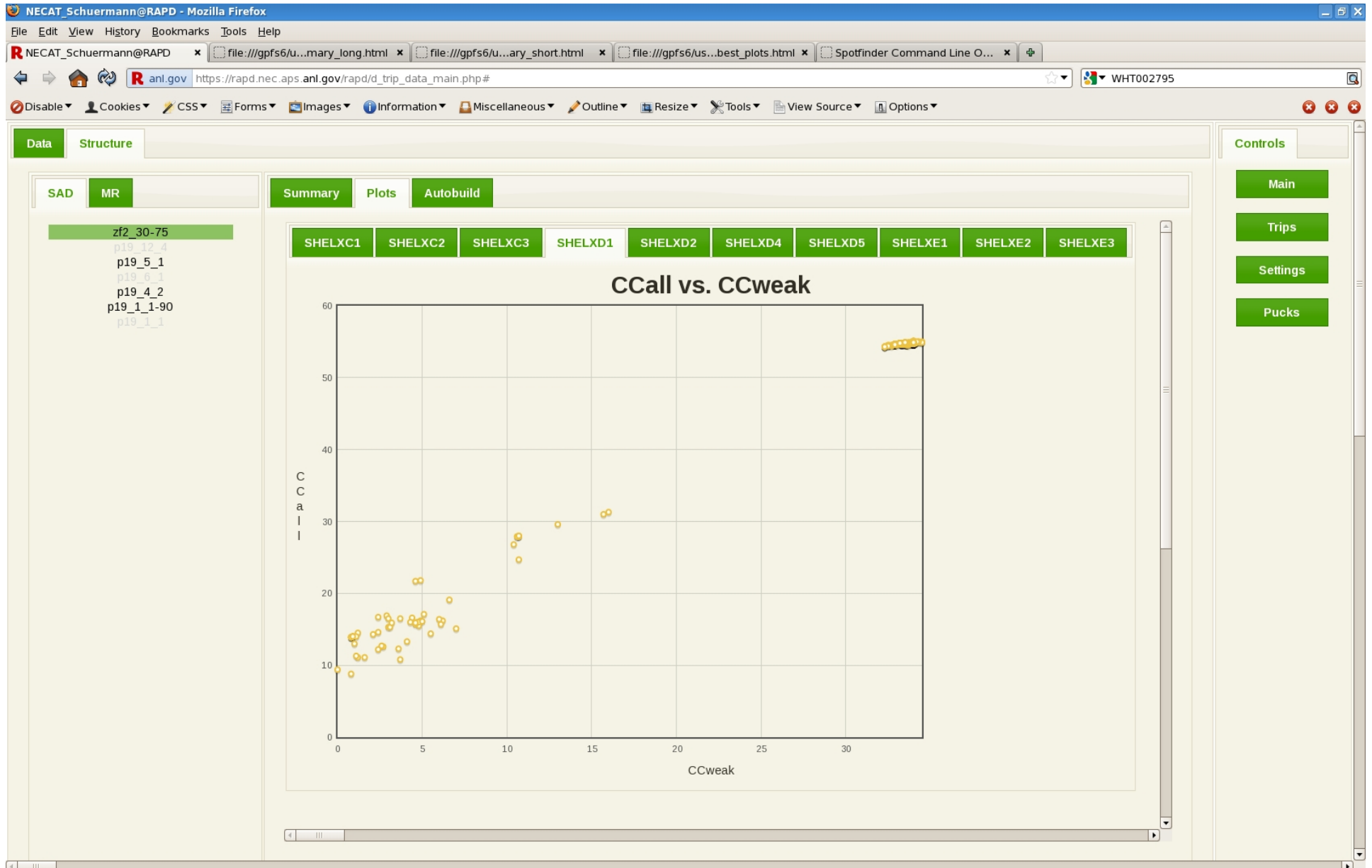
Main

Trips

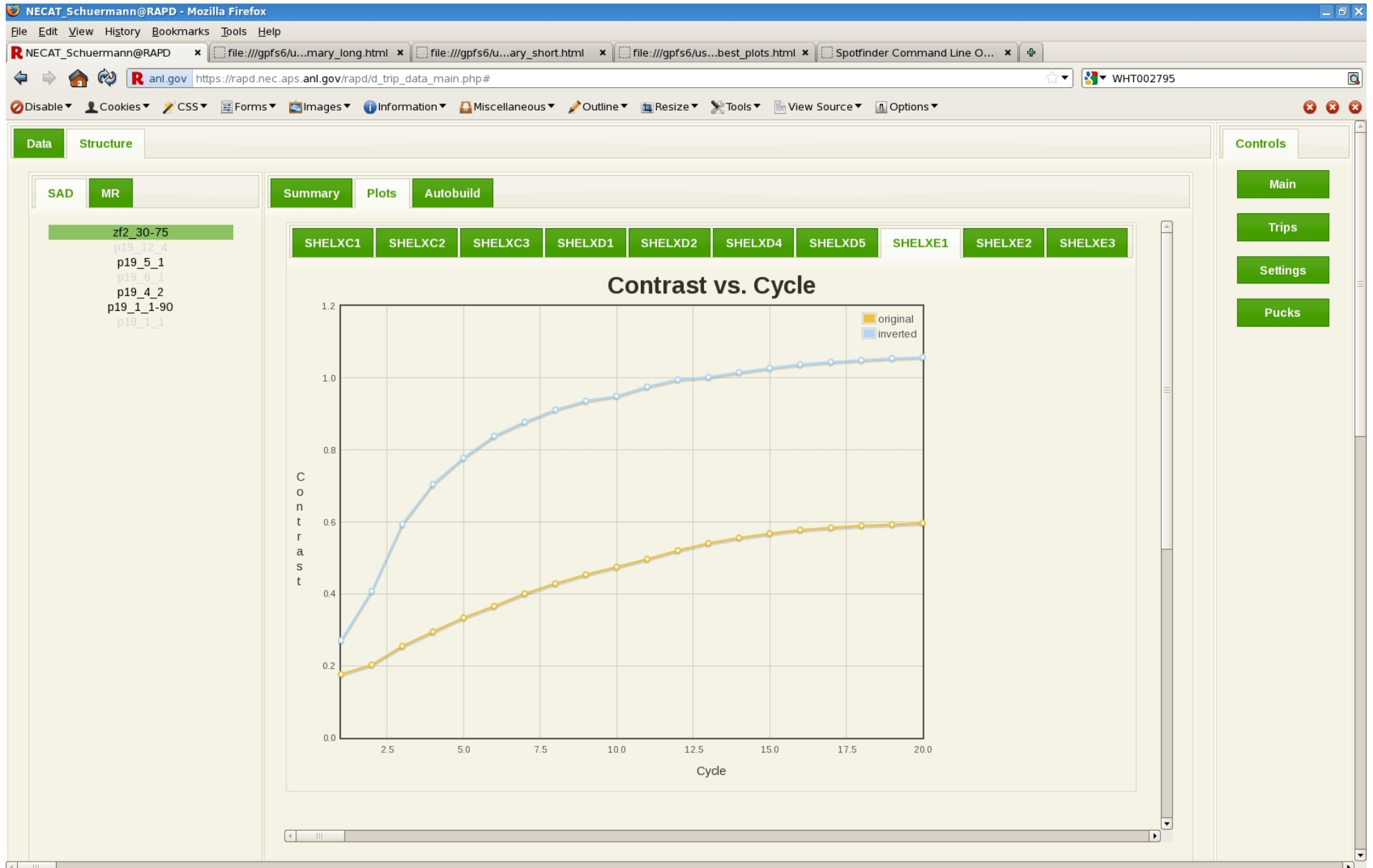
Settings

Pucks

SHELXD Plots



SHELXE Plots



Autosol Results

NECAT_Schuermann@RAPD - Mozilla Firefox

File Edit View History Bookmarks Tools Help

NECAT_Schuermann@RAPD x file:///gpfs6/u...mary_long.html x file:///gpfs6/u...ary_short.html x file:///gpfs6/us...best_plots.html x Spotfinder Command Line O... x

anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php# WHT002795

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Data Structure

SAD MR

zf2_30-75
p19_12_4
p19_5_1
p19_6_1
p19_4_2
p19_1_1-90
p19_1_1

Summary Plots Autobuild

Phenix AutoSol Results

Phasing Results	
Space Group	P4132
Bayesian CC	50.0
FOM	0.29
Number of starting sites	2
Number of refined sites	2
Building Results	
Number of residues built	117
Number of side-chains built	0
Total number of chains	17
model-map CC	0.41
Refined R/R-free	0.47/0.51

RAPD Logfile

Click to view log

Controls

Main

Trips

Settings

Pucks

RAPD Pipelines

- Autoindexing and strategy
- STAC
- Data (re)processing and merging (David Neau)
- Data analysis
- SAD
- **Molecular replacement**



Molecular Replacement

- Run in all possible SG's and cell permutations simultaneously
- Run Phaser filtering top 75% peaks greater than 4 sigma (rotation function) or 6 sigma (translation function)
- User can input PDB code or file
- Matthew's run to determine number of molecules in the AU automatically (user can override)
- If no solutions found, rerun allowing 10% clashes
- Statistics presented in RAPD GUI
- Results are downloadable



MR Pipeline Results

NECAT_Schuermann@RAPD - Mozilla Firefox

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NECAT_Schuermann@RAPD

anl.gov https://rapd.nec.aps.anl.gov/rapd/d_trip_data_main.php#

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Data Structure

SAD MR

dl1-1_1-140
dl2-1_20-140
mm15-3_1_1
mm15-3_1
mm14-2_1
mm13-2_1
mm13-3_1
mm13-4_1
mm12-4_1
mm11-2_1
mm11-3_1
mm10-4_1
lm20-2_2+lm20-2_1
lm20-2_1

Summary Plots Autobuild

Unit Cell Analysis

a	b	c	α	β	γ
89.3950	95.3540	225.7770	90.0000	90.0000	90.0000

Phaser Statistics

Space Group	Description	LL-Gain	RF Z-score	TF Z-score	# of Clashes
P21212	search model pdb	No solution	No solution	No solution	No solution
P222	search model pdb	No solution	No solution	No solution	No solution
P2122	search model pdb	No solution	No solution	No solution	No solution
P2212	search model pdb	No solution	No solution	No solution	No solution
P22121	search model pdb	No solution	No solution	No solution	No solution
P21221	search model pdb	No solution	No solution	No solution	No solution
P212121	search model pdb	5372	27.4	43.8	2
P2221	search model pdb	No solution	No solution	No solution	No solution

Download

RAPD Logfile

Click to view log

Controls

Main

Trips

Settings

Pucks

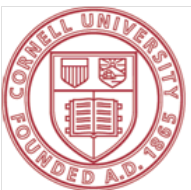
Current Capabilities of RAPD

- GUI can be viewed and results downloaded from an internet browser
- Automatic autoindex/strategy in ~20s
- Automatic data processing in 'real' time
- Automatic data analysis
- Automatic MR if similar structure in PDB
- Pipelines for SAD and MR
- Datasets can be reprocessed and merged
- Results stored in users directory
- Details of each result stored in MySQL database
- So far:
 - 276,444 autoindexing/strategy
 - 25,141 datasets processed
 - 1,539 SAD jobs
 - 773 MR jobs
 - 88,019 unit cell analysis runs (9,781 solutions with LL-gain > 100)



Future Goals/Wishes of RAPD

- Speed... much more speed (threading detector modules)
- XDS mosaicity calculated from small wedges of 'snapshots'
- Shift libraries to CCTBX for compatibility
- More database mining
- Run auto-beam center calculation in background
- MAD and MRSAD pipelines
- New GUI
- Better hooks for wrapping
- Multiple lattice integration
- Better support for multi-wedge data collection



Acknowledgments

- Frank Murphy – Core and user interface
- David Neau – data (re)processing
- Kay Perry, Surajit Banerjee
- RAPD
 - <https://rapd.nec.aps.anl.gov/rapd>
- Wiki
 - https://rapd.nec.aps.anl.gov/wiki/main_page

