

# High Data-Rate Macromolecular Crystallography (HDRMX) Meeting



Wednesday, March 15, 2017 - Friday, March 17, 2017

MAX IV

## Scientific Program

Mar. 15<sup>th</sup> 13:00 – 17<sup>th</sup> 16:00

Mar.15<sup>th</sup> afternoon @ **MAX Ia/Ib**, Status / Development report, Chair: Uwe Mueller

**Time**

**Duration (min)**

**Event**

13:00

30

Registration / Coffee

13:30

5

Welcome - Uwe Mueller

13:35

10

Introduction, review of last meeting and topics - Herbert J. Bernstein, slides

13:45

10 + 5

APS-GM/CA - Mark Hilgart, slides

14:00

10 + 5

Australian Synchrotron - Tom Caradoc-Davies / Jun Aishima, slides

14:15

10 + 5

DLS - Graeme Winter, slides

14:30

10 + 5

EMBL-HH - Maria Nikolova, slides

14:45

10 + 5

MAX IV - Jie Nan, slides

15:00

30

Coffee Break (MAX IV Matsal / Dining room)

15:30

10 + 5

NSLS-II - Jean Jakoncic, slides

15:45

10 + 5

SSRL - Thomas Eriksson, slides

16:00

10 + 5

SOLEIL - Martin Savko, slides

16:15

20 + 5

EIGER - Updates and Outlook - Stefan Brandstetter, slides

16:40

10

Summary

17:00

60

Tour of MAX IV (two groups)

19:30

Dinner at restaurant Godset in Lund center

Mar.16<sup>th</sup> morning @ **MAX Ia/Ib**, Software development updates, Chair: Gerard Bricogne

**Time**

**Duration (min)**

**Event**

9:00

20 + 5

Fast XDS processing of Eiger data - Kay Diederichs, slides

9:25

30 + 5

DIALS ; LABELIT / DISTL Spotfinder - Graeme Winter, slides1, slides2

10:00

30

Coffee Break (MAX IV Matsal / Dining room)

10:30

20 + 5

On-line evaluation of diffraction images with DOZOR - Gleb Bourenkov, slides

10:55

20 + 5

XDSAPP - Karine Röwer, slides

11:20

20 + 5

autoPROC - Claus Flensburg

11:45

20 + 5

LCLS2 Data Reduction Pipeline Preparation for Serial Femtosecond Crystallography - Chun Hong (Chuck) Yoon, slides

12: 10

10 + 5

Dectris Eiger HDF5 Stream Writer - Andrej Babic, slides

12:25

5

Summary

12:30

60

Lunch Break (MAX IV Matsal / Dining room)

Mar.16<sup>th</sup> afternoon @ **MAX Ia/Ib**

Session 1, IT infrastructure for Eiger data processing, Chair: Artur Barczyk

13:30

5

## Introduction

13:35

10 + 5

High speed detector software and IT infrastructure at Diamond - Ulrik Pedersen, slides

13:50

70

- internal/external network support
- computational support
- benchmark
- storage capacity and storage types
- the line between Dectris and beamline responsibility

15:00

30

Coffee Break (MAX IV Matsal / Dining room)

Session 2, Data handling (1), Chair: Andreas Förster

15:30

5



**Introduction**

15:35

10 + 5

NeXuS - Tobias Richter, slides

15:50

100

- Metadata alignment
- masterfile

19:30

Dinner at restaurant Glorias in Lund center

Mar.17<sup>th</sup> morning @ **MAX III**, Data handling (2), Chair: Herbert J. Bernstein

**Time**

**Duration (min)**

**Event**

9:00

60

slides1, slides2, slides3

- data manipulation, sum/binning/roi
- compression

10:00

30

Coffee Break (MAX IV Matsal / Dining room)

10:30

30

- formats and conversions

11:00

70

Open issues from Day 1 & 2

12:10

20

Next meeting

12:30

60

Lunch Break (MAX IV Matsal / Dining room)

Mar.17<sup>th</sup> afternoon @ **MAX III**, Summary and wrap up, Chair: Herbert J. Bernstein

**Time**

**Duration (min)**

**Event**

13:30

Summary and wrap up

15:30

30

Coffee Break (MAX IV Matsal / Dining room)

16:00

Departure