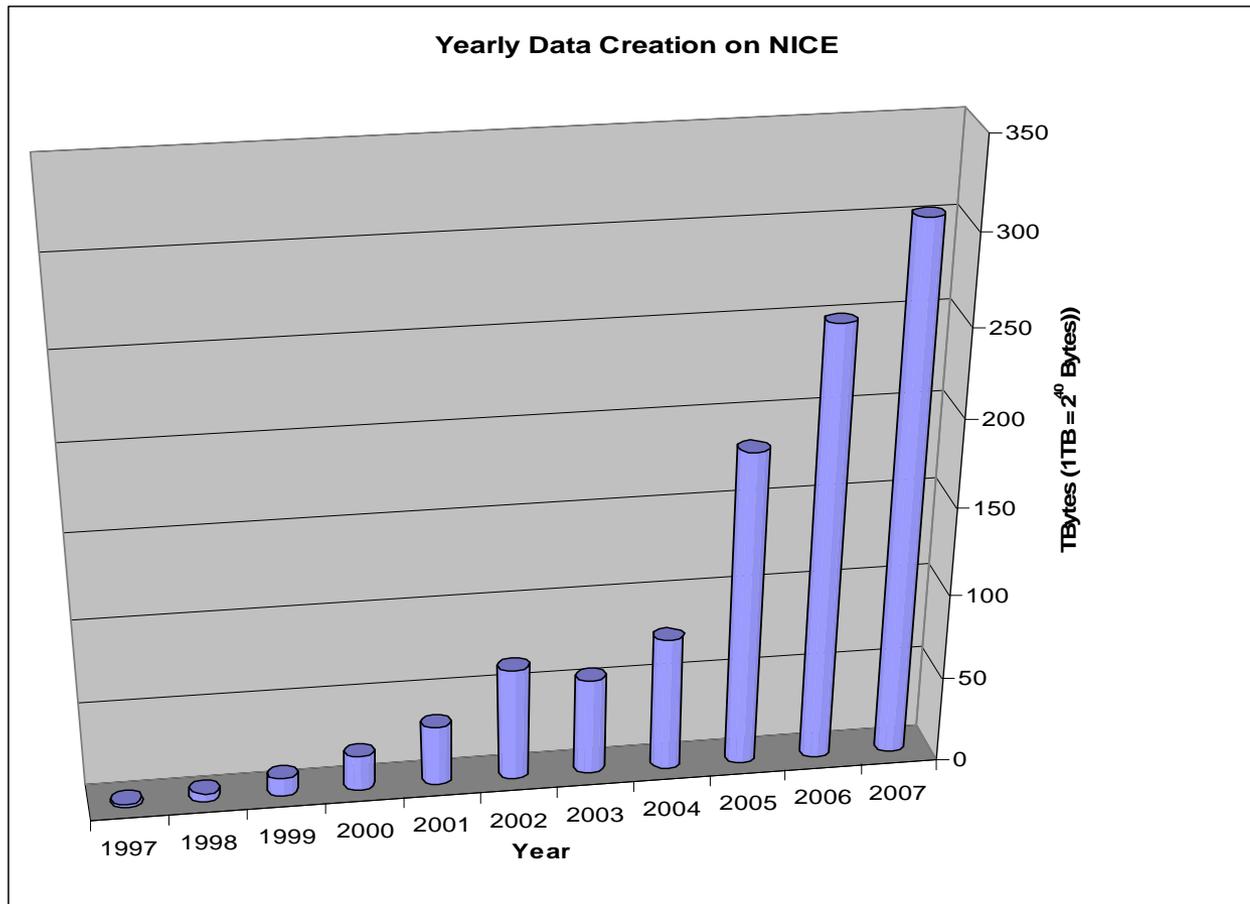


# **MX Data (& Sample) Handling (& Tracking) at the ESRF**

**Gordon Leonard**  
**ESRF Macromolecular Crystallography Group**

## Data Storage – 10 years evolution

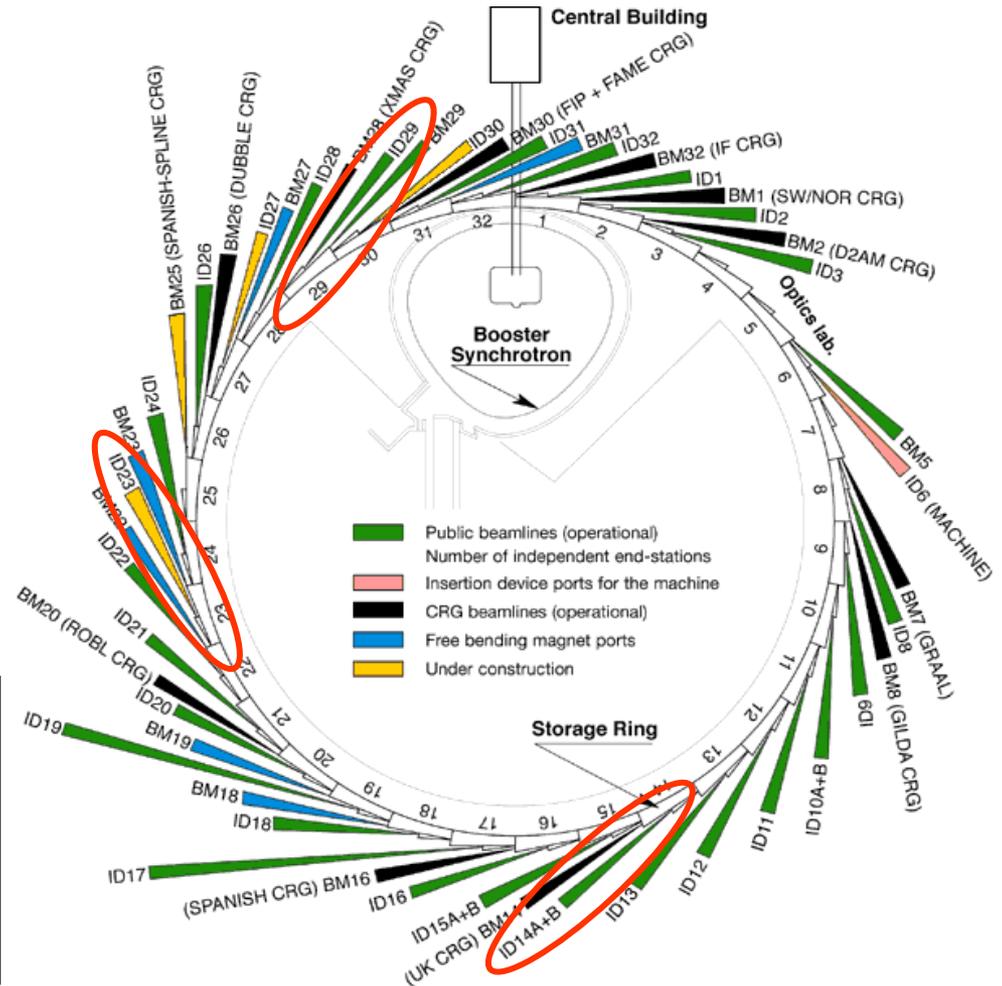


Data Production in 2007:  
 300 TB  
 (MX BLs ~45TB)

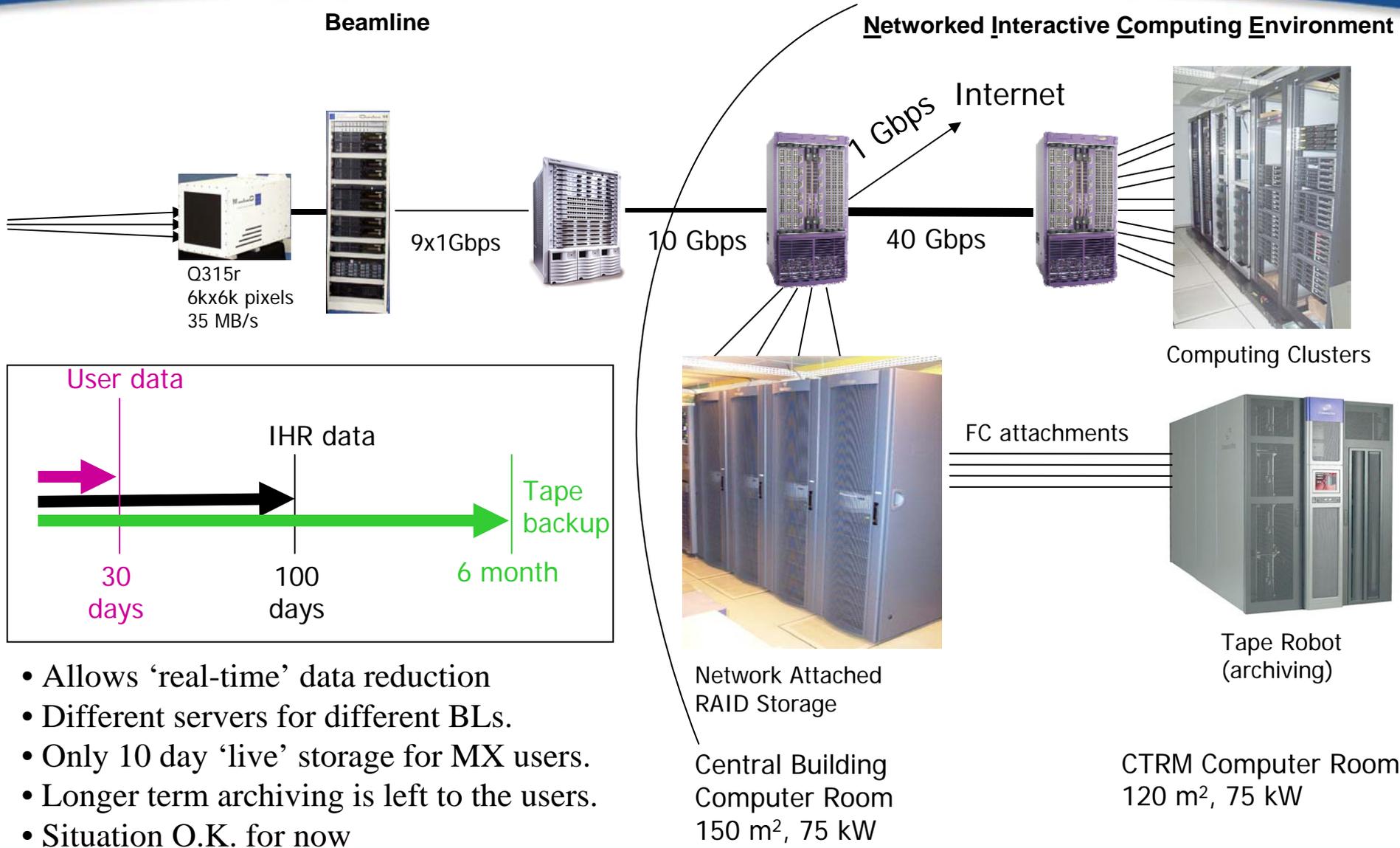
The data rate has increased 260-fold over the last ten years!

Stored on central servers – not on individual beam-lines

		# images '07
3 fixed $\lambda$ BL :	ID14-1	419,000
	ID14-2	335,000
	ID14-3*	223,000
3 MAD BL :	ID14-4*	290,000
	ID23-1	907,000
	ID29	720,000
1 $\mu$ focus BL :	ID23-2	382,000
<u>TOTAL</u>		<u>3,276,000</u>



High throughput. During data collection images produced every few seconds. Need ability to process/analyse/track these as they are produced

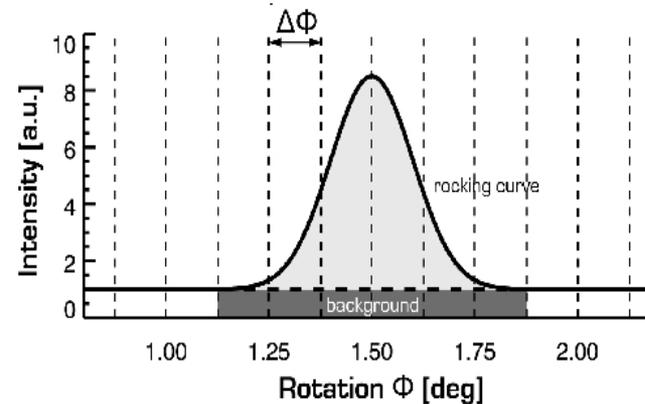


## PILATUS 6M detector



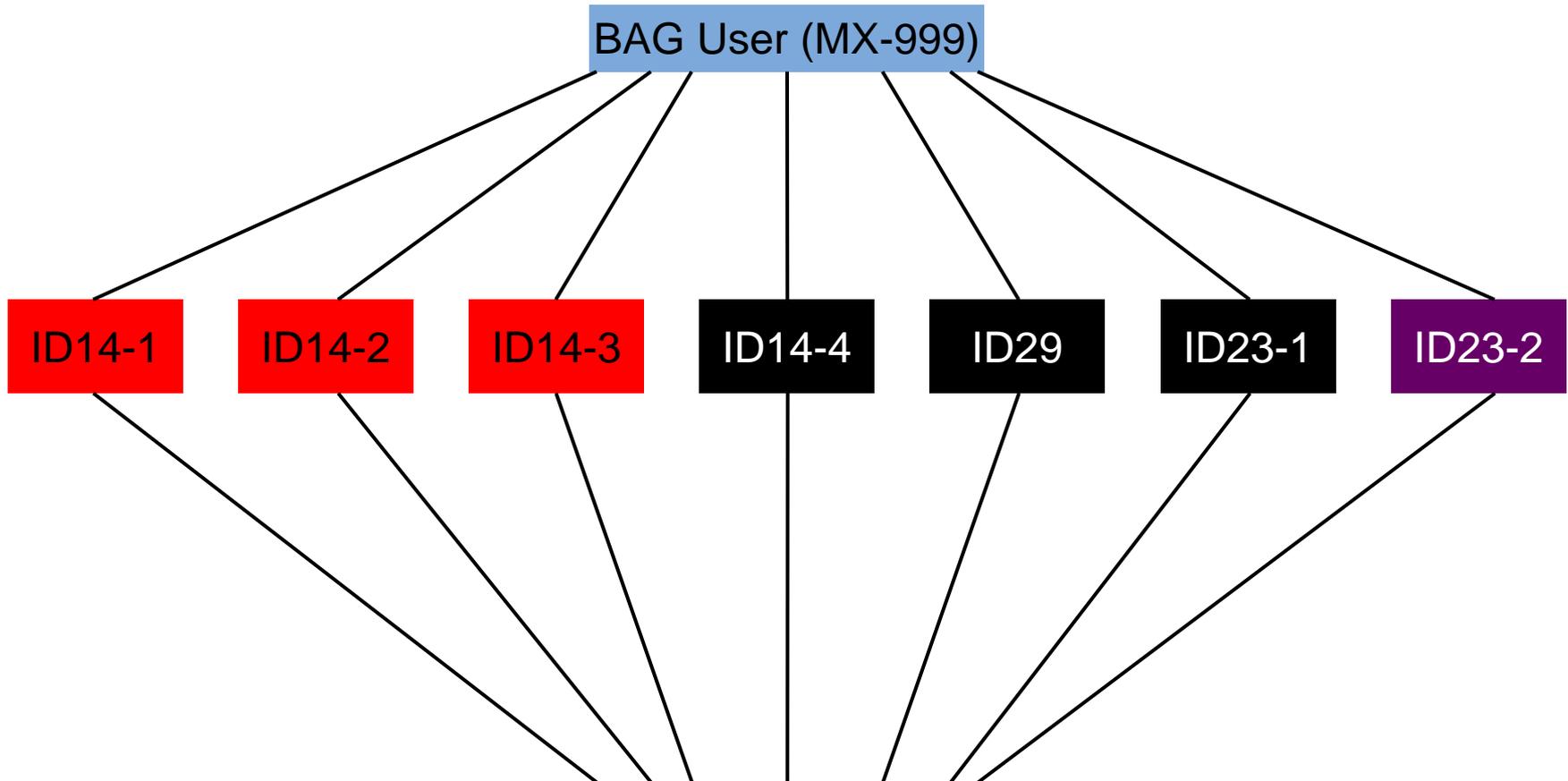
- Digital gating will allow shutter-less data collection.
- Fine phi-slicing will become routine.
- Image production rates will soar
- Will no longer be able to send images to central storage during data collection (?)

<b>Pixel size</b>	<b>172 x 172 <math>\mu\text{m}^2</math></b>
<b>Readout time</b>	<b>&lt;3.6 ms</b>
<b>Framing rate</b>	<b>10 Hz</b>

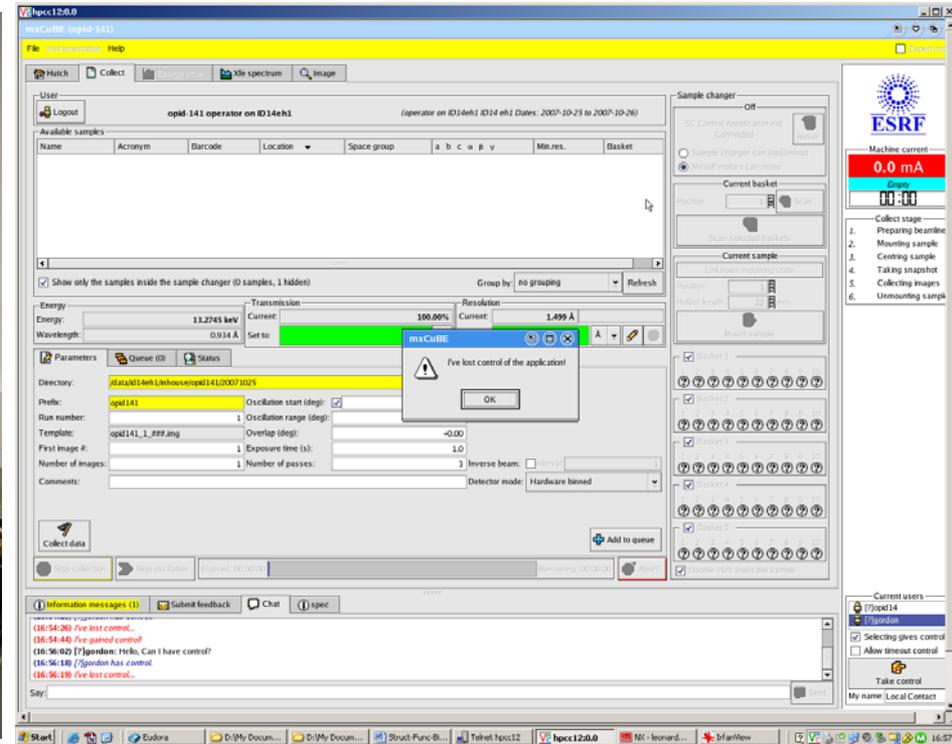
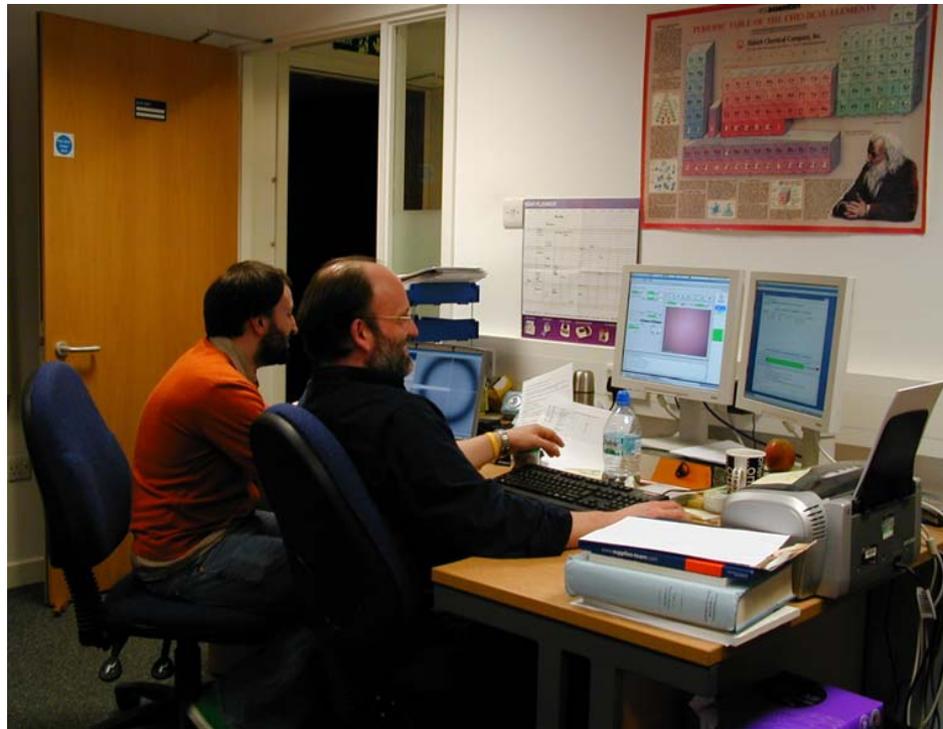


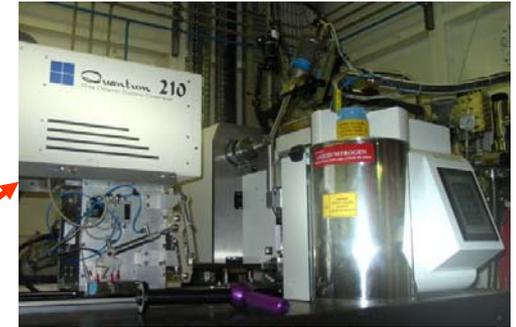
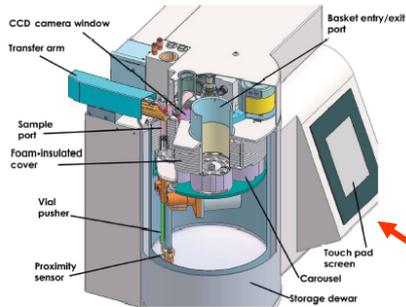
<http://pilatus.web.psi.ch/pilatus.htm>

MX BAGs collect ~25,000 data sets/year – also ~90,000 screening sets



Where's my data? Where did I collect it? When did I collect it?





SC

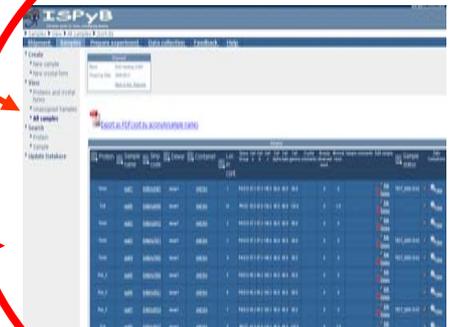
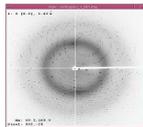
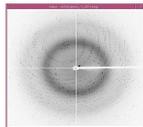
EH

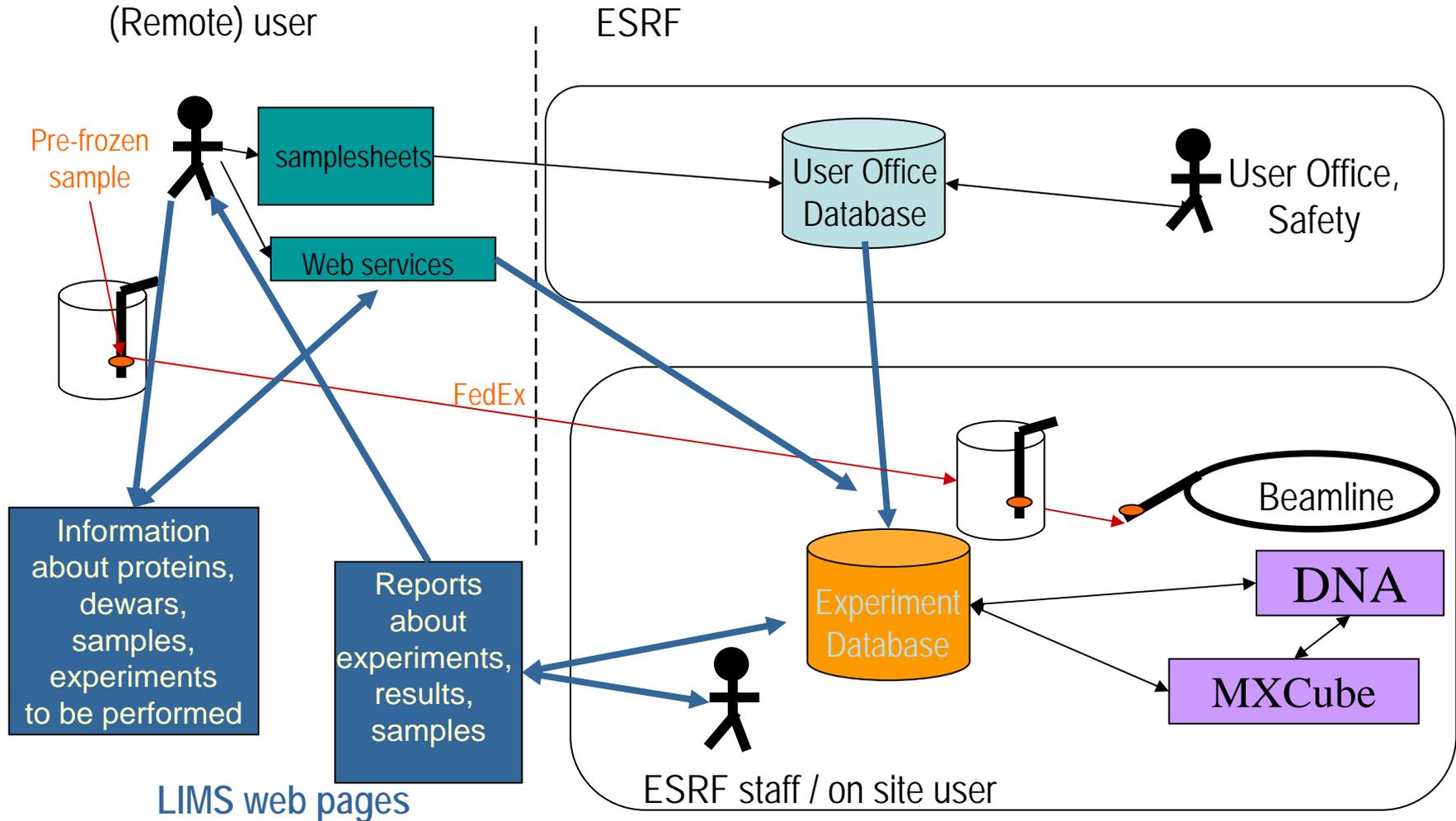


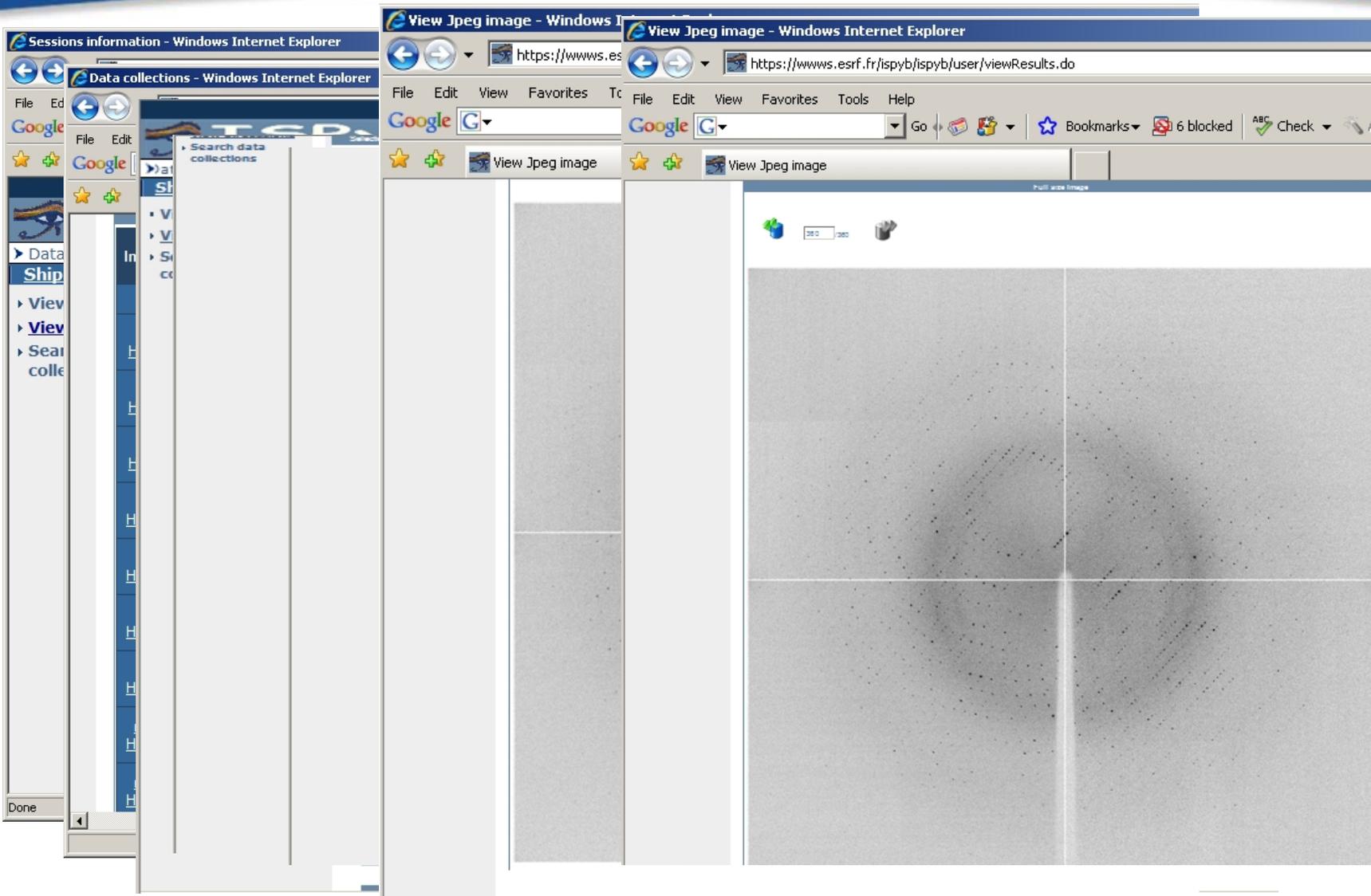
DNA

Database

MxCuBE GUI (all MX beam-lines)



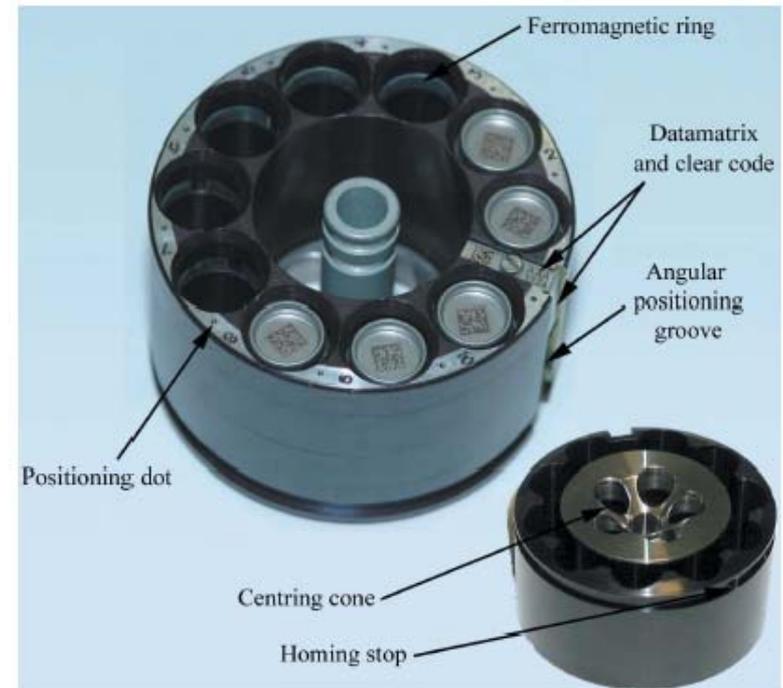




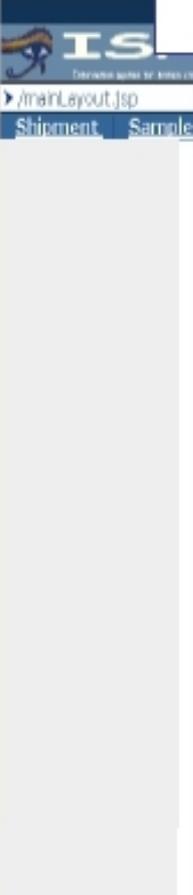
## European SPINE standard

Full specifications at <http://www.spineurope.org>, protocols menu

- 10 Character identification code:
  - DataMatrix on the base of Caps
  - Clear code near the DatatMatrix
- DataMatrices read by SC3 sample changer
- Datamatrices for SC3 pucks as well



Also need to consider tracking dewars inside & outside ESR. 850 dewars / year (2007). Need to make sure they're delivered to the right beamline. Will be done via ISPyB



IS  
/mainLayout.jsp  
Shipment Sample

## List of all parameters known for a shipment/dewars

- \* Shipment name
- \* Shipment status (saved, send to ESRF, at ESRF, send to User)
- \* Proposal number
- \* Creation date
- \* Sending date
- \* Expected ESRF arrival date
- \* Lab-contact card to ESRF
  - Contact person name
  - Contact person telephone
  - Contact person fax
  - Contact person email
  - Lab name
  - Lab address
- \* Lab-contact card to Home Lab
  - Contact person name
  - Contact person telephone
  - Contact person fax
  - Contact person email
  - Lab name
  - Lab address
- \* Courier company for return (if ESRF sends a dewar back)
- \* # dewars in the shipment
- \* For each dewar of the shipment:
  - Dewar name
  - Dewar number in the shipment (#total number)
  - Barcode
  - Average Customs value
  - Average Transport value
  - Location to be delivered at ESRF
  - Courier/ tracking number TO ESRF
  - Courier/ tracking number FROM ESRF
  - Experiment date
  - ESRF Local contact
  - ESRF arrival date
  - ESRF location (Stores, Beamline X)
  - Containers
  - Samples
- \* History of the shipment transport : will summary all transport steps = PDF

415

Sample tracking model
18/19



The ESRF introduced the MXpress service in 2002 offering companies the option of a 'mail-in' data collection service. MXpress offers clients an efficient & cost effective alternative to sending their staff to the synchrotron for data collection sessions that often lasts only a few hours. Currently, MXpress has a client base of around 20 companies with over 1000 samples being processed each year.



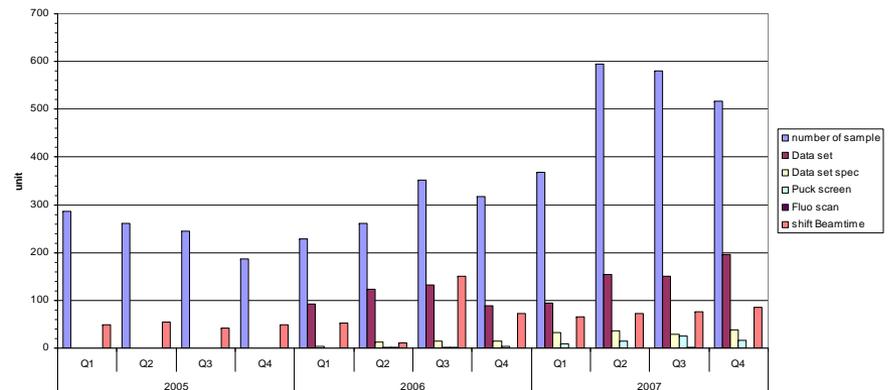
The provision of an efficient mxpress service has been one of the main driving forces for the automation of the MX beamlines at the ESRF.

MXpress has helped with the testing and development of sample changing robots, the automatic data collection system DNA & the ISPyB LIMS which is critical for sample tracking and subsequent reporting of results. All of these are now in routine use at the ESRF.

## MxPress activity in 2007 – by quarter with totals

# samples screened	368	595	580	516	~2,500
data set	94	154	151	196	595
data set special	32	36	29	38	135

Evolution of MXpress Service



- **MX data handling & storage at ESRF sufficient for current needs**
- **Needs will change if (when?) pixel detectors are installed on the BLs**
  - Initial storage at beam-lines?
  - Faster computers for on-site processing & analysis?
- **~25,000 datasets and ~90,000 screening sets per year**
  - Data & sample tracking becomes vital
  - ISPyB database/electronic logbook indispensable for this
- **Barcodes are a good way of ensuring proper tracking**
  - Individual samples
  - Pucks containing many samples
  - Dewars containing several pucks