

# Data Analysis Infrastructure for DLS MX/CX

M. Gerstel   R. Gildea   K. Levik   A. Ashton   G. Winter

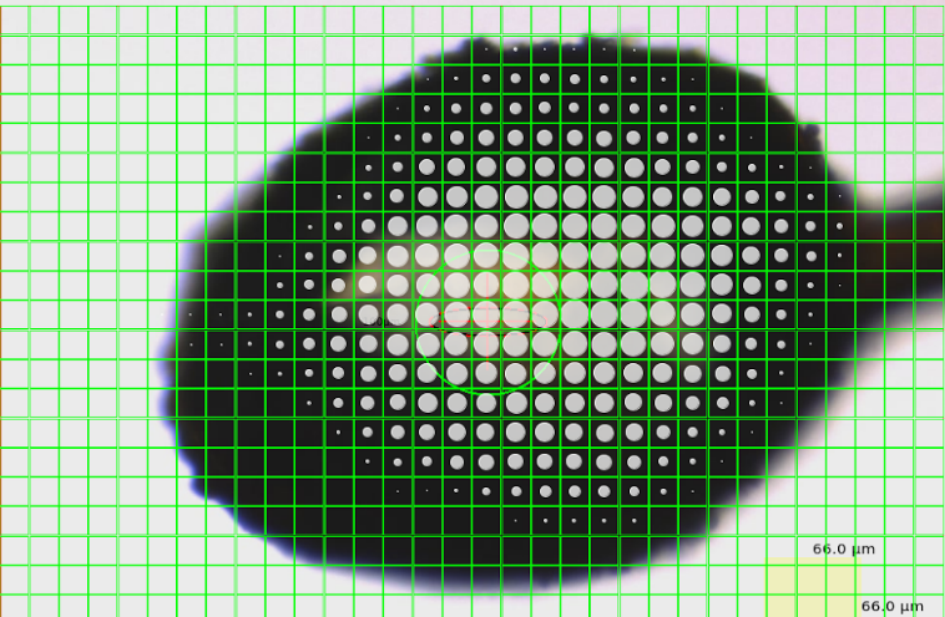
Diamond Light Source, Harwell, Oxfordshire, UK

NOBUGS 2016

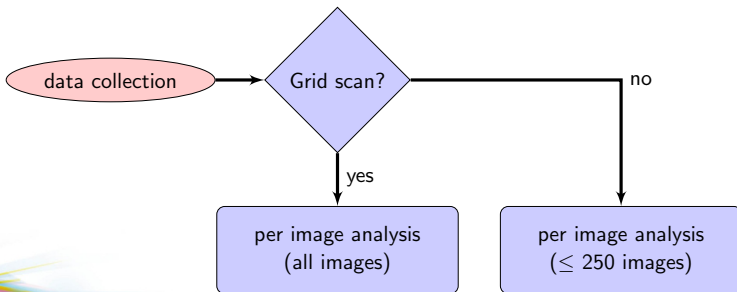
# Diamond Light Source



# GDA grid scan



# Grid scan processing







# Scripts run more scripts

```

#!/bin/sh
#script that is run at the end of every collect in RC
#original author of this script is Rijn Rubin 240608
#110351 added archiving to the end - awa

# input to script:
# automaticProcessing_Yes 4315 /dis/103/data/2008/0-0 test2_MISL_4_***.img /dis/103/data/2008/0-0/0

#create a full and proper log/script for re running preprocessing, RM 131022
# "date" >> $(3)/spool/RunEndOfCollectLog.sh
processing_dir="/dis_sw/apps/wc-scripts/misc/RunProcessingDir.sh $(2)"
echo "test -d '$(processing_dir)' && mv '$(processing_dir)' >> $(3)/spool/RunEndOfCollectLog.sh"
echo $0 $* >> $(3)/spool/RunEndOfCollectLog.sh
echo "sleep 120" >> $(3)/spool/RunEndOfCollectLog.sh

#
# Pause for nfs
#
umask 002
Pause=60

Visit='basename $(3)
ImageDirectory=$(5)
[[ $ImageDirectory != "/" ]] && ImageDirectory="$ImageDirectory/"
echo $RCID $ImageDirectory $ImageDirectory

set BEHLINE env or set
then BEHLINE : then
LINE= echo $3 | out -d/ -f3"

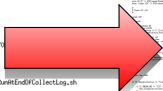
"/dis_sw/apps/wc-scripts/misc/isItDataCollection 2"
tion == "True" ]] ; then

appear in a separate job for monitoring reasons
t/autorun/run_all_images_there.sh $1 $2 $3 $4 $ImageDirectory $6

Run KIR2

IF [[ $DataCollection == "True" ]] ; then
if [[ $BEHLINE != "123" ]] ; then
/dis_sw/apps/wc-scripts/autorun-fast-dp-refactor.sh $1 $2 $3 $4 $ImageDirectory $6 > /tmp/date +%s %Z1 & /dev/null 2>&1
fi
if [[ $1 == "automaticProcessing_Yes" ]] ; then
rmdirirectia2 /dis_sw/apps/wc-scripts/autorun-fast-dp-refactor.sh
runautorPROC="/dis_sw/apps/wc-scripts/autorPROC/RunDirectFrom3R.sh
eval $rmdirirectia2 $1 $2 $3 $4 $ImageDirectory $6 > /dev/null 2>&1 &
eval $runautorPROC $1 $2 $3 $4 $ImageDirectory $6 > /dev/null 2>&1 &
fi
echo "date" >> $rmdirirectia2 $1 $2 $3 $4 $ImageDirectory $6 >> /dis_sw/BEHLINE/logs/RunEndOfCollectCommand.log
echo "date" >> $runautorPROC $1 $2 $3 $4 $ImageDirectory $6 >> /dis_sw/BEHLINE/logs/RunEndOfCollectCommand.log
fi
#
# Auto Run EDN
#
IF [[ $BEHLINE != "123" ]] ; then

```



qsub -cwd



qsub -cwd



qsub -cwd

```

-----
Date: 2008-09-18 10:00:00
User: root
Host: node01
JobID: 123456789
JobName: /dis_sw/apps/wc-scripts/misc/RunProcessingDir.sh
-----

```

```

-----
Date: 2008-09-18 10:00:00
User: root
Host: node01
JobID: 123456789
JobName: /dis_sw/apps/wc-scripts/misc/isItDataCollection 2
-----

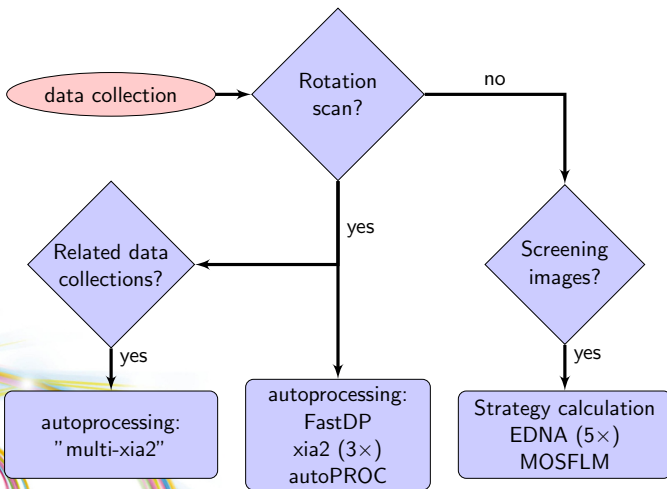
```

```

-----
Date: 2008-09-18 10:00:00
User: root
Host: node01
JobID: 123456789
JobName: /dis_sw/apps/wc-scripts/autorun-fast-dp-refactor.sh
-----

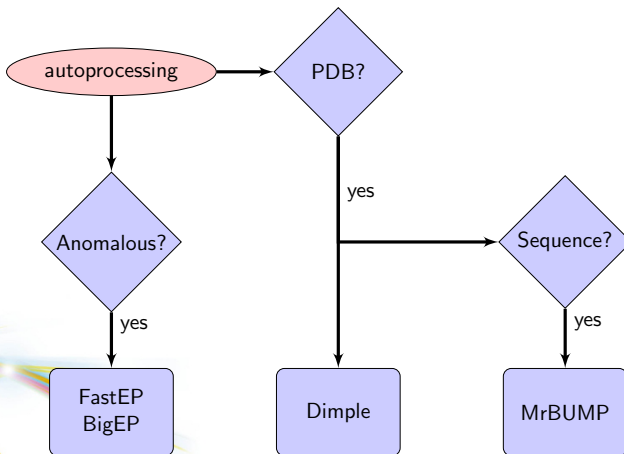
```

# Data set processing





# Data set processing II



# Limitations



# Limitations

- Maintainability



# Limitations

- Maintainability
- Testing



# Limitations

- Maintainability
- Testing
- Monitoring



# Limitations

- Maintainability
- Testing
- Monitoring
- Data reprocessing



# Limitations

- Maintainability
- Testing
- Monitoring
- Data reprocessing
- Efficient use of computing resources

# DECTRIS EIGER X





# DECTRIS EIGER X

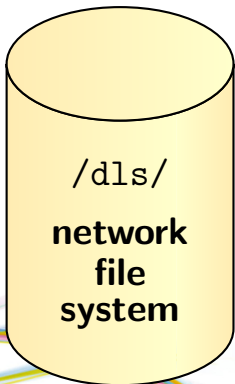


# DECTRIS EIGER X

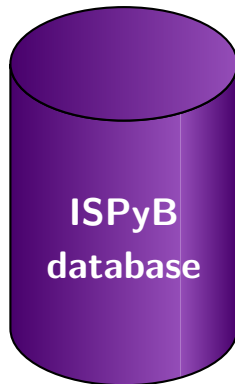


# ActiveMQ

## Data



## Metadata

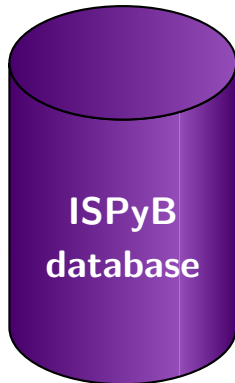
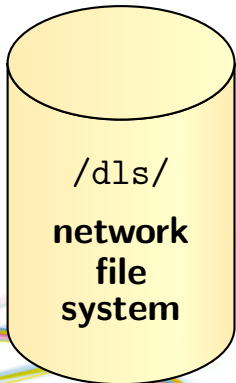


# ActiveMQ

**Data**

**Events**

**Metadata**



# ActiveMQ

- + Fast
- + Lightweight
- + Not invented here
- + Broad language support
- + Already used by other groups

— Documentation

# Terminology

- **Broker:** Central server



# Terminology

- **Broker:** Central server
- **Queue:** Producer–Consumer



# Terminology

- **Broker:** Central server
- **Queue:** Producer–Consumer
- **Topic:** Publish–Subscribe



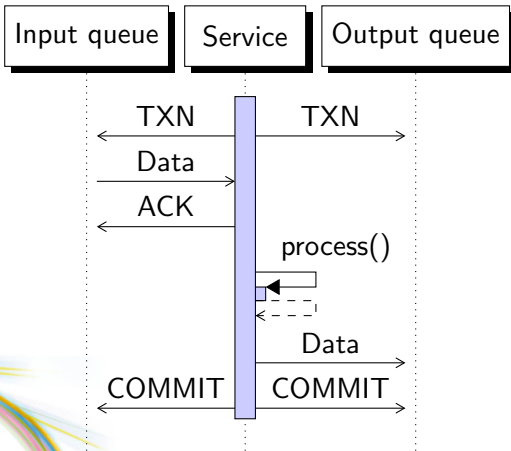


# Terminology

- **Broker:** Central server
- **Queue:** Producer–Consumer
- **Topic:** Publish–Subscribe
- **Transaction:** All or nothing



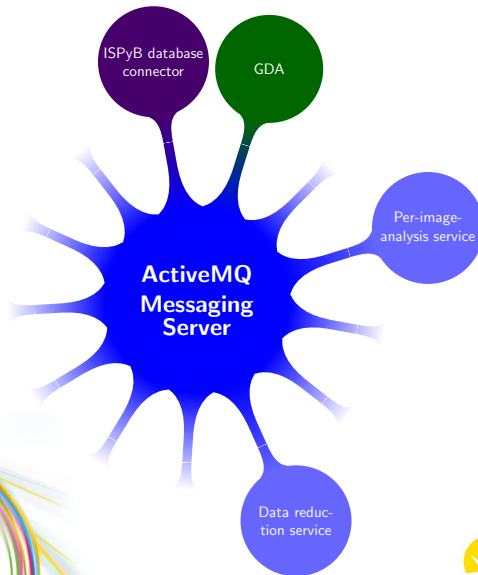
# Delivery guarantee with transactions



# ActiveMQ



# ActiveMQ



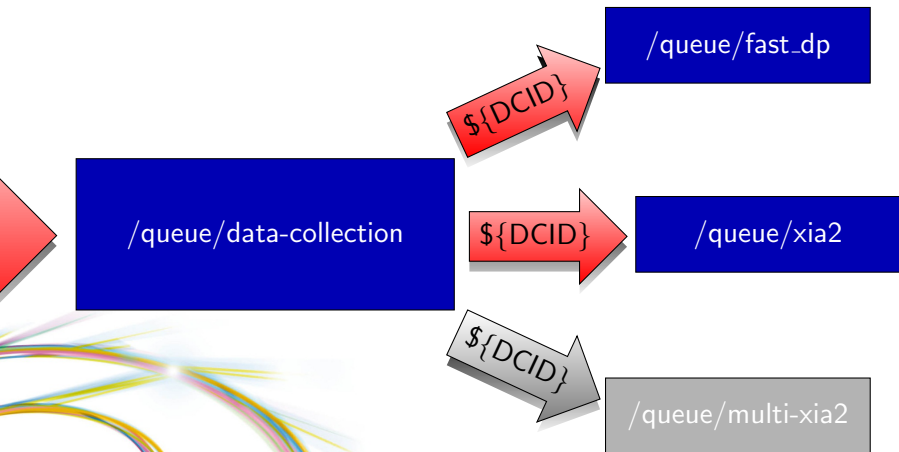
# GDA grid scan announces data collection

The screenshot shows the GDA Grid Scan Settings window. At the top, there are sections for 'Monitoring' (Beamline: idle, Script: [empty], Sample Control: idle) and 'User feedback' (Send feedback button). Below this is a toolbar with 'Tools', 'User Options', and 'Reset Layout'. The main area is titled 'Grid Scan Settings' and contains several sections: 'Scan Control' with a 'Run Scan' button; 'Files' with 'Visit directory' (idfr/i04/data/2016/cmi34452-2), 'Folder' (Configure Defaults), 'Prefix' (Configure Defaults), and 'thermo\_10'; 'Images' with 'Automatic run number' checked, 'Run number' (0), 'Exposure time' (0.1 s), 'Detector distance' (464.092 mm), 'Resolution' (2.333 Å), 'Transmission' (50 %), and 'Pilatus fast mode' checked; 'Grid' with 'Box width' (10 μm), 'Box height' (10 μm), and 'Number of images' (1,189); and 'Aperture and Beamstop' with 'Beamstop' set to 'Standard'. At the bottom, it shows 'No Script running' and 'Queue - waiting'.

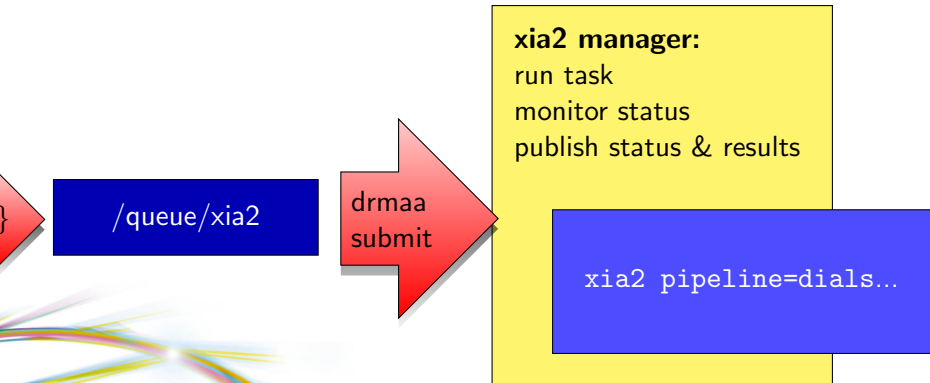


`/queue/data-collection`

# Data collection triggers processing



# Supervised & encapsulated processing



# Reporting results

## **xia2 manager:**

run task  
monitor status  
publish status & results

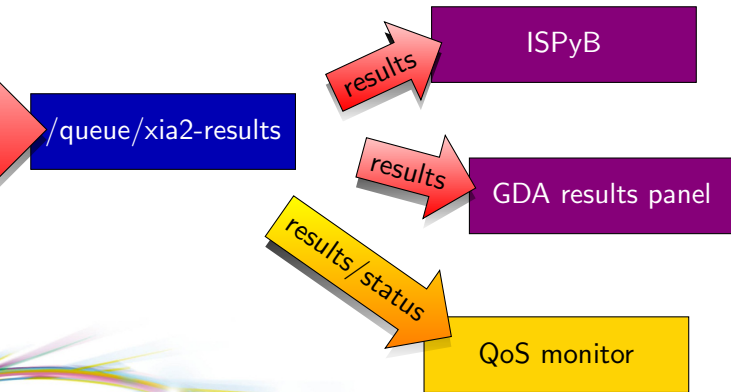
xia2 results

/queue/xia2-results

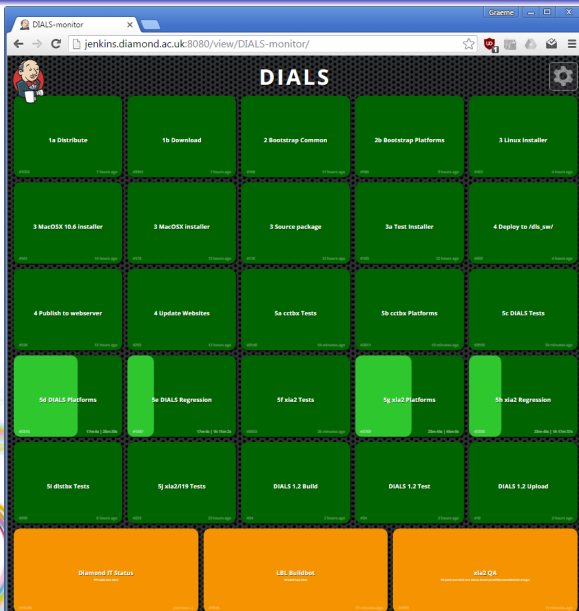
xia2 pipeline=dials...



# Reporting results



# Status monitor

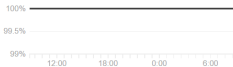


# Status monitor

Past Day   Past Week   Past Month

APP SERVER AVAILABILITY

100.0%



PAGES BUILDS FAILURE RATE

0.1618%



MEAN WEB RESPONSE TIME

158ms



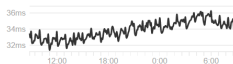
EXCEPTION PERCENTAGE

0.0001%



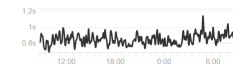
MEAN API RESPONSE TIME

33ms



MEAN HOOK DELIVERY TIME

0.85s



98TH PERC. WEB RESPONSE TIME

700ms

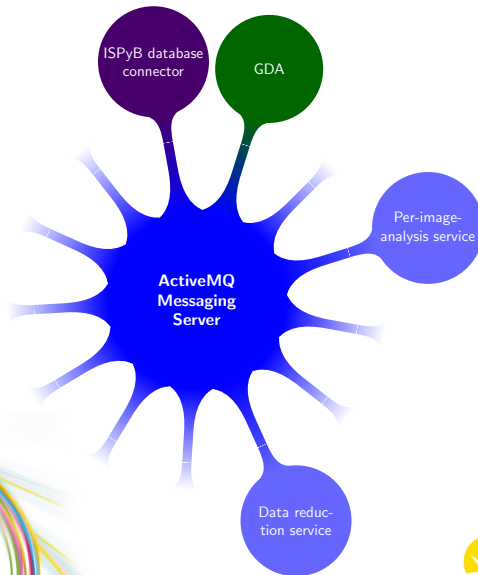


98TH PERC. BROWSER TIME TO FIRST BYTE

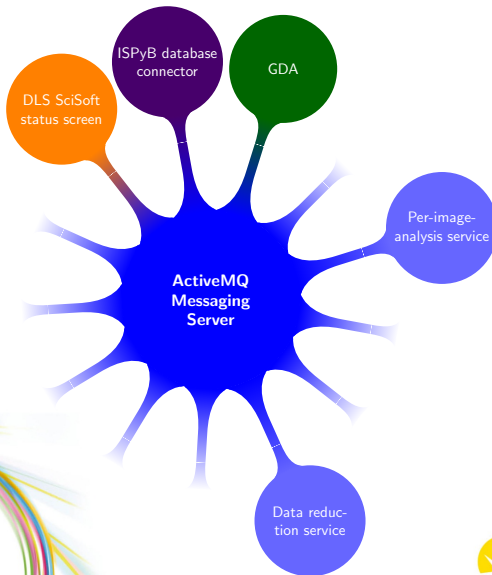
2458ms



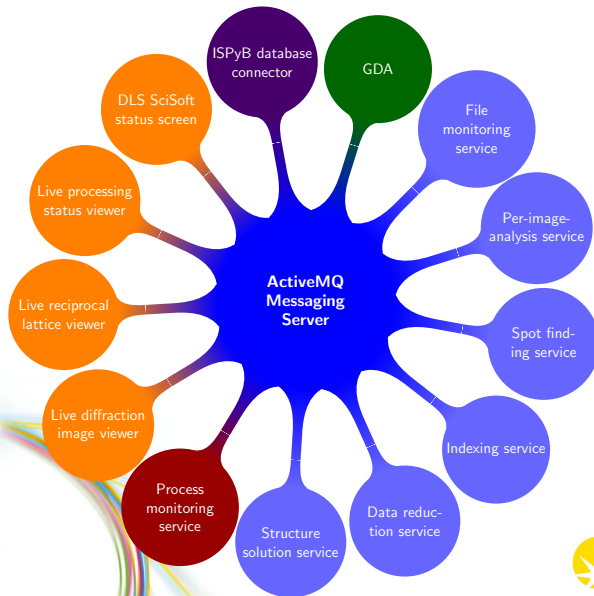
# Infrastructure Overview



# Infrastructure Overview



# Infrastructure Overview



# Timeframe

- Diamond currently in shutdown for ring upgrade
- Short (2 week) run in December 2016
- New infrastructure to be deployed on 2-3 beamlines
- Running in parallel to existing scripts
- Begin replacing existing infrastructure from early 2017

# Thank you

