



XXV IUCr Congress satellite workshop

Methods of Structural Biology



Joining CCP4/CCP-EM online workshop and CMS workshop

Dates: August 9 – 10, 2021 (CCP4/CCP-EM), August 12 – 13, 2021 (CMS)

Venue: Online + Institute of Biotechnology of the Czech Academy of Sciences, Biocev Centre, Prumyslova 595, Vestec near Prague

Aim: The **CMS workshop** will provide training and hands on experience in selected structural biology techniques available at the Centre of Molecular Structure (CMS) at IBT. Introductory talks will be accompanied by more advanced insights into biophysics, protein crystallization, X-ray diffraction, small angle X-ray scattering and structural mass spectrometry. Sessions at instruments will focus on training in selected techniques.

The **CCP4/CCP-EM online workshop** will focus on theory and practice in computational approaches in bio-crystallography and Cryo-EM single particle analysis.

Format: The CCP4/CCP-EM workshop will be organized online by the CCP4 and CCP-EM staff. The CMS workshop, organized by the CMS staff, will be on site. According to the epidemiological situation, we will confirm this format or announce changes.

There is a one-day break – August 11 – for travel of those who want to participate in both workshops.

Participation fee: **CCP4/CCP-EM** – free.

CMS workshop - 150 EUR (meals and course materials; does not cover accommodation and dinner on 11 Aug)

To apply: Please fill out the **preliminary registration form for both parts** at: <https://forms.biocev.org/index.php/891685?newtest=Y&lang=en>
You can register to one or both workshops. In the case of high interest, preference will be given to those registered to both workshops. You will receive confirmation (and payment details if applicable) before the end of June.

Application deadline: The deadline for preliminary registration is June 17, 2021. The payment deadline is July 31, 2021.

Jan Dohnálek – dohnalek -at- ibt.cas.cz, Magdalena Schneiderová - magdalena.schneiderova -at- ibt.cas.cz, Jan Stránský – jan.stransky -at- ibt.cas.cz
ccp4 -at- stfc.ac.uk

ciisb.org

ibt.cas.cz/core-facility/CMS

cssb.structbio.org

www.ccp4.ac.uk

www.ccpem.ac.uk

Preliminary programme (Prague, CEST time):

CCP4/CCP-EM online workshop

Monday, August 9

- 09:00-09:45 CCP4 Cloud Setup and General Introduction
- 09:45-10:45 Data processing and reduction
- 10:45-11:00 Break
- 11:00-12:00 Experimental Phasing and Density Modification
- 12:00-13:00 Lunch break
- 13:00-13:45 Molecular Replacement
- 13:45-14:45 Model Building and Refinement
- 14:45-15:00 Break
- 15:00-15:30 Automated Model Building
- 15:30-16:00 Validation and Deposition
- 16:00-16:30 Break
- 16:30-17:30 Introduction to CryoEM (talk)
- 17:30-18:00 CCP-EM (practical setup)

Tuesday, August 10

- 09:00-10:30 Single particle reconstruction (demo + short practical)
- 10:30-10:45 Coffee Break
- 10:45-11:15 Reconstructed volumes - interpretation, sharpening, noise reduction (practical)
- 11:15-12:00 De novo model building (practical)
- 12:00-13:00 Lunch
- 13:00-14:00 Model refinement and validation (practical)
- 14:00-15:00 Wrap-up / free time

CCP4/CCP-EM online workshop

Registration

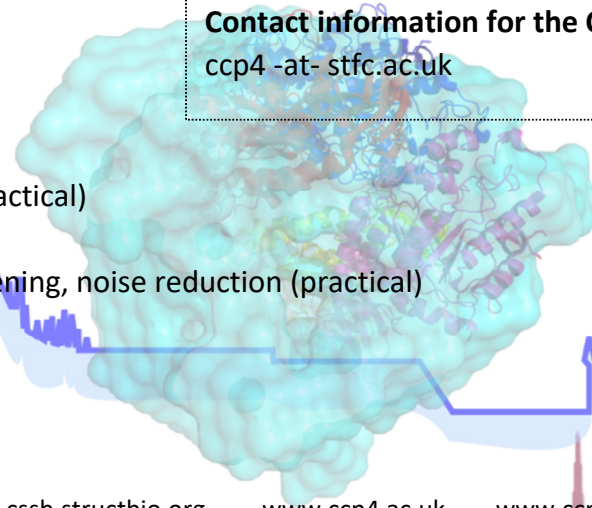
No fee is required for the CCP4/CCP-EM workshop. A webpage with details and registration information will be available soon. For now, please register your interest through the preliminary registration page.

Technical information/organizational

Participants will require access to a Linux or MacOS machine with CCP4 and CCP-EM installed. Access to Zoom and Slack will also be required.

Contact information for the CCP4/CCP-EM part

ccp4 -at- stfc.ac.uk





CMS workshop

Wednesday, August 11

Travel, get together dinner (paid individually)

Thursday, August 12

- 8:30 Arrival, coffee, instructions, meeting others
- 8:50-9:00 Welcome
- 9:00-9:30 Biophysics, introduction (Tatsiana Charnavets)
- 9:30-10:00 Biophysics, Advanced methods (TBA)
- 10:00-10:30 Basics of protein crystallisation (Jiří Pavlíček)
- 10:30-11:00 Crystallization of membrane proteins using lipidic systems (Martin Caffrey)
- 11:00-11:30 Coffee break
- 11:30-12:00 Basics of X-ray diffraction in structural biology (Jan Stránský)
- 12:00-12:30 Protein crystallography at XFELs (Arwen Pearson)
- 12:30-13:00 Application talk – TBA

13:00-14:00 Lunch (local canteen)

Practicals at instruments

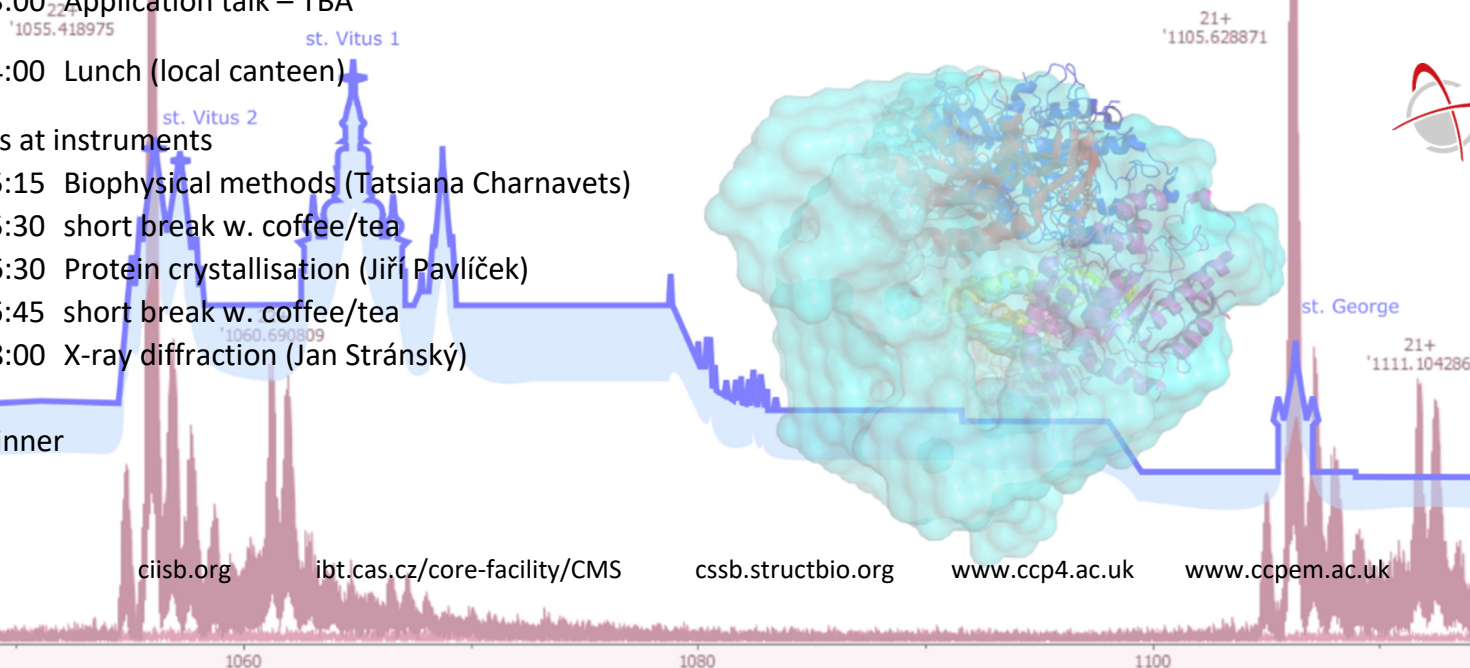
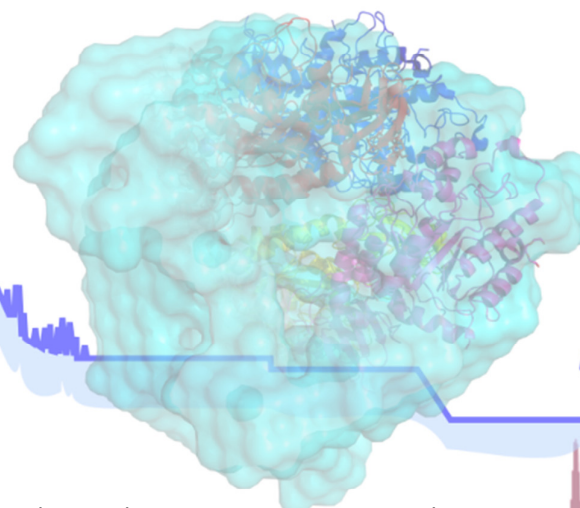
- 14:00-15:15 Biophysical methods (Tatsiana Charnavets)
- 15:15-15:30 short break w. coffee/tea
- 15:30-16:30 Protein crystallisation (Jiří Pavlíček)
- 16:30-16:45 short break w. coffee/tea
- 16:45-18:00 X-ray diffraction (Jan Stránský)

19:00 Dinner

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Friday, August 13

- 8:30-9:00 Introduction to Small angle X-ray scattering and its application in-house (Jan Stránský)
- 9:00-9:30 Advanced SAXS modeling techniques for biological macromolecules in solution (Dima Molodenskyi)
- 9:30-10:30 Mass Spectrometry (Julien Marcoux + Petr Pompach)
- 10:30-11:00 Coffee break
- 11:00-12:00 Bioinformatics (TBA)
- 12:00-12:30 Application talk (TBA)

- 12:30-13:30 Lunch (local canteen)



Practicals at instruments/computers

- 13:30-14:45 Laboratory Small angle X-ray scattering (Jan Stránský)
- 14:45-15:00 short break w. coffee/tea
- 15:00-16:15 Native Mass Spectrometry (Petr Pompach)
- 16:15-16:30 short break w. coffee/tea
- 16:30-17:45 Bioinformatics (TBC)

19:00 Dinner

Confirmed speakers/tutors:

Martin Caffrey (Trinity College, Dublin); Julien Marcoux (CNRS, Toulouse); Dima Molodenskyi (EMBL, Hamburg); Arwen Pearson (Universität Hamburg); Tatsiana Charnavets (IBT); Jiří Pavlíček (IBT); Petr Pompach (IBT); Jan Stránský (IBT)

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