

HDRMX

High Data-Rate Macromolecular Crystallography
MAX IV Meeting, 15 – 17 March 2017
<https://indico.maxiv.lu.se/event/233/>

Introduction

Review of the Basel Meeting

Topics for This Meeting

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Work supported in part by Dectris, Ltd.
Meeting supported in part by Dectris and by Max IV



Introduction

This is the fourth in a series of meetings that began in spring 2016 on changes needed to existing major software packages for support of very high data rate macromolecular crystallography.

- The first HDRMX meeting was held at Brookhaven National Laboratory, 26 – 28 May 2016
- The second meeting held at an informal dinner gathering during the meeting of the American Crystallographic Association in Denver Colorado, 22 – 26 July 2016.
- The third meeting was held at Biozentrum in Basel on 2 September 2016.

See <http://www.hdrmx.medsbio.org/>



Issues and Conclusions from Basel

Issues

- Compression Issues, both faithful and lossy
- Data Volume Reduction in the Detector Control Unit (DCU)
- Direct reading of HDF5
- Touch-once approaches
- 40 Gigabit per second network support

Conclusions

- Dectris is only responsible for providing the currently specified HDF5 FileWriter output and the streaming interface; and
- The beamlines are responsible for processing the streaming interface to other formats;
- But what should be archived or distributed should be NXmx compliant

Topics for Lund

The agenda for this fourth meeting will focus on tools and approaches to efficient processing of streamed images, including handling of regions of interest, compression, binning and summing.

Organizers:

Herbert J. Bernstein, Rochester Institute of Technology (co-chair)

Jie Nan, The MAX IV Laboratory (co-chair, local organizer)

Uwe Mueller, The MAX IV Laboratory (local organizer)

Jean Jakoncic, Brookhaven National Laboratory

Nicholas K. Sauter, Lawrence Berkeley National Laboratory

Robert M. Sweet, Brookhaven National Laboratory

Sean McSweeney, Brookhaven National Laboratory

Andreas Förster (Dectris, Ltd.)

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Session Topics

13:00 – 18:00 **Wed, 15 March 17** at MAX lab **Meeting Starts**

13:00 – 13:30 **Registration, Coffee**

13:30 – 15:00 **Status & Development Reports**, Uwe Miller, Chair

15:00 – 15:30 **Coffee Break**

15:30 – 16:50 **Status & Development Reports**, continued

17:00 – 18:00 **Tour of MAX IV** (2 groups)

19:30 Godset in Lund Center **Dinner**

09:00 – 18:00 **Thurs, 16 March 17** at MAX lab **Meeting Continues**

09:00 – 10:00 **Software Development Updates**, Gerard Bricogne, Chair

10:00 – 10:30 **Coffee Break**

10:30 – 12:30 **Software Development Updates**, continued

12:30 – 13:30 **Lunch**

13:30 – 15:00 **IT Infrastructure for Eiger Data Processing**, Artur Barczyk, Chair

15:00 – 15:30 **Coffee Break**

15:30 – 17:30 **Data Handling I**, Andreas Förster, Chair

19:30 Godset in Lund Center **Dinner**



Session Topics (cont.)

09:00 – 16:00 **Fri, 17 March 17** at MAX lab **Meeting Continues**

09:00 – 11:00 **Data Handling II**, Herbert J. Bernstein, Chair

10:00 – 10:30 **Coffee Break**

10:30 – 11:00 **Data Handling II**, continued

11:00 – 12:10 **Open Issues**

12:10 – 12:30 **Next Meeting Planning**

12:30 – 13:30 **Lunch**

13:30 – 15:30 **Summary and Wrap-up**, Herbert J. Bernstein, Chair

15:30 – 16:00 **Coffee Break**

16:00 **Meeting Ends**

See [https://indico/maxiv.lu.se/event/233/program](https://indico.maxiv.lu.se/event/233/program) for the detailed agenda



Questions for the Meeting

We hope for answers to the following questions

- What successes and what problems are being seen in handling HDRMX data?
- Which tools and which approaches are best used for efficient processing of streamed images, including handling of regions of interest, compression, binning and summing?
- What format and metadata conventions are best suited to process and archive data in an interoperable manner at synchrotrons, at user institutions and in archives?
- What tasks should we focus on next?