
High Data-Rate Macromolecular Crystallography
NSLS-II Brookhaven National Laboratory
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# Statement of the Problem and Charge to the Meeting

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# Statement of the Problem

- Macromolecular crystallography (MX) is the gold standard for the determination of the atomic-resolution three-dimensional structure of large biologically active molecules.
- MX is becoming a big data science straining the capabilities of computers and networks.
- New techniques of serial crystallography are allowing new science to be done but they are increasing the heterogeneity of the data that must be handled.

# Statement of the Problem (cont.)

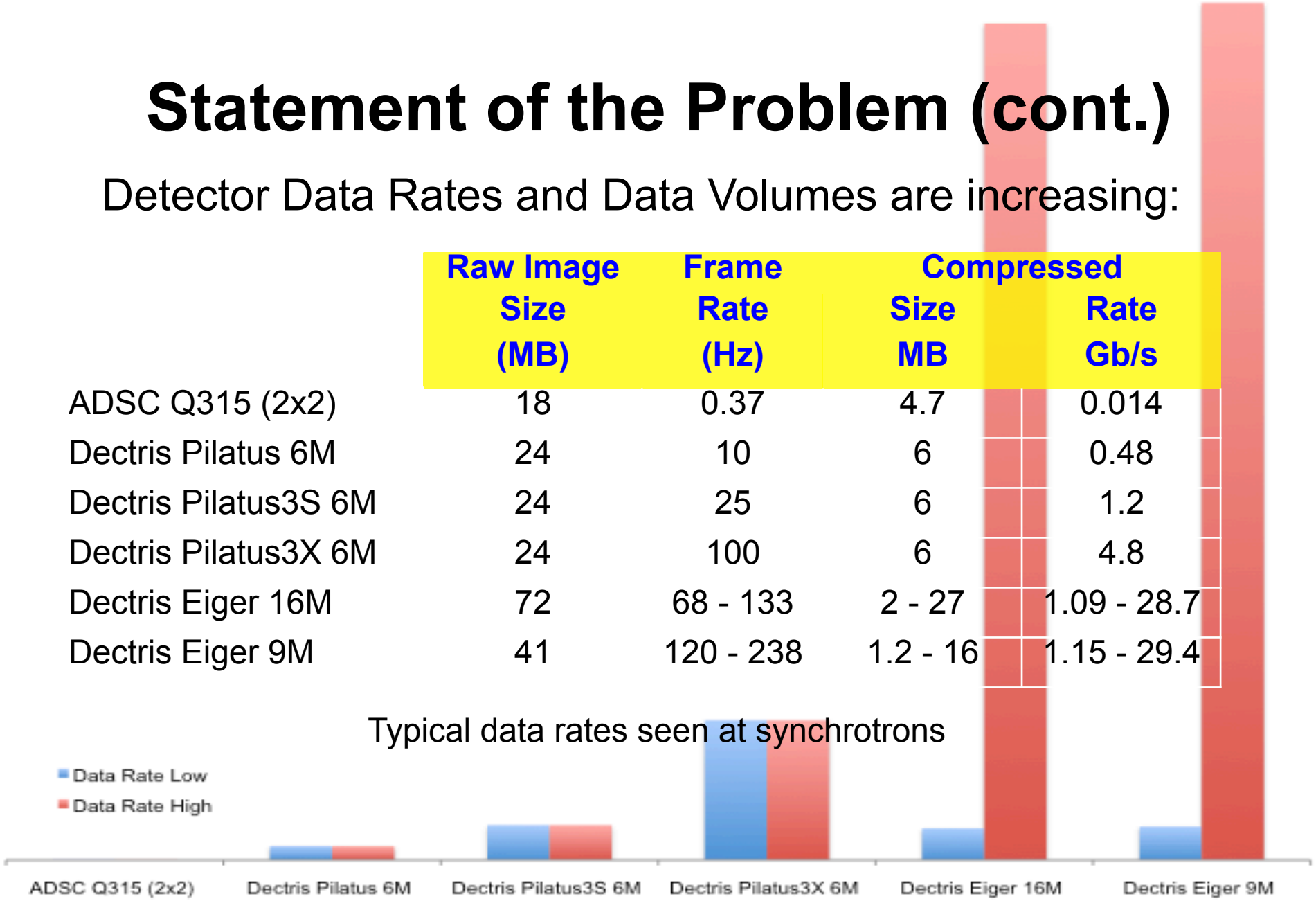
- Issues in Archiving
  - We are dealing with much more data than in the past.
  - In the short term we need to store a lot of data that is retrievable quickly.
  - In the medium term we need to store some version of much of the same data for processing and for users to take home.
  - In the longer term we may need to store the publishable data.
  - We need to consider issues of compression and background removal.

# Statement of the Problem (cont.)

Detector Data Rates and Data Volumes are increasing:

| | Raw Image Size (MB) | Frame Rate (Hz) | Compressed Size MB | Compressed Rate Gb/s |
|---|---|---|---|---|
| ADSC Q315 (2x2) | 18 | 0.37 | 4.7 | 0.014 |
| Dectris Pilatus 6M | 24 | 10 | 6 | 0.48 |
| Dectris Pilatus3S 6M | 24 | 25 | 6 | 1.2 |
| Dectris Pilatus3X 6M | 24 | 100 | 6 | 4.8 |
| Dectris Eiger 16M | 72 | 68 - 133 | 2 - 27 | 1.09 - 28.7 |
| Dectris Eiger 9M | 41 | 120 - 238 | 1.2 - 16 | 1.15 - 29.4 |

Typical data rates seen at synchrotrons



# Statement of the Problem (cont.)

- Eiger 16M detectors produce
  - 2.4 gigapixels per second
  - 76 raw gigabits per second
  - often more than 10 Gb/s networks can handle
  - even when compressed 4:1
- Increasingly daunting flood of image data
- We should try to
  - Reduce movement of data
  - Reduce transformations of data
  - Move data in large blocks

# Statement of the Problem (cont.)

- Compressions could be improved, but that will not be sufficient

| | bzip2 | bslz4 | nibble-offset | Byte-offset | packed | Lz4**2 |
|---|---|---|---|---|---|---|
| Avg Ratio | 5 | 4 | 4 | 3 | 3 | 2 |
| Max Ratio | 37059 | 114 | 16 | 4 | 647 | 333 |
| Min Ratio | 3 | 3 | 3 | 1 | 2 | 2 |
| Avg fps | 11 | 56 | 33 | 53 | 26 | 20 |

Compression ratios in the presence of varying amounts of water

- No single compression is ideal
- No single compression is sufficient

# Why Be Concerned

- **For any stochastic system**, the delays and lengths of queues rise sharply as the rate of arrival of information to process approaches the rate at which it can be processed.
- **For any information processing system**, the rate at which you can move information through the system is limited by the capacity of the narrowest bottle neck.
- **When you work close to the capacity of a system you are dancing on the edge of a cliff.**

# Charge to the Meeting

We hope for answers to the following questions

- What stumbling blocks inhibit direct processing of HDF5 data?
- Is there a way to have the data produced by the detector processed by all the major packages without conversion?
- What are best practices to process Eiger images?
  - Using C, Fortran, Python?
  - In large compute clusters at synchrotrons?
  - In users' home lab computers?