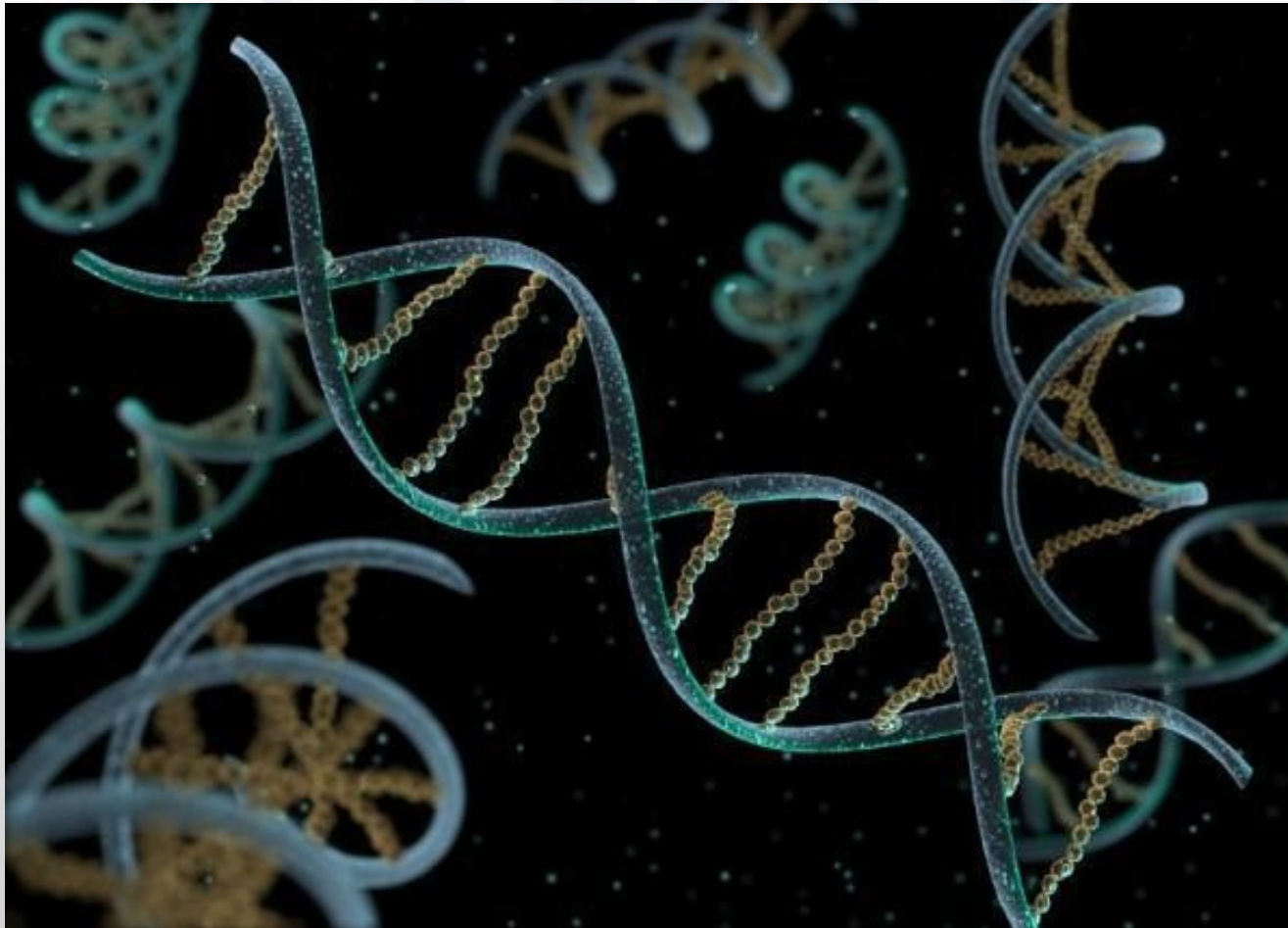




EDNA MX:

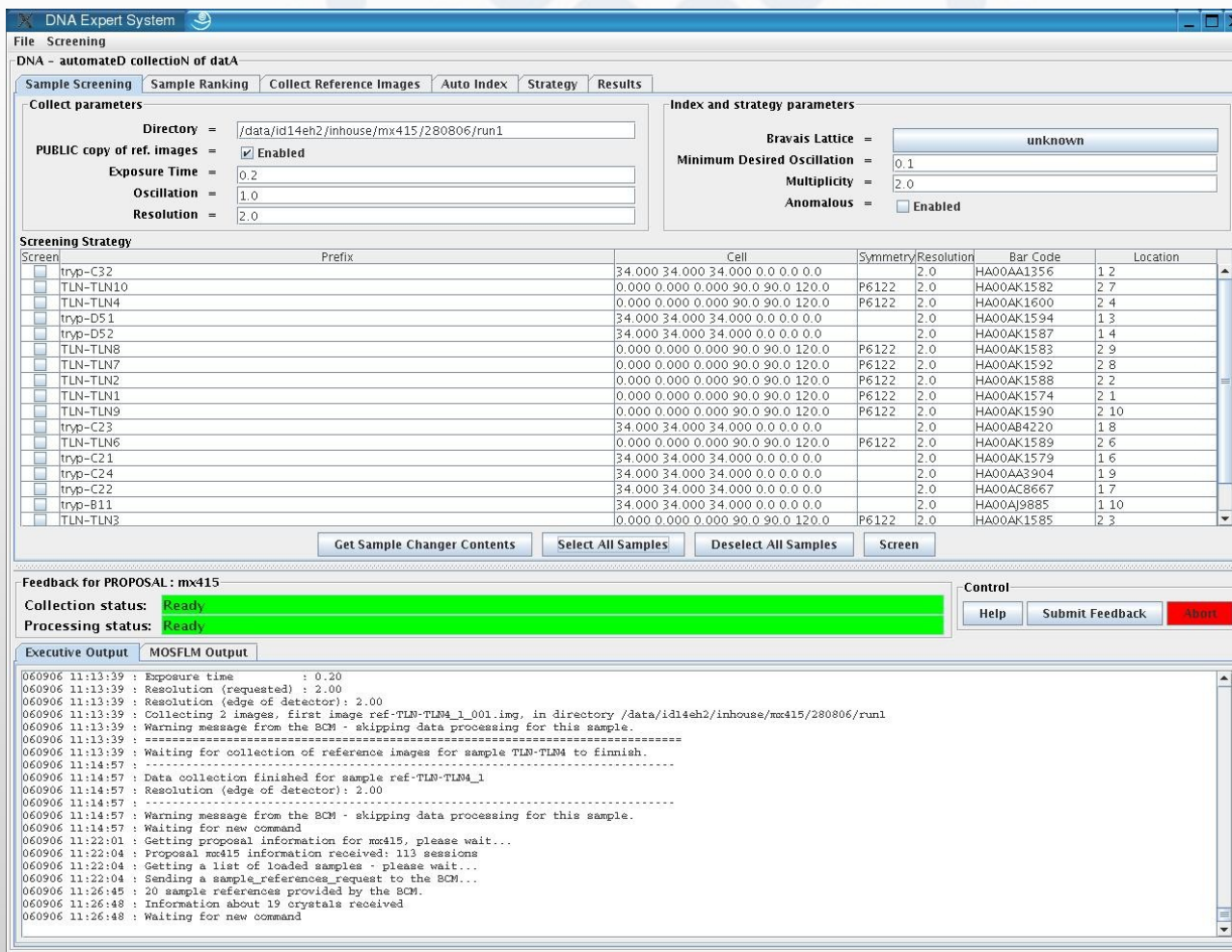
MXv1 → MXv2

In the beginning there was DNA...



... or RNA or something else, if you speak about life...

In the beginning there was DNA...



DNA Expert System

File Screening

DNA - automateD collection of data

Sample Screening | Sample Ranking | Collect Reference Images | Auto Index | Strategy | Results

Collect parameters

Directory = /data/id14eh2/inhouse/mx415/280806/run1

PUBLIC copy of ref. images = Enabled

Exposure Time = 0.2

Oscillation = 1.0

Resolution = 2.0

Index and strategy parameters

Bravais Lattice = unknown

Minimum Desired Oscillation = 0.1

Multiplicity = 2.0

Anomalous = Enabled

Screening Strategy

Screen	Prefix	Cell	Symmetry	Resolution	Bar Code	Location
<input type="checkbox"/>	tryp-C32	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AA1356	12
<input type="checkbox"/>	TLN-TLN10	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1582	27
<input type="checkbox"/>	TLN-TLN4	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1600	24
<input type="checkbox"/>	tryp-D51	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AK1594	13
<input type="checkbox"/>	tryp-D52	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AK1587	14
<input type="checkbox"/>	TLN-TLN8	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1583	29
<input type="checkbox"/>	TLN-TLN7	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1592	28
<input type="checkbox"/>	TLN-TLN2	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1588	22
<input type="checkbox"/>	TLN-TLN1	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1574	21
<input type="checkbox"/>	TLN-TLN9	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1590	210
<input type="checkbox"/>	tryp-C23	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AB4220	18
<input type="checkbox"/>	TLN-TLN6	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1589	26
<input type="checkbox"/>	tryp-C21	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AK1579	16
<input type="checkbox"/>	tryp-C24	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AA3904	19
<input type="checkbox"/>	tryp-C22	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AC8667	17
<input type="checkbox"/>	tryp-B11	34.000 34.000 34.000 0.0 0.0 0.0		2.0	HA00AJ9885	110
<input type="checkbox"/>	TLN-TLN3	0.000 0.000 0.000 90.0 90.0 120.0	P6122	2.0	HA00AK1585	23

Get Sample Changer Contents | Select All Samples | Deselect All Samples | Screen

Feedback for PROPOSAL : mx415

Collection status: **Ready**

Processing status: **Ready**

Control: Help | Submit Feedback | Abort

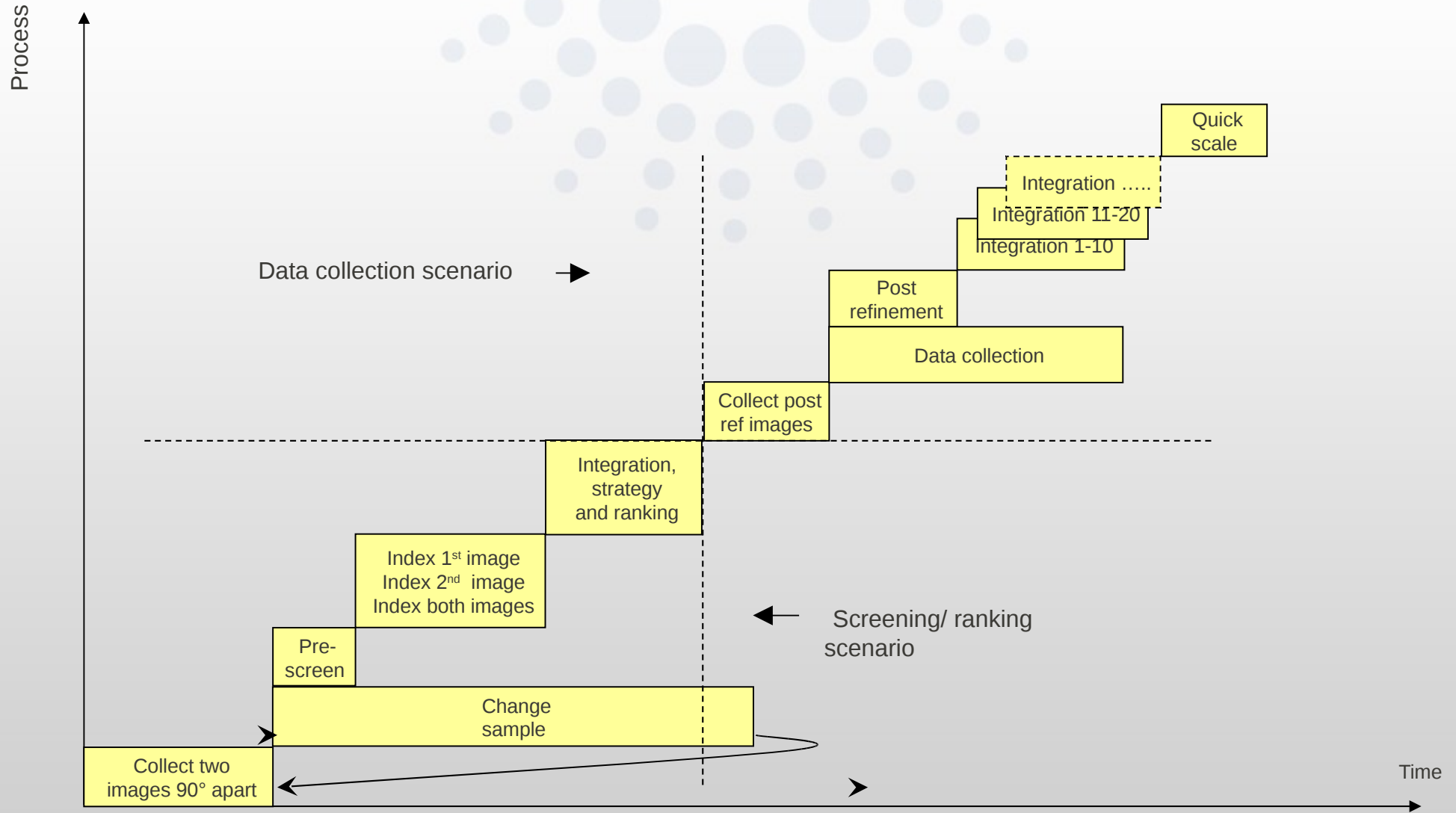
Executive Output

```

060906 11:13:39 : Exposure time : 0.20
060906 11:13:39 : Resolution (requested) : 2.00
060906 11:13:39 : Resolution (edge of detector): 2.00
060906 11:13:39 : Collecting 2 images. first image ref-TLN-TLN4_1_001.img. in directory /data/id14eh2/inhouse/mx415/280806/run1
060906 11:13:39 : Warning message from the BCM - skipping data processing for this sample.
060906 11:13:39 : =====
060906 11:13:39 : Waiting for collection of reference images for sample TLN-TLN4 to finish.
060906 11:14:57 : =====
060906 11:14:57 : Data collection finished for sample ref-TLN-TLN4_1
060906 11:14:57 : Resolution (edge of detector): 2.00
060906 11:14:57 : =====
060906 11:14:57 : Warning message from the BCM - skipping data processing for this sample.
060906 11:14:57 : Waiting for new command
060906 11:22:01 : Getting proposal information for mx415, please wait...
060906 11:22:04 : Proposal mx415 information received: 113 sessions
060906 11:22:04 : Getting a list of loaded samples - please wait...
060906 11:22:04 : Sending a sample_references_request to the BCM...
060906 11:26:45 : 20 sample references provided by the BCM.
060906 11:26:48 : Information about 19 crystals received
060906 11:26:48 : Waiting for new command
  
```

... if you speak about EDNA!

DNA screening / data collection scenarios



What is MXv1? And MXv2???

- DNA → EDNA (2005 - 2007)
- The EDNA project started with the spike. There were immediately conflicts in the development team concerning the data model.
- In 2008 it was decided to develop a MX prototype with a simplified data model
- After the release of the prototype (July 2008) we agreed to split up the development:
 - The prototype execute plugins (MOSFLM, BEST, RADDPOSE etc) become the “**mxPluginExec**” project
 - The prototype “generic” data model and its control plugins (Indexing etc) became the “**mxv1**” project
 - The more advanced data model developments became the “**mxv2**” project

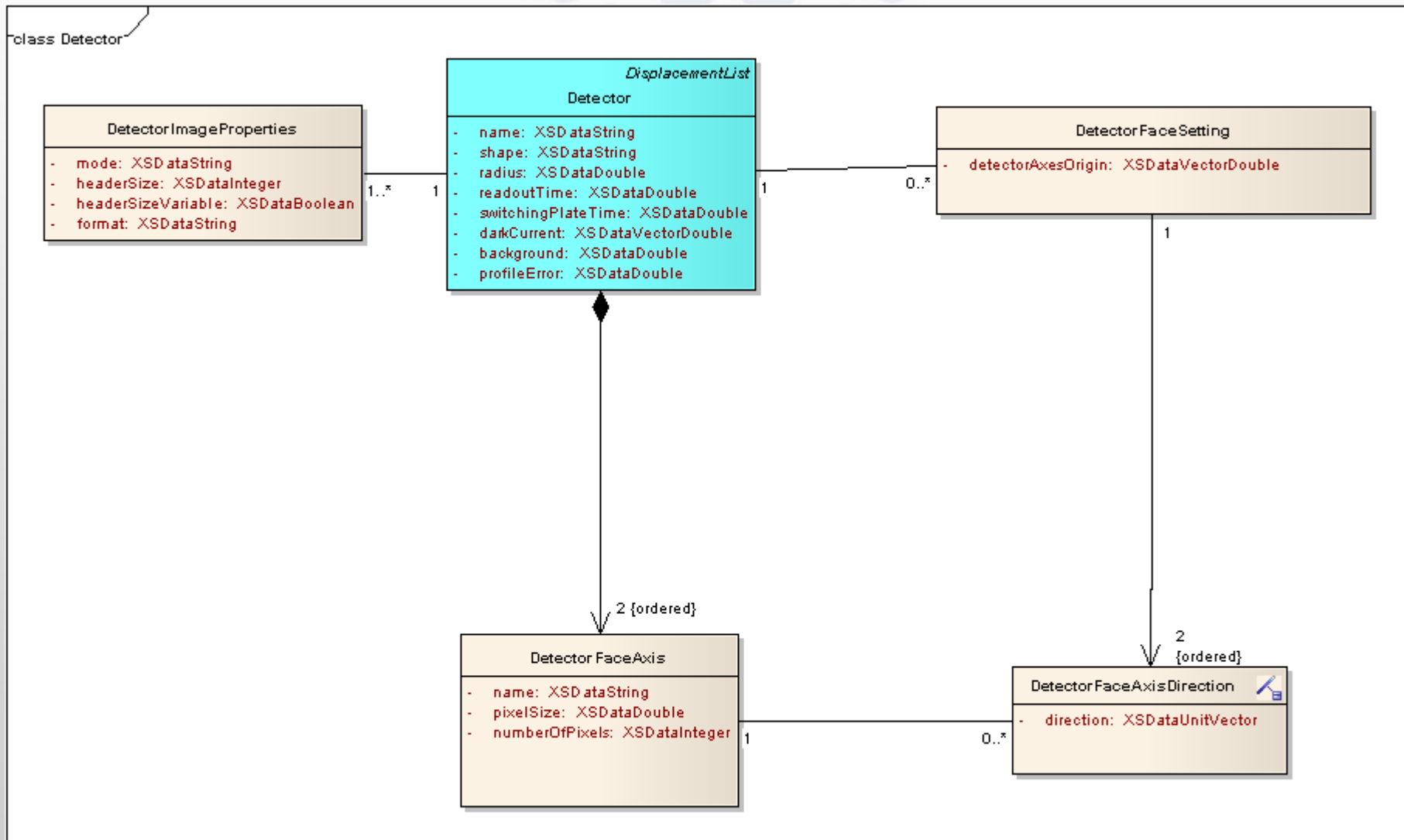
What is the difference between MXv1 and MXv2?

- The differences between MXv1 and MXv2 are in the data model
- MXv2 data model has:
 - More advanced detector geometry
 - More advanced goniostat geometry
 - Many more things that I'm not aware of...
- The MXv2 is though not yet fully developed:
 - Many MXv1 parameters missing like transmission etc.

Example : MXv1 data model, detector

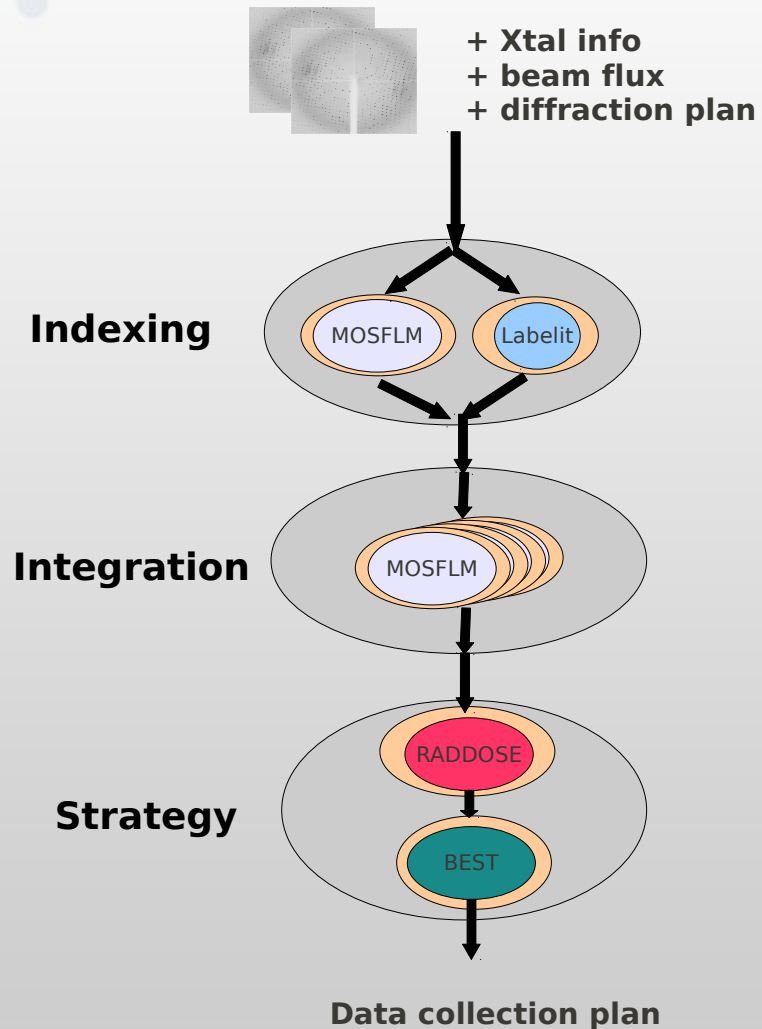
<i>XSData</i>	
XSDataDetector	
+	beamPositionX: XSDataLength
+	beamPositionY: XSDataLength
+	bin: XSDataString
+	byteOrder: XSDataString
+	dataType: XSDataString
+	distance: XSDataLength
+	gain: XSDataFloat
+	imageSaturation: XSDataInteger
+	name: XSDataString
+	numberBytesInHeader: XSDataInteger
+	numberPixelX: XSDataInteger
+	numberPixelY: XSDataInteger
+	pixelSizeX: XSDataFloat
+	pixelSizeY: XSDataFloat
+	serialNumber: XSDataString
+	twoTheta: XSDataAngle
+	type: XSDataString

Example MXv2 data model, detector:

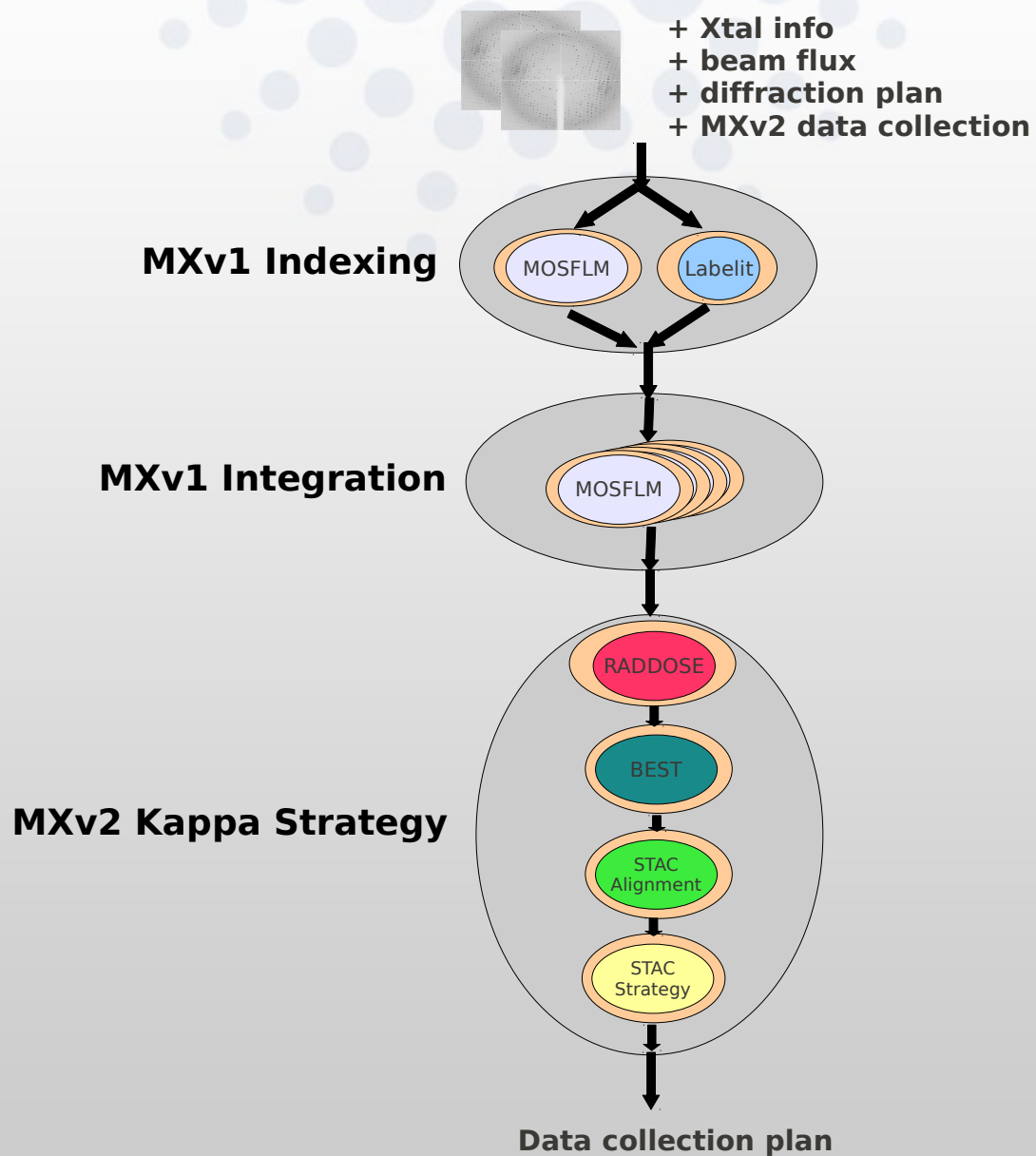


MXv1 Characterisation v1.1

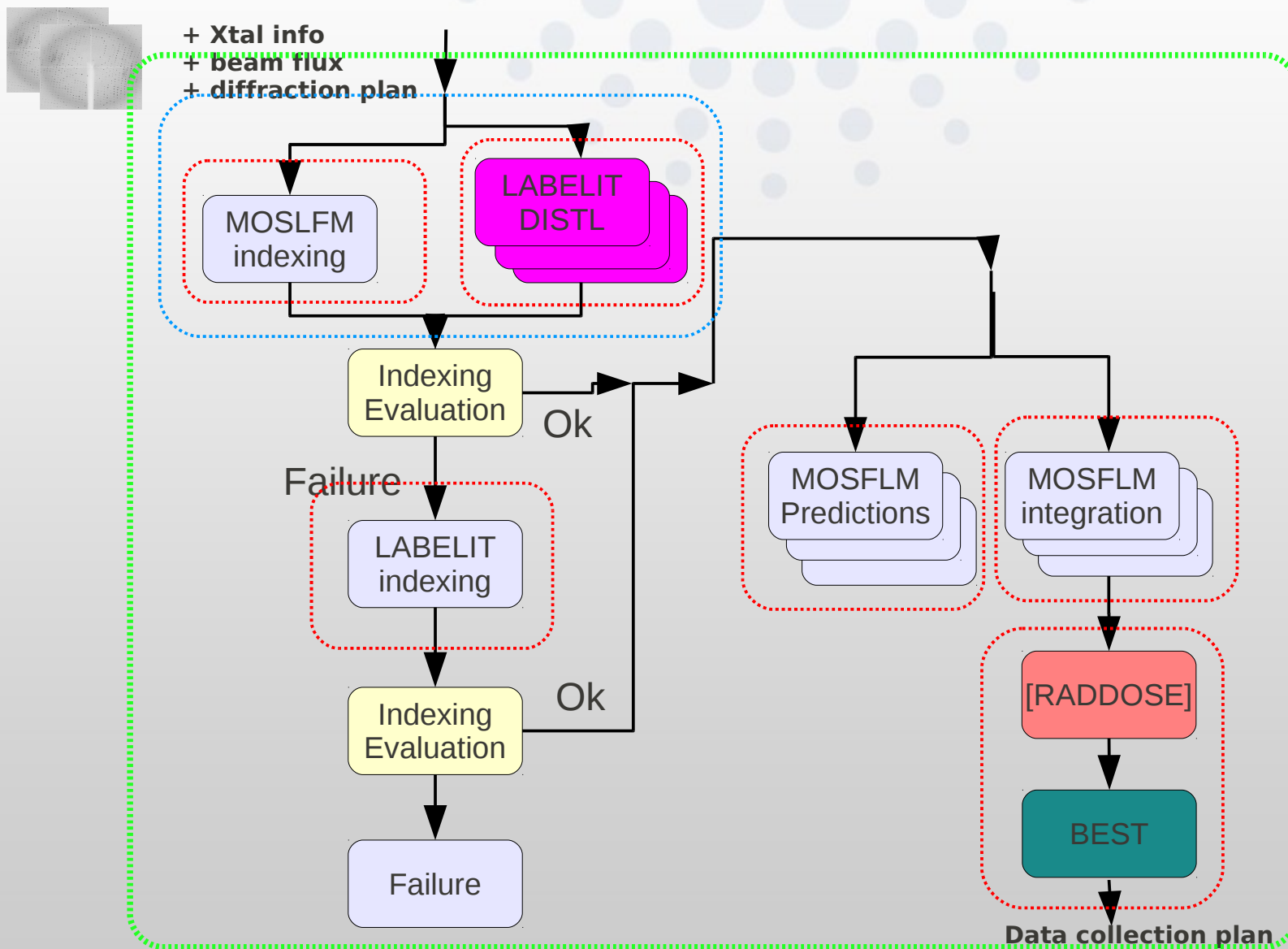
- MX sample characterisation taking into account radiation damage
- Indexing using MOSFLM or Labelit
- Parallel integration of reference images
- If flux + beamsize:
 - RADDOSE for estimating radiation damage
- BEST strategy calculation
 - taking into account radiation damage
 - multi-subwedge data collection strategies



MXv2 Characterisation v2.0



MXv1 Characterisation v1.2



Example of edna-mxv2-characterisation output

```

> Strategy : Best : Crystal
> Strategy : Best : Space Group : P 2 2 2
> Strategy : Best : Cell : 54.81 59.08 66.96 90.00 90.00 90.00
> Strategy : Best : Mosaicity : 0.69 degree
> Strategy : Best :
> Strategy :
> Strategy : -----
> Strategy : STAC - Alignment : <!--SUMMARY_BEGIN-->
> Strategy : STAC - Alignment : Version 2 by Sandor Brockhauser
> Strategy : STAC - Alignment :
> Strategy : STAC - Alignment : Calculation performed by STAC (using gonset from Phil Evans)
> Strategy : STAC - Alignment : -----
> Strategy : STAC - Alignment : --v1-----v2-----O-----K-----P-----
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (1.0;0.0;0.0) : 115.705 128.411 259.323
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (1.0;0.0;0.0) : 58.489 234.548 201.831
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (1.0;0.0;0.0) : 295.705 128.411 259.323
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (1.0;0.0;0.0) : 238.489 234.548 201.831
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (0.0;1.0;0.0) : 25.703 128.411 259.323
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (0.0;1.0;0.0) : 328.488 234.548 201.831
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (0.0;1.0;0.0) : 205.703 128.411 259.323
> Strategy : STAC - Alignment : (0.0;0.0;1.0) (0.0;1.0;0.0) : 148.488 234.548 201.831
> Strategy : STAC - Alignment : -----
> Strategy : STAC - Alignment : <!--SUMMARY_END-->
> Strategy :
> Strategy : -----
> Strategy : STAC - Strategy : <!--SUMMARY_BEGIN-->
> Strategy : STAC - Strategy : Version 2 by Sandor Brockhauser
> Strategy : STAC - Strategy :
> Strategy : STAC - Strategy : Calculation performed by STAC (using strategy from Raimond Ravelli)
> Strategy : STAC - Strategy : -----
> Strategy : STAC - Strategy : --ID-----OStart-----OEnd-----K-----P----#Img-----Compl%-----
> Strategy : STAC - Strategy : 1 : 26.75 <-> 114.728 128.411 259.323 88 97.245
> Strategy : STAC - Strategy : 1 : 132.996 <-> 198.621 90.0 40.0 66 99.883
> Strategy : STAC - Strategy : 2 : 59.431 <-> 147.437 234.548 201.831 89 97.245

```

Future?

- Current situation :
 - edna-mxv2-characterisation is using the MXv1 data model for indexing and integration but the MXv2 data model for the strategy
- Future directions :
 - We continue to develop MXv1 and slowly migrate functionality to MXv2
 - We stop developing MXv1 and all new developments are done in MXv2