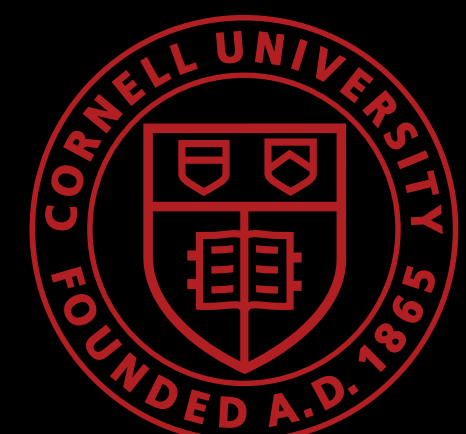


# **RAPD** Data Analysis at NE-CAT

MCE2021 Workshop

Frank Murphy – March 17, 2021



# Agenda

NE-CAT

Automated data analysis @ NE-CAT

Current capabilities

Development of version 2

Design & implementation

~~Problems~~ Opportunities

# Acknowledgements

## Contributors

Jon Schuermann\*

David Neau

Kay Perry

Jim Withrow

## NE-CAT Support Staff

Surajit Banerjee

Ali Kaya

Igor Kourinov

N. Sukumar

## Support

NIGMS P30 GM124165

# NE-CAT Beamlines

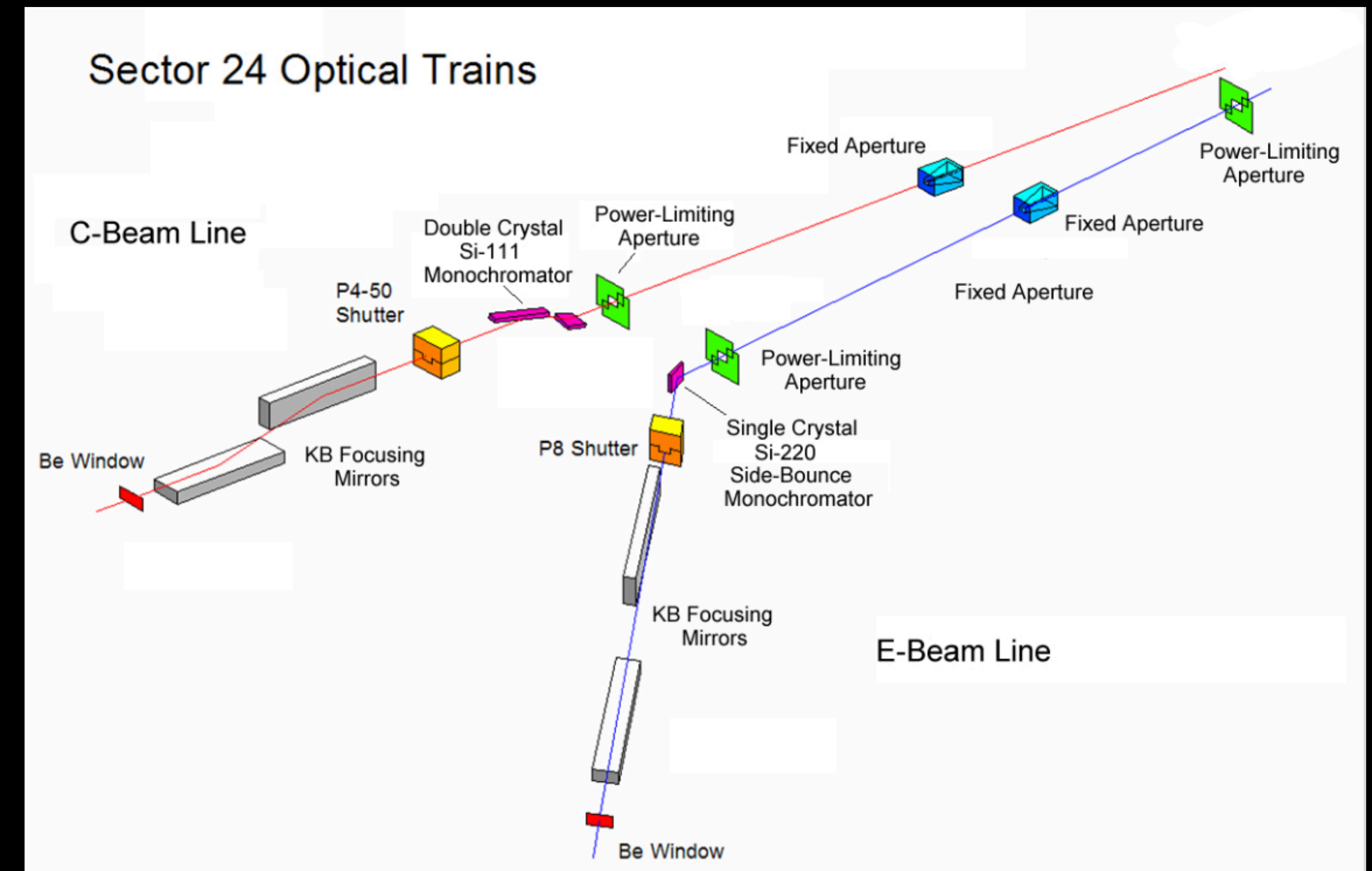
## APS Sector 24

### 24-ID-C

Tunable 6.5-20keV  
 $1.5 \times 10^{13}$  photons/sec  
 $25 \mu\text{mH} \times 10 \mu\text{mV}$   
Eiger2 X 16M

### 24-ID-E

Fixed 12,663eV  
 $1.0 \times 10^{13}$  photons/sec  
 $35 \mu\text{mH} \times 5 \mu\text{mV}$   
Eiger 16M





# Our Goals For Automated Data Analysis

- Help users collect better data faster
- Enable collaboration with off-site users
- Project started in 2009

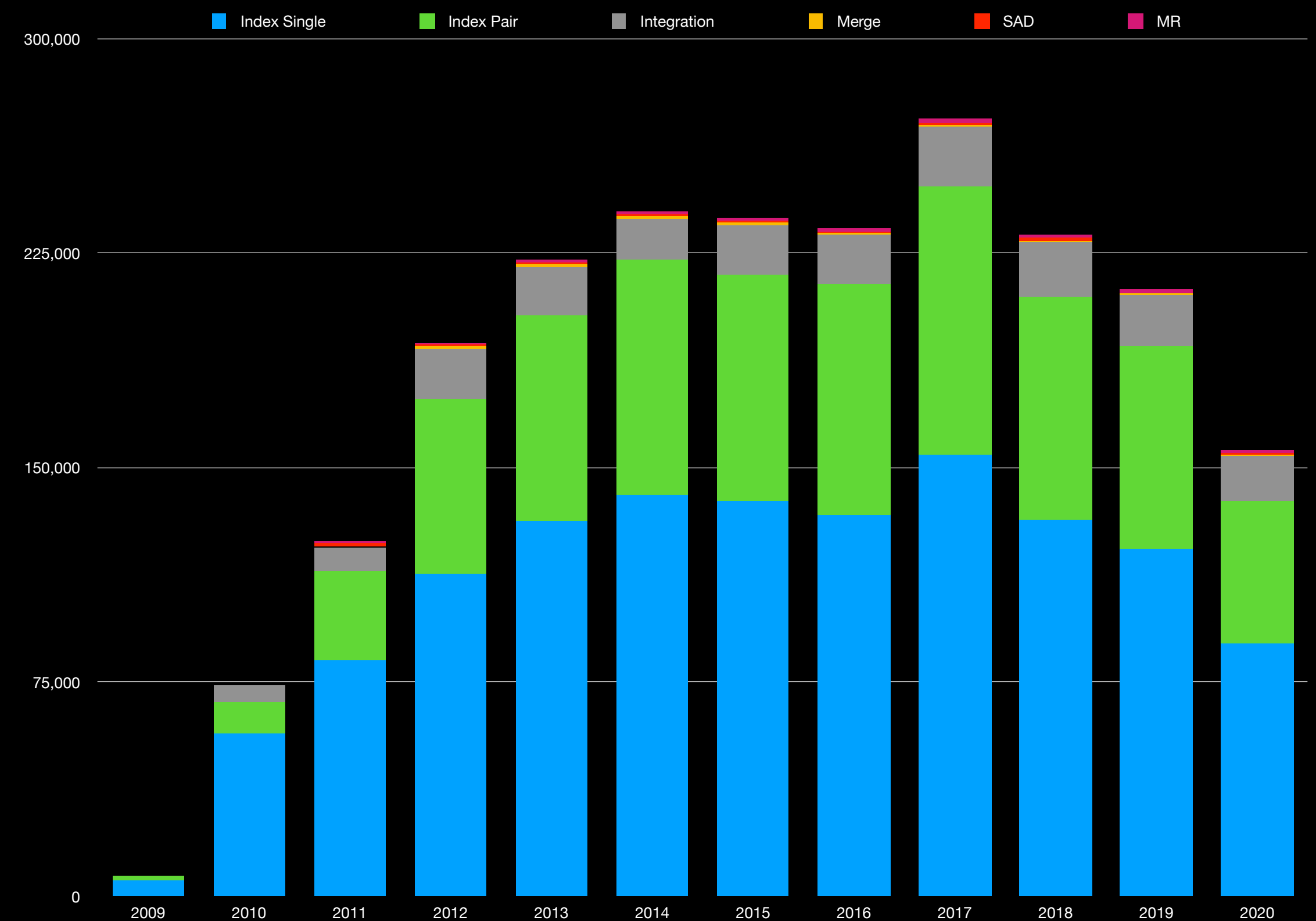
**Current Status – RAPDv1**

# RAPD Capabilities

- Indexing & Strategy
- Integration, Scaling & Analysis
- Merging
- SAD
- MR

# RAPD Capabilities

- Indexing & Strategy – DISTL, Labelit, BEST, Mosflm
- Integration, Scaling & Analysis – XDS, Aimless, Pointless, Phaser, Xtrriage
- Merging – Aimless, Pointless
- SAD – SHELX, Phenix
- MR – Phaser



# RAPD Index

rapd.nec.aps.anl.gov

Data Structure

Snaps Runs

NE38\_7\_PAIR\_0\_1+2.img  
 NE38\_7\_PAIR\_0\_000002.img  
 NE38\_7\_PAIR\_0\_000001.img  
 NE38\_6\_PAIR\_0\_1+2.img  
 NE38\_6\_PAIR\_0\_000002.img  
 NE38\_6\_PAIR\_0\_000001.img  
 NE38\_5\_PAIR\_0\_1+2.img  
 NE38\_5\_PAIR\_0\_000002.img  
 NE38\_5\_PAIR\_0\_000001.img  
 NE38\_4\_PAIR\_0\_1+2.img  
 NE38\_4\_PAIR\_0\_000002.img  
 NE38\_4\_PAIR\_0\_000001.img  
 NE38\_3\_PAIR\_0\_1+2.img  
 NE38\_3\_PAIR\_0\_000002.img  
 NE38\_3\_PAIR\_0\_000001.img  
 NE38\_2\_0\_000002.img  
 NE38\_2\_0\_000001.img  
 NE38\_1\_PAIR\_0\_1+2.img  
 NE38\_1\_PAIR\_0\_000002.img  
 NE38\_1\_PAIR\_0\_000001.img

Summary Detail Plots Snaps Runs Samples

### Labelit autoindexing summary for:

Image: /gpfs1/users/cornell/chem7880\_C\_5704/images/haoyue/snaps/NE38\_7\_PAIR\_0\_000001.cbf  
 Image: /gpfs1/users/cornell/chem7880\_C\_5704/images/haoyue/snaps/NE38\_7\_PAIR\_0\_000002.cbf

Space Group	a	b	c	$\alpha$	$\beta$	$\gamma$	mosaicity	resolution
P4	57.83	57.83	150.13	90.00	90.00	90.00	0.100000	1.25

### Detector distance

Resolution limit at edge	Detector distance
1.2	150
1.3	180.0
1.4	200.0

### Data collection strategy from BEST

N	Omega Start	Omega End	Rot Range	N of Images	Delta Omega	Exposure time	% Transmission
1	82.00	140.0	58.0	290	0.20	0.3	1.5

### ANOMALOUS data collection strategy from BEST

N	Omega Start	Omega End	Rot Range	N of Images	Delta Omega	Exposure time	% Transmission
1	78.00	170.0	92.0	368	0.25	0.2	1.5

Controls

Main  
 Trips  
 Settings  
 Pucks

rapd.nec.aps.anl.gov

Data Structure

Snaps Runs

NE38\_7\_PAIR\_0\_000002.img  
 NE38\_7\_PAIR\_0\_000001.img  
 NE38\_6\_PAIR\_0\_1+2.img  
 NE38\_6\_PAIR\_0\_000002.img  
 NE38\_6\_PAIR\_0\_000001.img  
 NE38\_5\_PAIR\_0\_1+2.img  
 NE38\_5\_PAIR\_0\_000002.img  
 NE38\_5\_PAIR\_0\_000001.img  
 NE38\_4\_PAIR\_0\_1+2.img  
 NE38\_4\_PAIR\_0\_000002.img  
 NE38\_4\_PAIR\_0\_000001.img  
 NE38\_3\_PAIR\_0\_1+2.img  
 NE38\_3\_PAIR\_0\_000002.img  
 NE38\_3\_PAIR\_0\_000001.img  
 NE38\_2\_0\_000002.img  
 NE38\_2\_0\_000001.img  
 NE38\_1\_PAIR\_0\_1+2.img  
 NE38\_1\_PAIR\_0\_000002.img  
 NE38\_1\_PAIR\_0\_000001.img

Summary Detail Plots Snaps Runs Samples

Omega start ANOM Omega start Max delta Omega Wilson Plot Rad damage1 Rad damage2

### Min osc range for different completenesses

Omega Start

Omega

Controls

Main  
 Trips  
 Settings  
 Pucks

rapd.nec.aps.anl.gov

Data Structure

Snaps Runs

NE38\_7\_PAIR\_0\_000002.img  
 NE38\_7\_PAIR\_0\_000001.img  
 NE38\_6\_PAIR\_0\_1+2.img  
 NE38\_6\_PAIR\_0\_000002.img  
 NE38\_6\_PAIR\_0\_000001.img  
 NE38\_5\_PAIR\_0\_1+2.img  
 NE38\_5\_PAIR\_0\_000002.img  
 NE38\_5\_PAIR\_0\_000001.img  
 NE38\_4\_PAIR\_0\_1+2.img  
 NE38\_4\_PAIR\_0\_000002.img  
 NE38\_4\_PAIR\_0\_000001.img  
 NE38\_3\_PAIR\_0\_1+2.img  
 NE38\_3\_PAIR\_0\_000002.img  
 NE38\_3\_PAIR\_0\_000001.img  
 NE38\_2\_0\_000002.img  
 NE38\_2\_0\_000001.img  
 NE38\_1\_PAIR\_0\_1+2.img  
 NE38\_1\_PAIR\_0\_000002.img  
 NE38\_1\_PAIR\_0\_000001.img

Summary Detail Plots Snaps Runs Samples

Omega start ANOM Omega start Max delta Omega Wilson Plot Rad damage1 Rad damage2

### Maximal Oscillation Width

Omega Start

Omega

Controls

Main  
 Trips  
 Settings  
 Pucks

# RAPD Integrate

rapd.nec.aps.anl.gov

Data Structure

Summary Detail Plots Analysis Snaps Runs Samples

NE38\_7\_1  
 NE38\_1\_1  
 NE38\_5\_1  
 NE38\_4\_1  
 NE38\_3\_1  
 NE38\_2\_1

### Processing Results for NE38\_1\_1

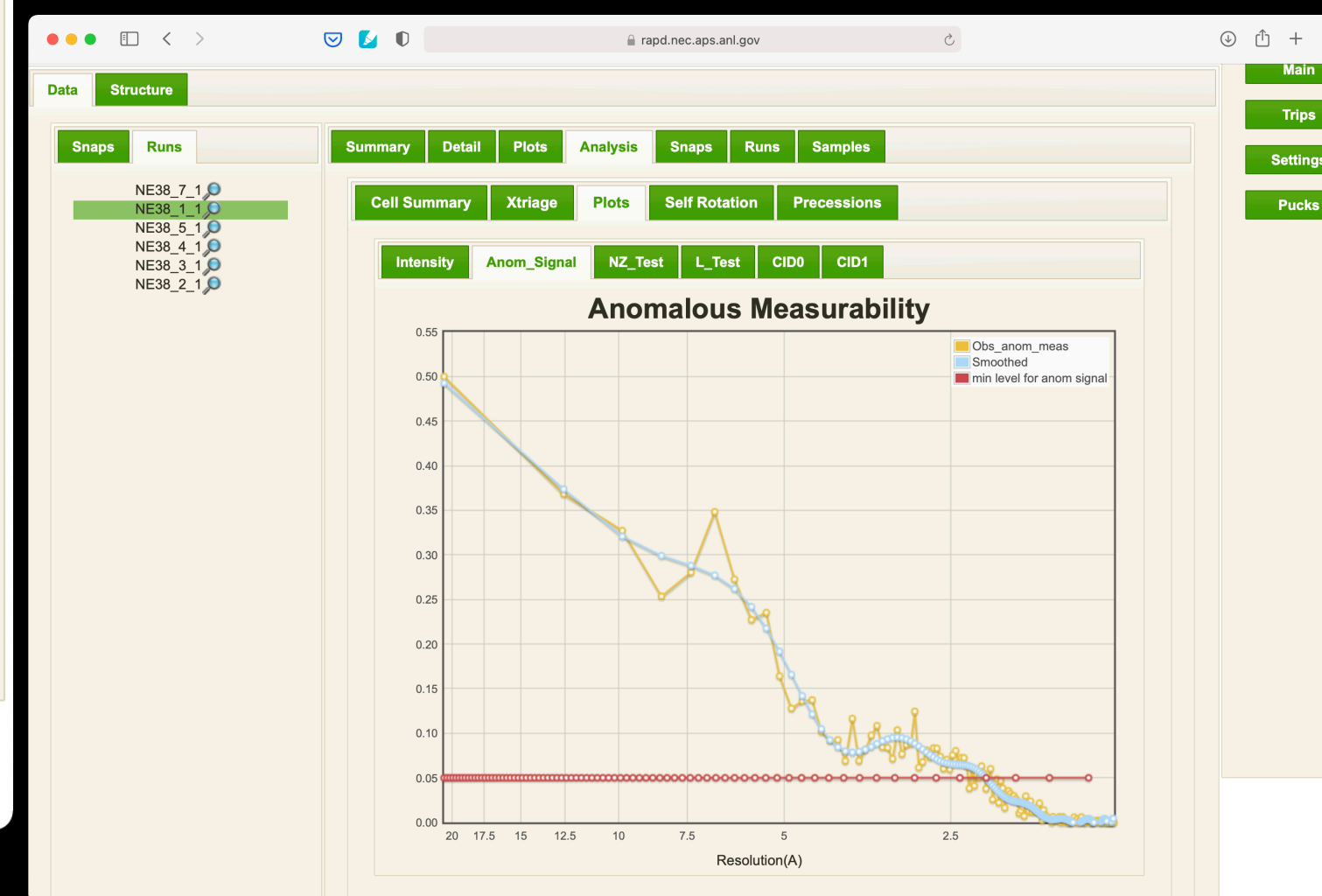
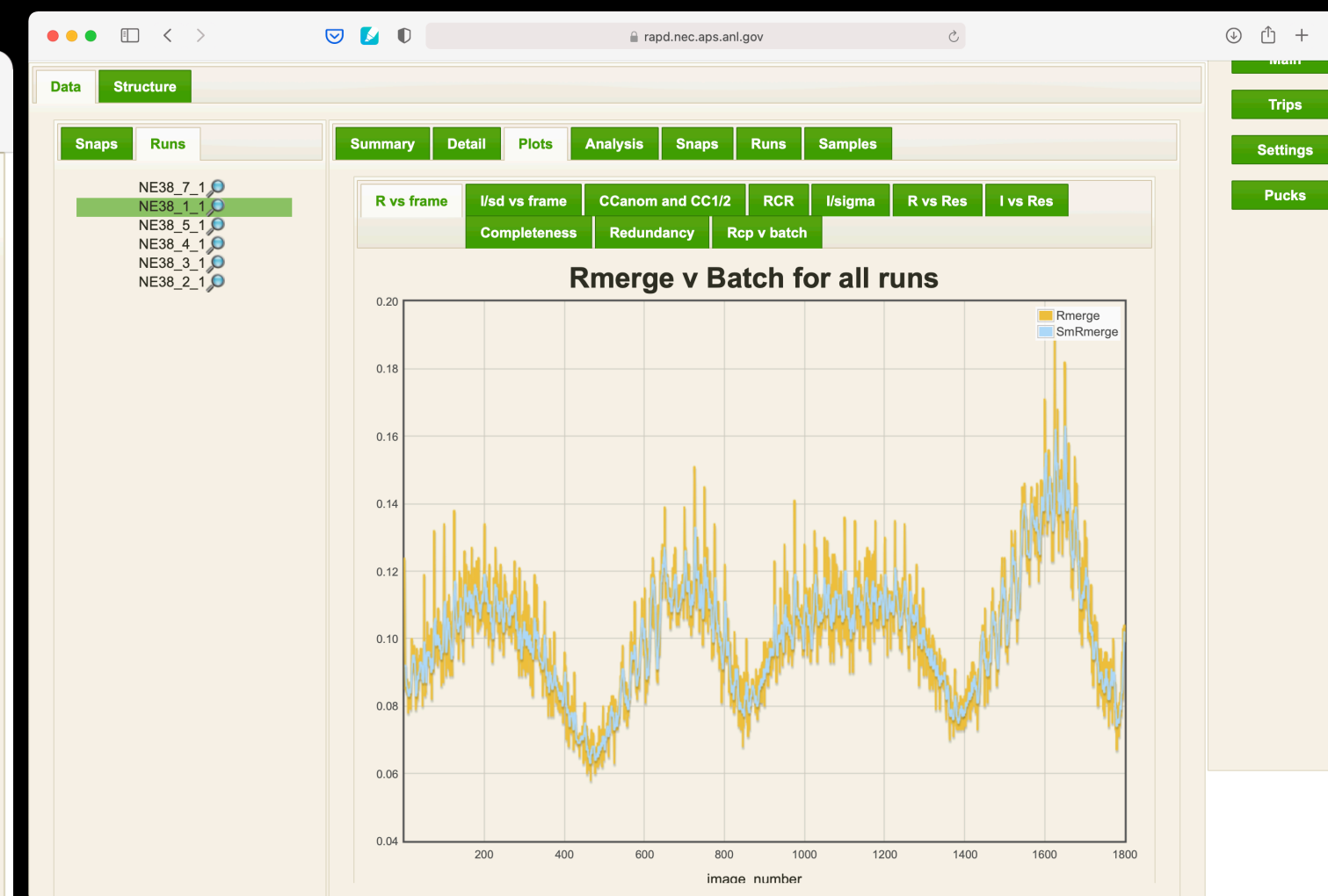
#### Images 1-1800

Spacegroup: P 41 21 2  
 Unit Cell: 57.85 57.85 150.15 90.00 90.00 90.00  
 SIGMAR (Mosaicity): 0.09329°  
 Asymptotic limit of I/sigma (ISa) = 23.81

	Overall	Inner Shell	Outer Shell
High resolution limit	1.27	6.94	1.27
Low resolution limit	150.15	150.15	1.29
Completeness	99.9	100.0	98.6
Multiplicity	25.7	18.2	24.0
I/sigma	30.2	81.7	3.5
CC(1/2)	0.999	0.999	0.875
Rmerge	0.102	0.081	1.055
Rmerge (anomalous)	0.100	0.079	1.037
Rmeas	0.104	0.083	1.078
Rmeas (anomalous)	0.104	0.082	1.080
Rpim	0.020	0.018	0.215
Rpim (anomalous)	0.028	0.023	0.299
Anomalous completeness	99.8	100.0	96.8
Anomalous multiplicity	13.7	12.1	12.7
Anomalous correlation	-0.131	0.047	-0.089
Anomalous slope	1.060	--	--
Total observations	1763371	9851	78787

Controls

Main  
 Trips  
 Settings  
 Pucks





# RAPD SAD

rapd.nec.aps.anl.gov

Data Structure

SAD MR MAD

NE38\_7\_1  
NE38\_1\_1

Summary Plots Autobuild

### SHELXC Results

SAD

Resolution	5.73	3.53	2.66	2.17	1.86	1.64	1.47	1.34	1.23	1.14	1.07
N(data)	906	2616	4392	6311	8030	9896	12142	13801	16625	18748	19463
Chi <sup>2</sup>	1.19	1.02	1.04	1.18	1.35	1.53	1.54	1.51	1.45	1.35	0.80
<l/sig>	162.3	182.0	154.5	135.7	107.4	67.3	44.3	26.5	16.7	11.5	5.2
% Complete	99.9	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	98.1
<d"/sig>	3.60	2.37	2.13	2.07	1.72	1.32	1.04	0.85	0.77	0.73	0.69
CC(1/2)	95.7	93.4	79.4	70.1	52.1	31.7	19.4	10.4	5.1	2.5	-3.0

### SHELXD Results

Space Group	Max CCall	Max CCweak	Max CFOM	Max PATFOM
P41212 (P43212)	29.41	20.27	49.68	9.61
P4122 (P4322)	22.39	14.72	37.11	3.61
P4212	9.13	5.02	14.14	2.94
P422	8.55	4.53	13.08	3.1
P42212	8.55	4.71	13.27	2.79
P4222	10.61	6.00	16.6	2.63

### SHELXE Results

SHELXE may have found a solution in P41212 with a solvent fraction of 0.55

Site	x	y	z	occ*Z	density
1	0.5121	0.0412	0.0813	34.0000	70.78
2	0.4828	-0.2186	-0.0078	31.8478	63.24
3	0.2879	-0.0853	-0.0604	22.9296	43.89
4	0.5232	0.1897	0.0867	19.9104	38.48
5	0.5288	-0.0034	0.0945	17.0748	29.60
6	0.4847	0.0388	0.1893	14.4772	30.83
7	0.8224	-0.0473	0.1008	11.0296	18.88
8	0.1737	0.0207	-0.0578	8.6598	15.94

SHELXE FOM 0.842

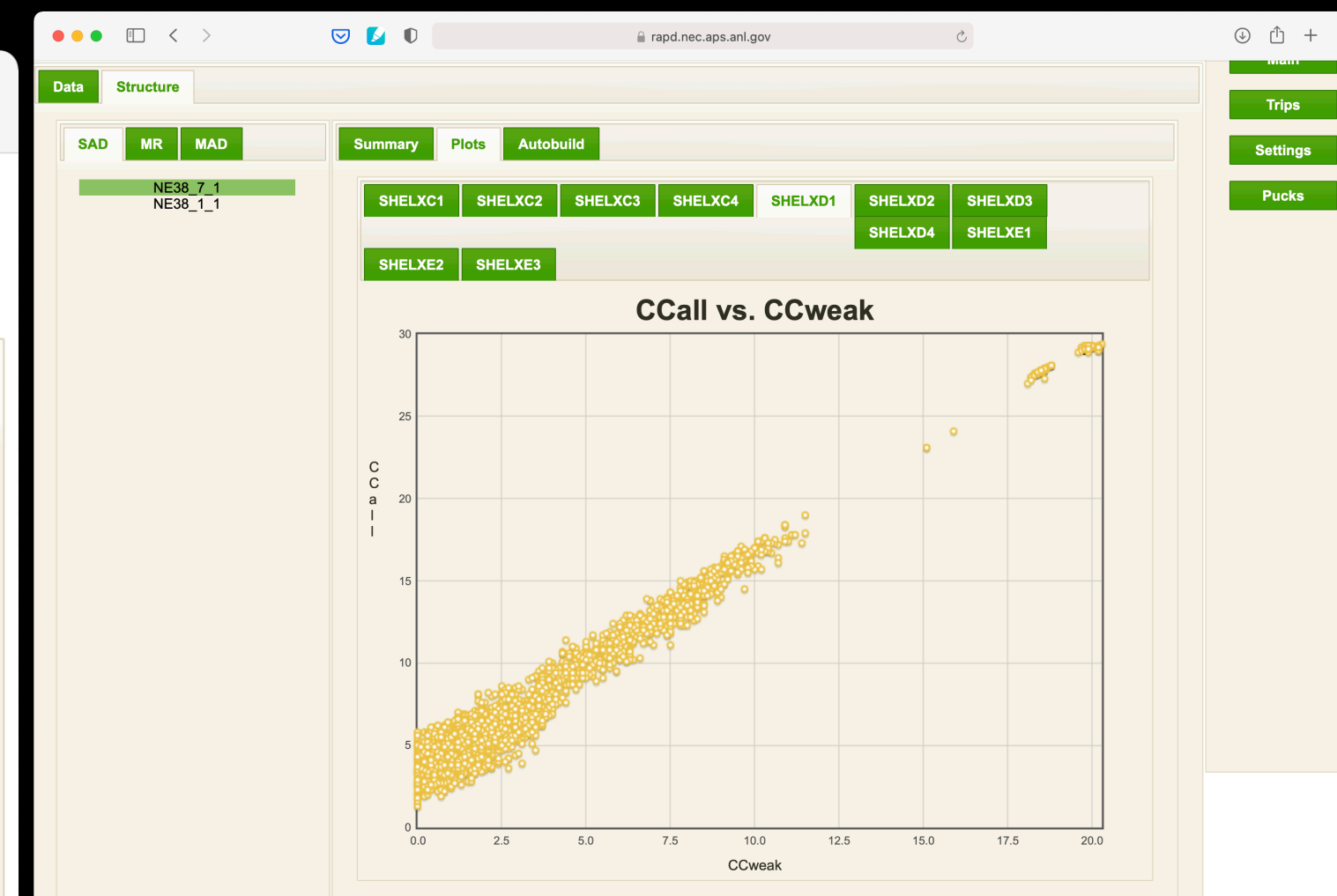
Controls

Main

Trips

Settings

Pucks



rapd.nec.aps.anl.gov

Data Structure

SAD MR MAD

NE38\_7\_1  
NE38\_1\_1

Summary Plots Autobuild

### Phenix AutoSol Results

Statistics	
Space Group	P41212
Bayesian CC	41.9
FOM	0.21
Number of starting sites	46
Number of refined sites	40
Number of residues built	135
Number of side-chains built	0
Total number of chains	3
model-map CC	0.53
Refined R/R-free	0.41/0.42

RAPD Logfile

Click to view log

Trips

Settings

Pucks

# That's All Great But...

- Very difficult to add new features
- NE-CAT specific code throughout
- PHP UI was outdated



# An Interruption to Our Regularly Scheduled Program









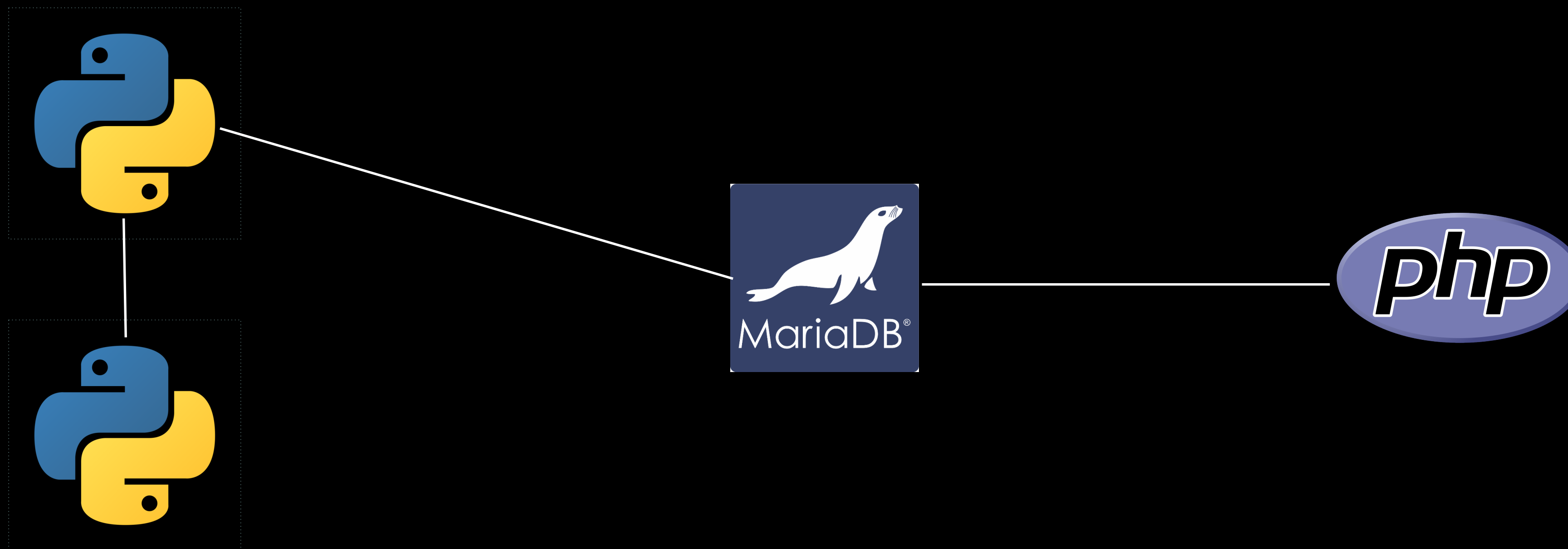


# RAPDv2 Development

# Our Goals For **RAPDv2**

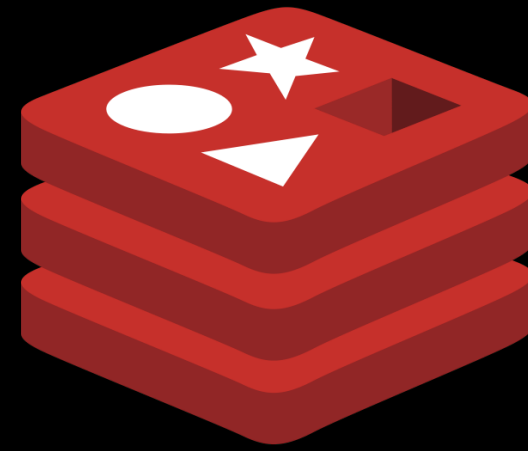
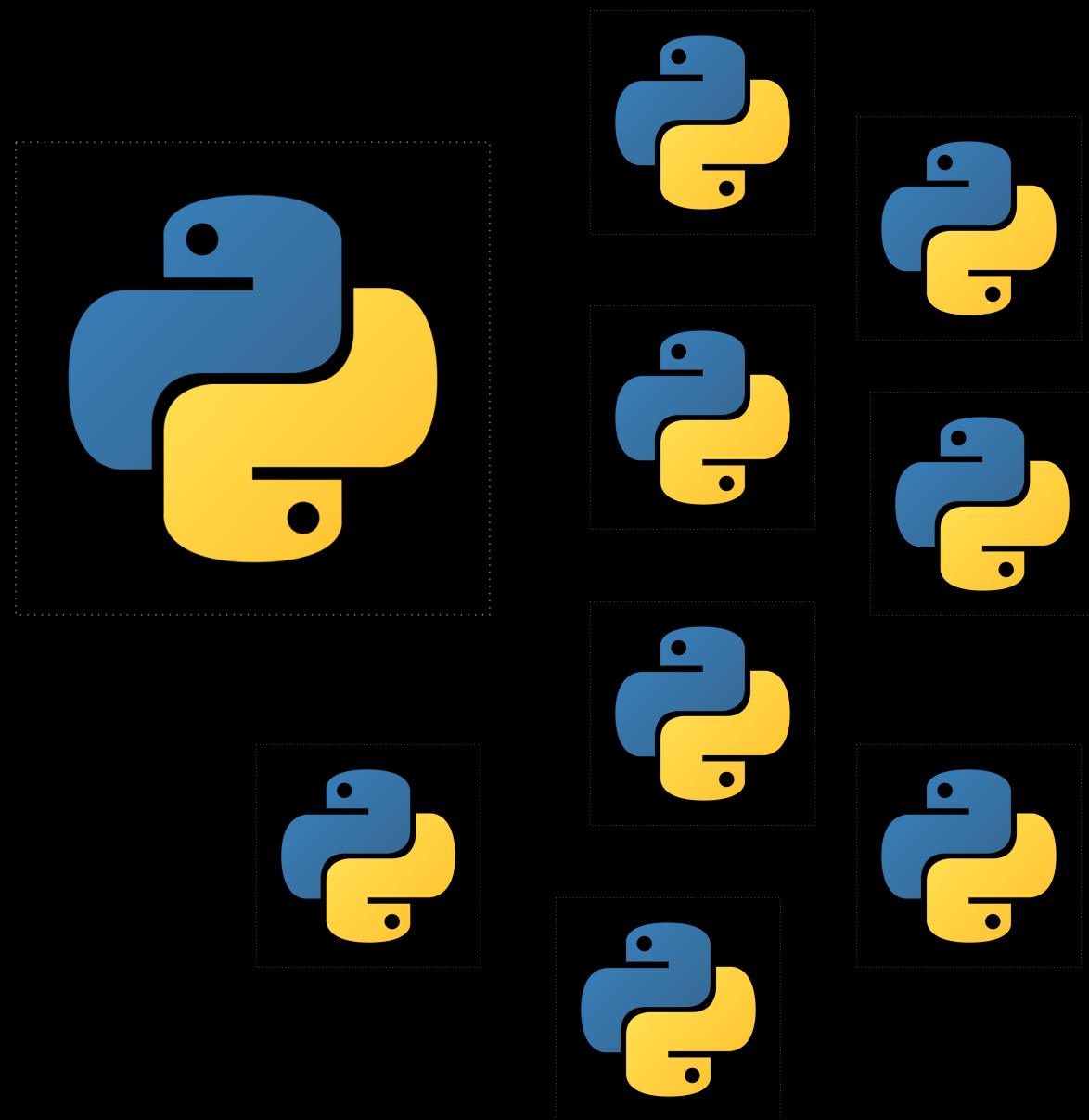
- Take the best of **RAPDv1** and throw out the rest
- Borrow knowledge from remote access program
- Flexible design
- Multiple modes of use
- Modern UI

# RAPDv1 Design



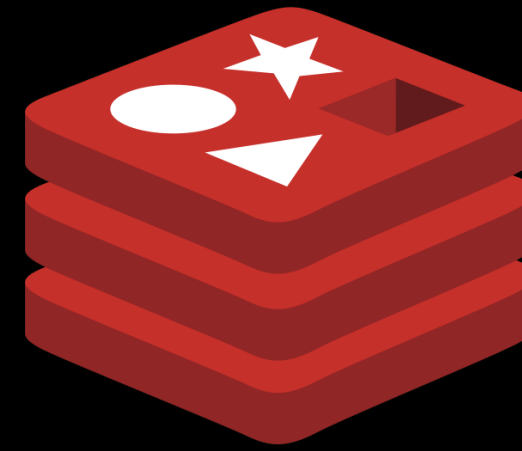
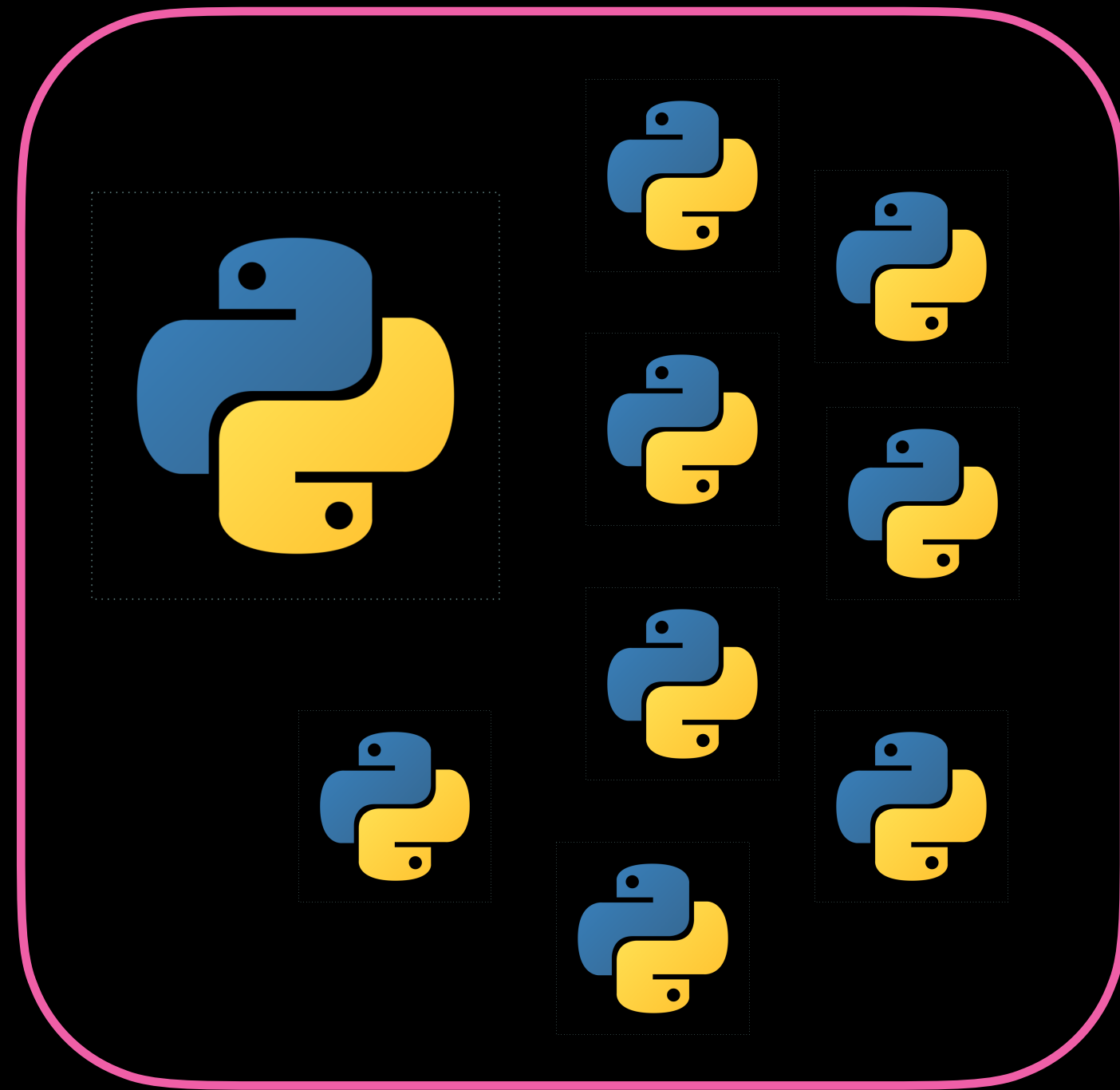


# RAPDv2 Design



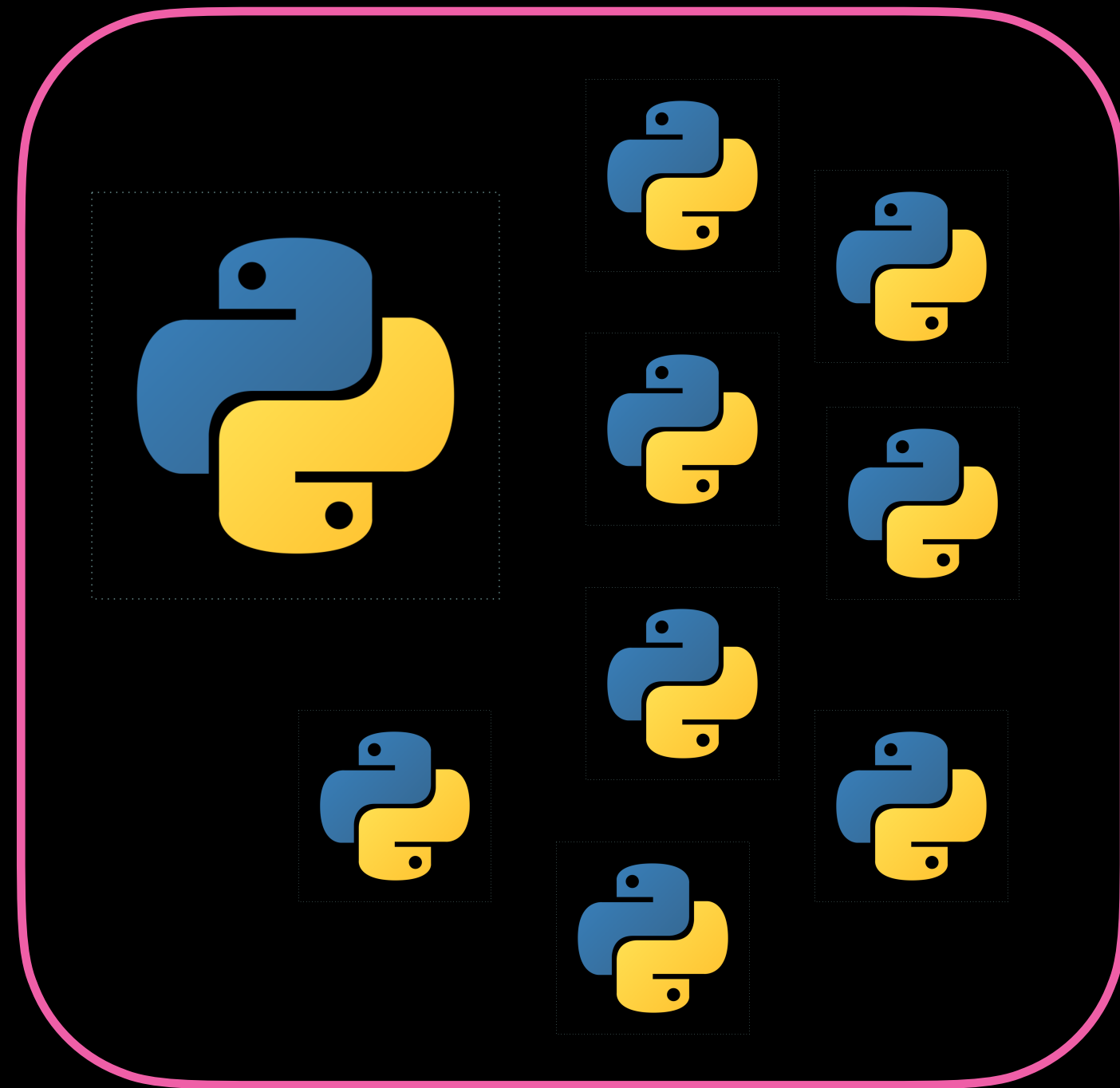


# RAPDv2 Design



Plugin-based architecture  
Python 2.7

# RAPDv2 Design



Plugin-based architecture  
Python 2.7

Core Python code is beamline-agnostic

Where does specificity come from?

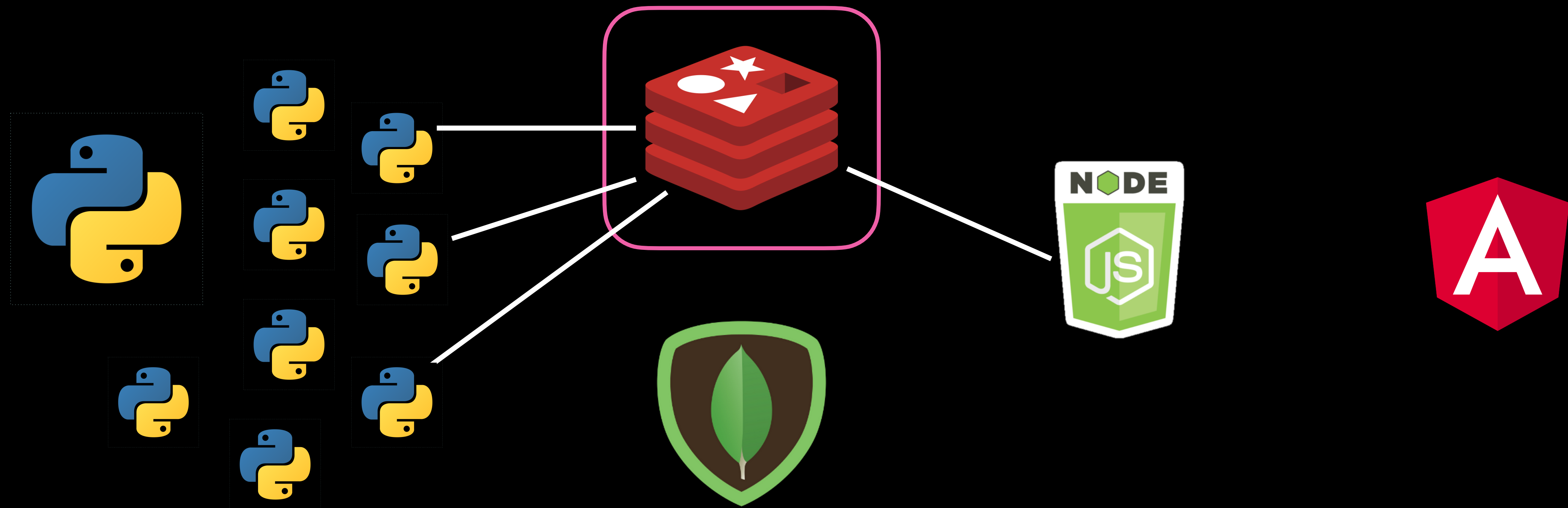
- Configuration file
- Site-specific plugins - detector, gatherers

Data processing plugins now run in CLI

What's a plugin?

- Connection to databases
- Data gatherers
- Connection to cluster
- Processing pipelines

# RAPDv2 Design



Redis-based inter-process  
communication

# RAPDv2 Design

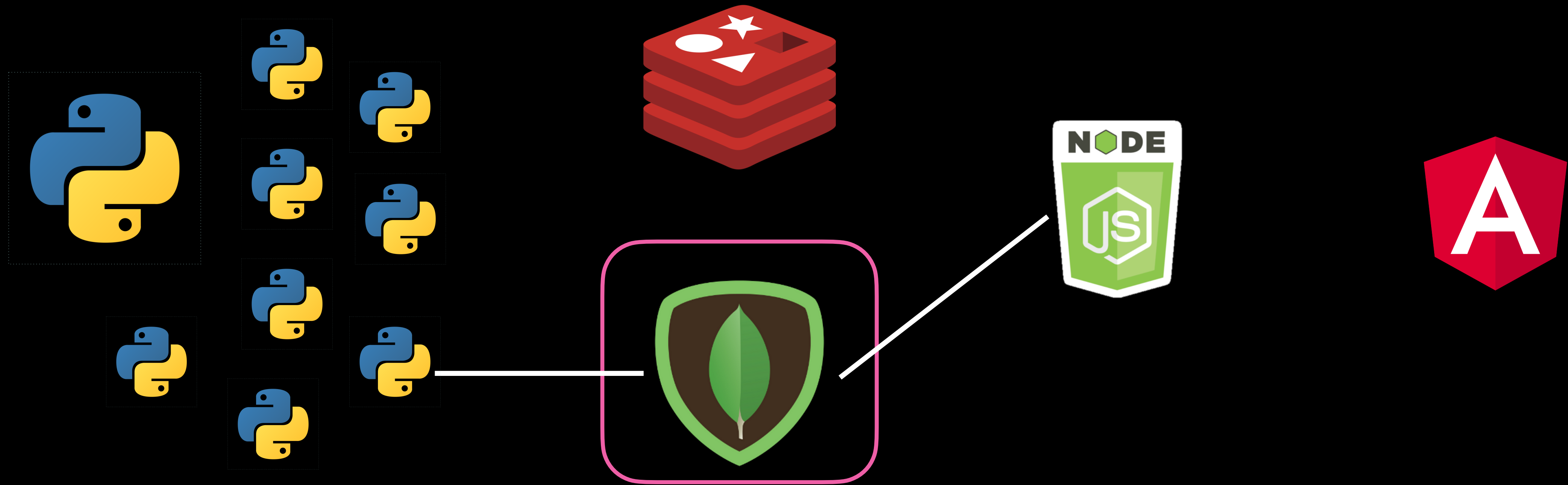


Redis-based inter-process  
communication

Redis is an indispensable tool for us.

- key-value store
- publication-subscribe interprocess communication
- [redis.io](https://redis.io)

# RAPDv2 Design



Document-based database  
MongoDB

# RAPDv2 Design

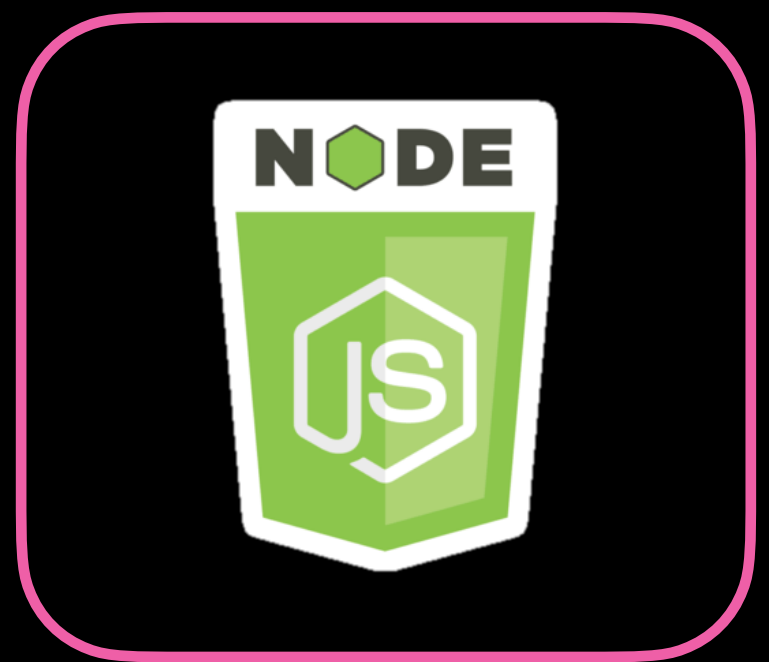
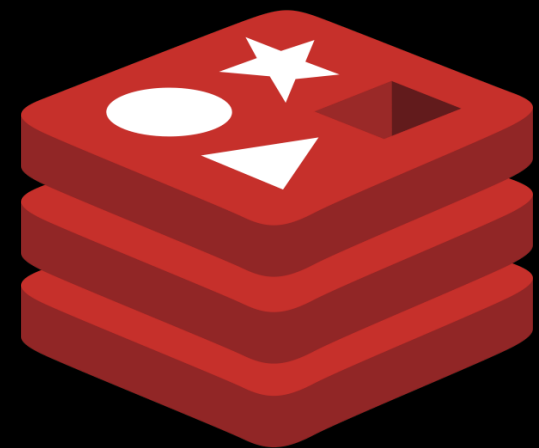
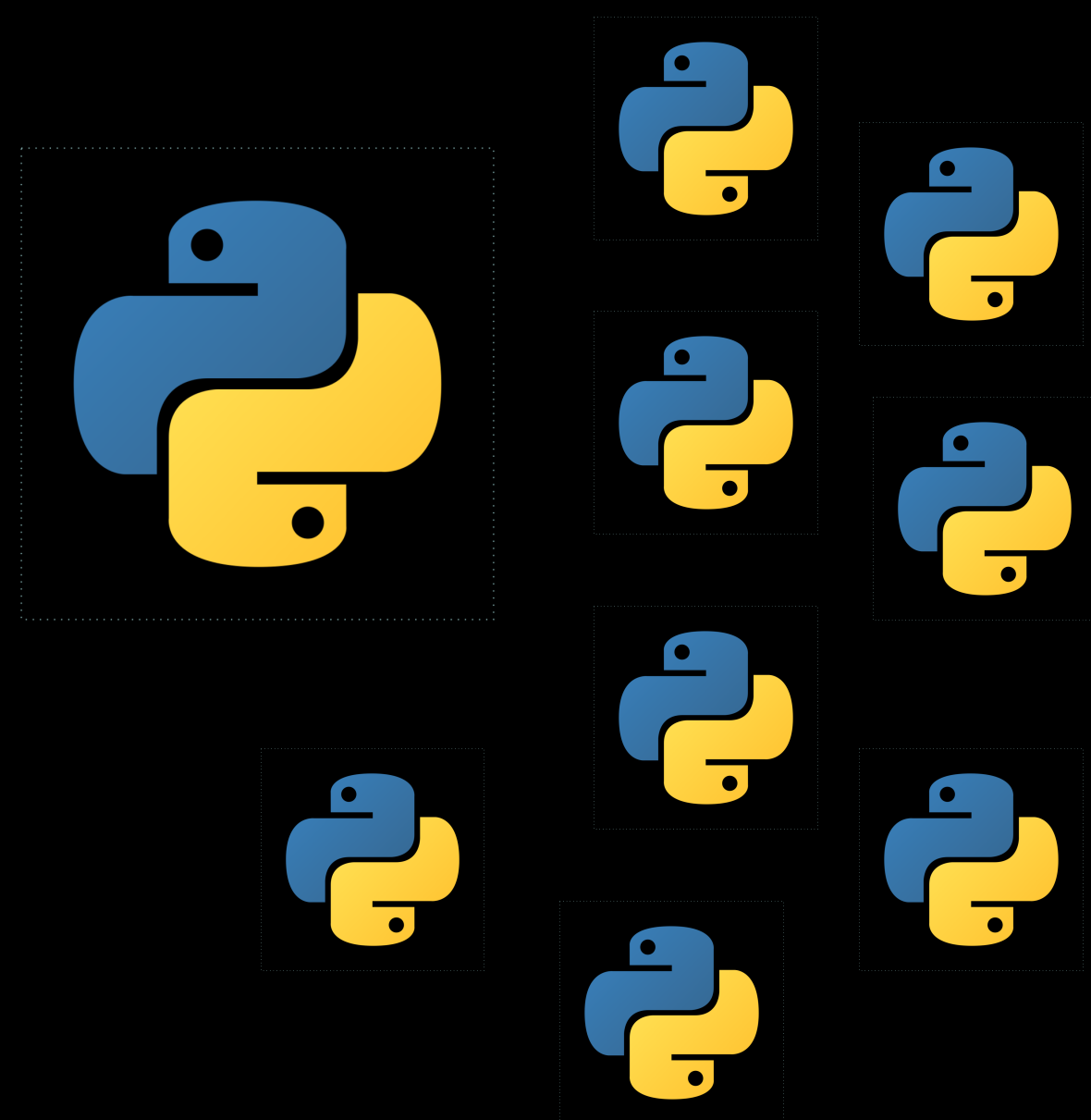


Document-based database  
MongoDB

MongoDB much more flexible than SQL-based solutions

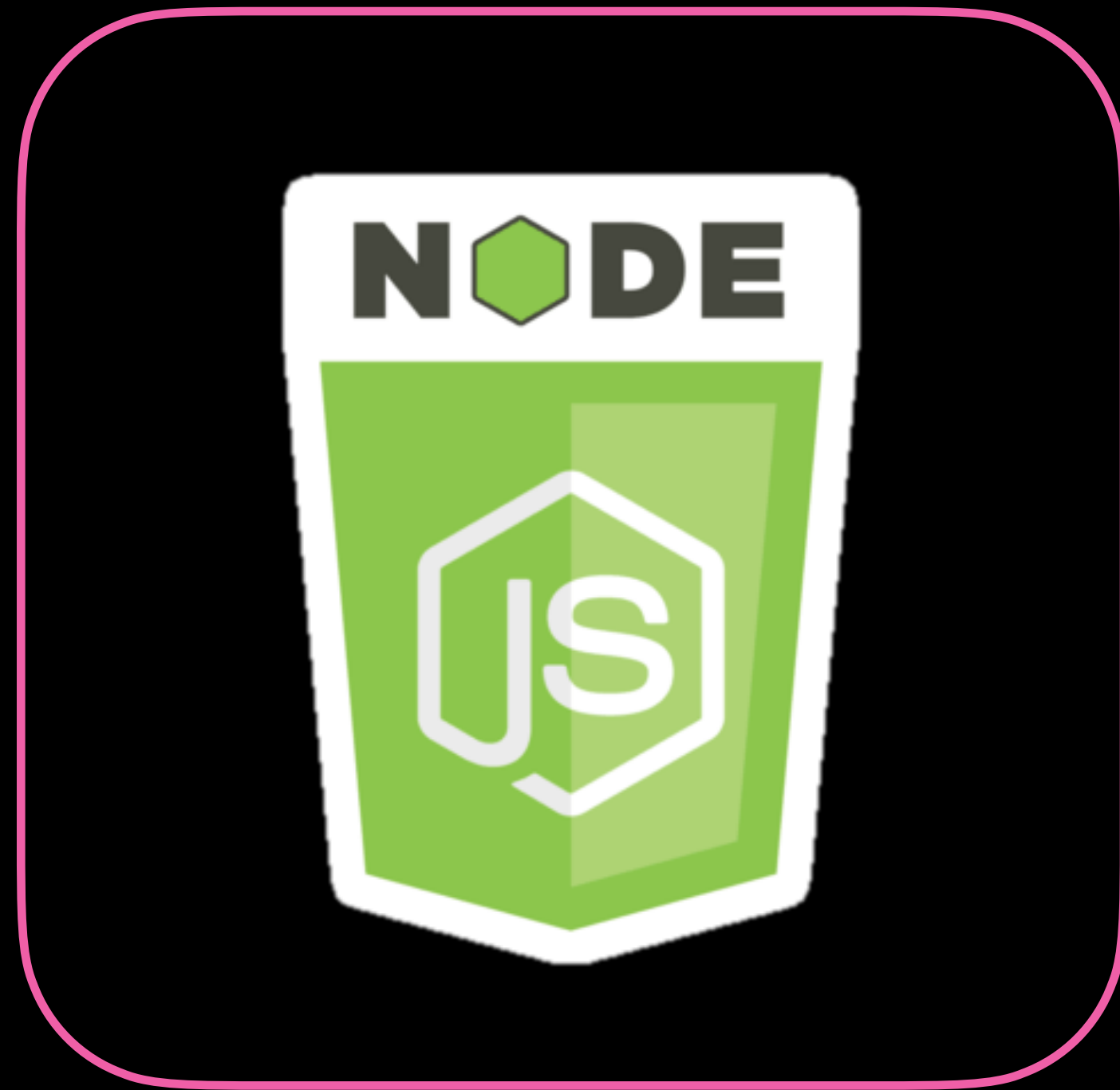
- Stores documents & files
- More flexibility
- Meshes well with modern UI design
- [mongodb.com](https://www.mongodb.com)

# RAPDv2 Design



NodeJS  
Application server

# RAPDv2 Design



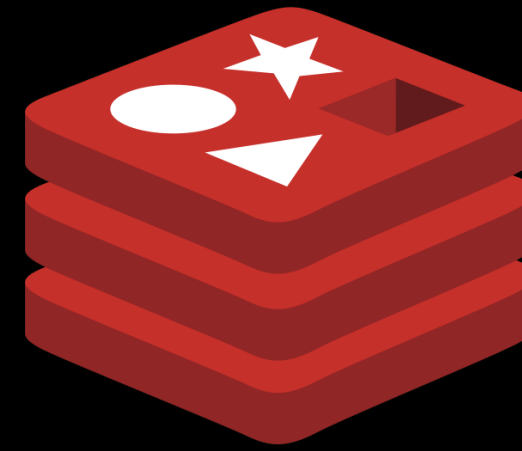
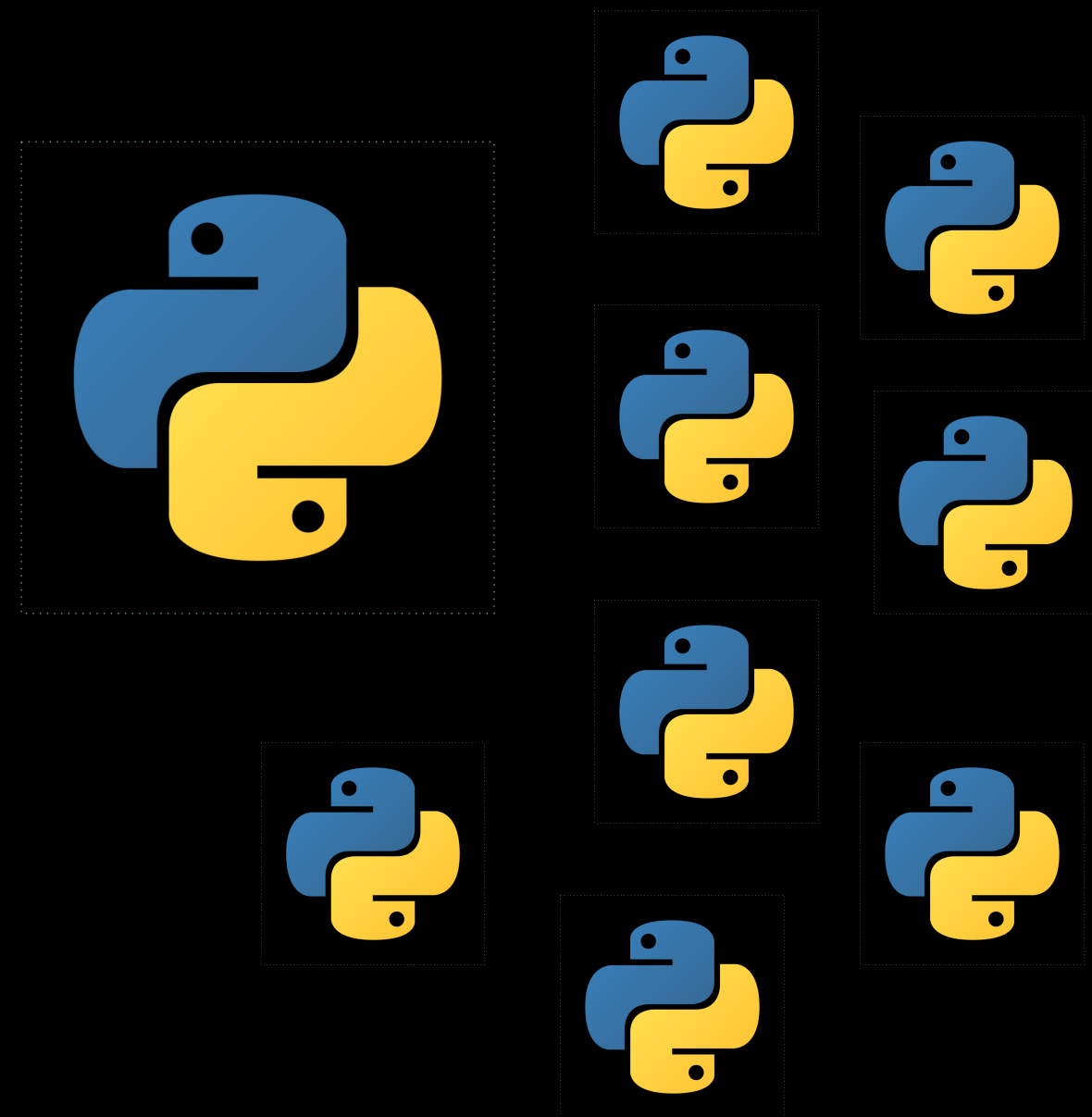
NodeJS  
Application server

NodeJS offers a lot of power & flexibility

- Powerful, flexible & fast
- Tight integration with UI
- Provides REST & Websocket access to **RAPDv2**
- [nodejs.org](https://nodejs.org)



# RAPDv2 Design



Angular UI

# RAPDv2 Design



Angular UI

Modern web development platform

- Very powerful
- Steep learning curve
- Actively developed & large community
- [angular.io](https://angular.io)

# RAPDv2 Current Capabilities

- Indexing & Strategy – DISTL, Labelit, BEST, Mosflm
- Integration, Scaling & Analysis – XDS, Aimless, Pointless, Phaser, Xtrriage
- Merging – Aimless, Pointless
- SAD – SHELX, Phenix
- MR – Phaser

# RAPDv2 Index

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_PAIR\_0\_000001.cbf

NE38\_6\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_1+2.cbf

NE38\_5\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_000001.cbf

NE38\_4\_PAIR\_0\_1+2.cbf

NE38\_4\_PAIR\_0\_000002.cbf

NE38\_4\_PAIR\_0\_000001.cbf

NE38\_3\_PAIR\_0\_1+2.cbf

NE38\_3\_PAIR\_0\_000002.cbf

NE38\_3\_PAIR\_0\_000001.cbf

NE38\_2\_0\_000002.cbf

NE38\_2\_0\_000001.cbf

NE38\_1\_PAIR\_0\_000002.cbf

### Indexing Results for NE38\_7\_PAIR\_0\_000001.cbf

Summary

#### Indexing Solution

Spacegroup	Unit Cell			Mos. (°)	Res. (Å)
P4	57.86	57.86	150.21	90.00 90.00 90.00	0.025 1.11

#### Data Collection Strategies

##### Normal by Best

N	$\Omega$ Start	$\Delta\Omega$	# Images	Exposure time	Distance	Transmission
1	82	0.1	580	0.05	170	3

##### Anomalous by Best

N	$\Omega$ Start	$\Delta\Omega$	# Images	Exposure time	Distance	Transmission
1	78	0.1	920	0.05	170	3

Reindex + Project ↑ Pin 🗑️ Junk

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_PAIR\_0\_000001.cbf

NE38\_6\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_1+2.cbf

NE38\_5\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_000001.cbf

NE38\_4\_PAIR\_0\_1+2.cbf

NE38\_4\_PAIR\_0\_000002.cbf

NE38\_4\_PAIR\_0\_000001.cbf

NE38\_3\_PAIR\_0\_1+2.cbf

NE38\_3\_PAIR\_0\_000002.cbf

NE38\_3\_PAIR\_0\_000001.cbf

NE38\_2\_0\_000002.cbf

NE38\_2\_0\_000001.cbf

NE38\_1\_PAIR\_0\_000002.cbf

### Indexing Results for NE38\_7\_PAIR\_0\_000001.cbf

Details

#### Data Collection Strategy from Best Normal

N	$\Omega$ Start	$\Delta\Omega$	# Images	Exposure time	Distance	Transmission
1	82°	0.1°	580	0.05s	168mm	2.9%

Resolution Limit	1.22 Å
$\Omega_{start}$ - $\Omega_{finish}$	82° - 140°
Rotation Range	58.0°
Number of Images	580
Completeness (outer)	0.99 (1)
Redundancy (outer)	2.44 (2.36)
R factor (outer)	12.3 (129.1)
I/σ (outer)	7.7 (0.8)

#### Data Collection Strategy from Best ANOMALOUS

N	$\Omega$ Start	$\Delta\Omega$	# Images	Exposure time	Distance	Transmission
1	78.0°	0.1°	920	0.05s	168mm	3%

Resolution Limit	1.22 Å
$\Omega_{start}$ - $\Omega_{finish}$	78° - 170°
Rotation Range	92.0°
Number of Images	920

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_PAIR\_0\_000001.cbf

NE38\_6\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_1+2.cbf

NE38\_5\_PAIR\_0\_000002.cbf

NE38\_5\_PAIR\_0\_000001.cbf

NE38\_4\_PAIR\_0\_1+2.cbf

NE38\_4\_PAIR\_0\_000002.cbf

NE38\_4\_PAIR\_0\_000001.cbf

NE38\_3\_PAIR\_0\_1+2.cbf

NE38\_3\_PAIR\_0\_000002.cbf

NE38\_3\_PAIR\_0\_000001.cbf

NE38\_2\_0\_000002.cbf

NE38\_2\_0\_000001.cbf

NE38\_1\_PAIR\_0\_000002.cbf

### Indexing Results for NE38\_7\_PAIR\_0\_000001.cbf

Logs

#### Best Strategy Normal

Program Best /A.Popov & G.Boarenkov/  
Version 3.4.4 // 10.06.2011  
Copyright 2004-11 by Alexander Popov and Gleb Boarenkov  
<B><FONT COLOR="#FF0000"><!--SUMMARY\_BEGIN-->  
Main Wedge  
\*\*\*\*\*  
Resolution limit is set by the initial image resolution  
Resolution limit =1.22 Angstrom Transmission = 2.9% Distance = 168.2mm

#### Best Strategy ANOMALOUS

Program Best /A.Popov & G.Boarenkov/  
Version 3.4.4 // 10.06.2011  
Copyright 2004-11 by Alexander Popov and Gleb Boarenkov  
<B><FONT COLOR="#FF0000"><!--SUMMARY\_BEGIN-->  
Main Wedge  
\*\*\*\*\*  
Resolution limit is set by the initial image resolution  
Resolution limit =1.22 Angstrom Transmission = 3.1% Distance = 168.2mm

# RAPDv2 Integrate

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_1\_[1-3600].cbf

NE38\_5\_1\_[1-3600].cbf

NE38\_4\_1\_[1-3600].cbf

NE38\_3\_1\_[1-3600].cbf

NE38\_2\_1\_[1-3600].cbf

NE38\_1\_1\_[1-1800].cbf

### Integration Results for NE38\_7\_1\_[1-3600].cbf

Summary

#### Indexing Solution

Spacegroup	Unit Cell	Mosaicity	ISA
P 41 21 2	57.77 Å 57.77 Å 150.01 Å 90.0° 90.0° 90.0°	0.06°	28.83

#### Table 1

	Overall	Inner Shell	Outer Shell
Res Limits (Å)	75.01-1.05	75.01-5.76	1.07-1.05
Completeness (%)	99.3	100	87.6
Multiplicity	45.8	40.4	17.6
$I/\sigma(I)$	36.5	149.4	0.4
CC 1/2	1	1	0.161
R merge	0.064	0.028	5.768
R merge Anomalous	0.063	0.027	5.661
R meas	0.064	0.029	5.936
R meas Anomalous	0.064	0.028	5.986
R pim	0.009	0.004	1.355
R pim Anomalous	0.013	0.005	1.894
Anomalous Completeness	99.1	100	83.9
Anomalous Multiplicity	23.9	26	9.4
Anomalous Correlation	0.356	0.622	0.104
Anomalous Slope	1.084		

#### Rmerge vs Batch

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_1\_[1-3600].cbf

NE38\_5\_1\_[1-3600].cbf

NE38\_4\_1\_[1-3600].cbf

NE38\_3\_1\_[1-3600].cbf

NE38\_2\_1\_[1-3600].cbf

NE38\_1\_1\_[1-1800].cbf

### Integration Results for NE38\_7\_1\_[1-3600].cbf

Analysis

Summary Self-Rotation Logs

#### Unit Cell

Spacegroup	Unit Cell
P 41 21 2 (92)	57.77 Å 57.77 Å 150.01 Å 90.0° 90.0° 90.0°

#### Patterson Analysis

% Origin	p-value	X	Y	Z
5.94	0.727	0.0	0.33	0.0

#### Twinning Analysis

No twinning suspected

#### Xtriage Summary

The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected. The results of the L-test indicate that the intensity statistics behave as expected. No twinning is suspected.

Download + Project Reintegrate MR SAD Pin Junk

rapd.nec.aps.anl.gov

## RAPD @ NECAT

Sessions Projects Dashboard Admin Log Out

Snaps Runs

NE38\_7\_1\_[1-3600].cbf

NE38\_5\_1\_[1-3600].cbf

NE38\_4\_1\_[1-3600].cbf

NE38\_3\_1\_[1-3600].cbf

NE38\_2\_1\_[1-3600].cbf

NE38\_1\_1\_[1-1800].cbf

### Integration Results for NE38\_7\_1\_[1-3600].cbf

PDB Query

Cell Search Contaminants Raw

#### Search Based On Unit Cell Similarity

ID	Description	LL Gain ↓	RF Z-score↑	Z-score#	Clashes	Actions
3ALD	Thaumatococcus	45,587.1	8.4	17.6	0	Download Search
5Y9R	Thaumatococcus	45,361.6	8.6	15.9	0	Download Search
5X9L	Thaumatococcus	45,120.4	7.8	16.6	0	Download Search
4BAL	Thaumatococcus	44,995.9	9.5	19.8	0	Download Search
3AL7	Thaumatococcus	44,947.4	8.1	17.0	0	Download Search
5Y9Q	Thaumatococcus	44,812.0	8.0	17.6	0	Download Search
4BAR	Thaumatococcus	44,663.6	9.7	20.5	0	Download Search
2VHR	Thaumatococcus	44,512.8	9.4	19.6	0	Download Search
1RQW	Thaumatococcus	44,175.4	9.8	20.4	0	Download Search
2VHK	Thaumatococcus	44,032.5	9.7	21.2	0	Download Search

# Our Goals For **RAPDv2**

Take the best of **RAPDv1** and throw out the rest

- Much of the data processing code was adapted
- Some UI elements that we liked were kept

# Our Goals For **RAPDv2**

Borrow knowledge from remote access program

- Use of Redis & MongoDB
- NodeJS as application server



# Our Goals For **RAPDv2**

## Flexible design

- Core programs are not site-specific
- Config file determines variables and plugins that define site



# Our Goals For **RAPDv2**

## Multiple modes of use

- CLI for data processing & development
- REST interface
- WebSocket interface

# RAPDv2 Status

## Now

- RAPDv2 running as secondary
- Final steps of UI implementation for SAD & MR

## Mid 2021

- Replace RAPDv1 as primary
- Built-out operations control

## Late 2021

- Merging and Cluster Merging tools

# Can I Use **RAPDv2**?

- If you really like the *bleeding edge*, have at it.
- Waiting until NE-CAT is using as primary (mid-2021) is recommended.

github.com

RAPD / RAPD

<> Code Issues 34 Pull requests 3 Actions Projects 1 Wiki Security 1 Insights

⚠ We found potential security vulnerabilities in your dependencies. You can see this message because you have been granted [access to Dependabot alerts for this repository](#). [See Dependabot alerts](#)

master 20 branches 0 tags [Go to file](#) [Add file](#) [Code](#)

Commit Message	Commit Hash	Time Ago	Commits
schuerjp1 Moved distl to subcontractor for use in other plugins.	d060b1b	21 days ago	3,272
install Add mysolr to install		2 years ago	
src Moved distl to subcontractor for use in other plugins.		21 days ago	
.gitignore Fixed MR.transfer_files.		5 months ago	
.pylintrc Tweak the results from indexing		4 years ago	
.travis.yml Trying to test TravisCI		4 years ago	
AUTHORS.txt Change authors file		5 years ago	
CONTRIBUTING.md Update to the MongoDB tool, create a script for it, and add to contri...		3 years ago	
LICENSE.txt Changing the license		5 years ago	
README.md Fix conflicts in README.md		4 years ago	
notes Need pkg_config for ubuntu		4 years ago	

README.md

## RAPD

A package for automated indexing, strategy, integration, analysis, & structure solution of macromolecular

# Acknowledgements

## Contributors

Jon Schuermann

David Neau

Kay Perry

Jim Withrow

## NE-CAT Support Staff

Surajit Banerjee

Ali Kaya

Igor Kourinov

N. Sukumar

## Support

NIGMS P30 GM124165