

## CCP4/APS School in Macromolecular Crystallography: From Data Collection to Structure Refinement and Beyond

Argonne National Laboratory

June 23 Monday - June 30 Monday 2025

### Chicago Time (CDT)

Virtual Day 1 (Mon June 2): Cryocrystallography and Bioinformatics (zoom link)

|          |      |                                                        |                |
|----------|------|--------------------------------------------------------|----------------|
| 9:00 AM  | 0:30 | Introduction: Outline resources and SLACK Arrangements |                |
| 9:30 AM  | 0:45 | Cryo-crystallography                                   | Elspeth Garman |
| 10:15 AM | 0:45 | Radiation Damage                                       | Elspeth Garman |
| 11:00 AM | 0:15 | Break                                                  |                |
| 11:15 AM | 1:15 | Bioinformatics                                         | Dan Rigden     |
| 12:30 AM | 0:45 | Generating Your Models                                 | Adam Simpkin   |
| 1:15 PM  | 1:00 | Lunch Break                                            |                |

Virtual day 2 (Mon June 16): Introduction to CCP4 and X-ray Diffraction (zoom link)

|          |      |                                                                   |                                  |
|----------|------|-------------------------------------------------------------------|----------------------------------|
| 9:00 AM  | 1:30 | Introduction to CCP4                                              | Charles Ballard /<br>Maria Fando |
| 10:30 AM | 0:15 | Break                                                             |                                  |
| 10:45 AM | 1:00 | Basic Diffraction Theory                                          | Kamel El Omari                   |
| 11:45 AM | 1:15 | Introduction to data processing                                   | David Waterman                   |
| 1:00 PM  | 1:00 | Lunch Break                                                       |                                  |
| 2:00 PM  | 0:30 | Introduction to data processing - demo                            | David Waterman                   |
| 2:30 PM  | 1:00 | How to Collect the Best Macromolecular Diffraction Data - Dectris | Sofia Trampari                   |
| 3:30 PM  | 1:00 | Enabling Crystallography with Developments from MiTeGen           | Joyce Frank/Mitegen              |

Day 1 (Mon June 23): Data Collection and Processing

|          |      |                                                      |                                                    |
|----------|------|------------------------------------------------------|----------------------------------------------------|
| 8:30 AM  | 0:05 | Welcome and Introduction                             | Qingping Xu                                        |
| 8:35 PM  | 0:45 | Introduction to the Upgraded APS and MX Capabilities | Bob Fischetti                                      |
| 9:20 AM  | 1:10 | Data Collection Concepts and Tips                    | Zheng-Qing (Albert) Fu - SERCAT                    |
| 10:30 AM | 0:15 | Break                                                |                                                    |
| 10:45 AM | 1:00 | Assessing Diffraction Data Quality                   | Kay Diederichs                                     |
| 11:45 AM | 0:45 | Data Processing with DIALS - demo-lecture            | Graeme Winter                                      |
| 12:30 AM | 0:10 | Group Photo                                          |                                                    |
| 12:40 AM | 0:50 | Lunch break                                          |                                                    |
| 1:30 PM  | 1:15 | Data Processing with HKL3000 - demo-lecture          | Dominika Borek                                     |
| 2:45 PM  | 1:15 | Data Processing with XDS - demo-lecture              | Kay Diederichs                                     |
| 4:00 PM  | 0:15 | Break                                                |                                                    |
| 4:15 PM  | 1:45 | GMCA after APS-U<br>Beamline Tour                    | David Kissick, Naga Venugopalan,<br>Michael Becker |
| 6:00 PM  | 1:30 | Student Presentations Part 1                         | Students                                           |
| 7:30 PM  | 1:00 | Dinner Break                                         |                                                    |
| 8:30 PM  | 1:30 | Student Presentations Part 2                         | Students                                           |

Day 2 (Tue June 24): Data Collection and Processing

|          |      |                                                   |                                   |
|----------|------|---------------------------------------------------|-----------------------------------|
| 8:30 AM  | 1:30 | Scaling and Merging the Data (Multi-crystal Data) | Graeme Winter                     |
| 10:00 AM | 2:30 | Data Collection                                   | Michael Becker / Naga Venugopalan |
| 12:30 PM | 1:00 | Lunch Break                                       |                                   |
| 1:30 PM  | 3:00 | Data Collection (coffee available from 4pm)       | Michael Becker / Naga Venugopalan |
| 4:30 PM  | 3:00 | Data Collection                                   | David / Qingping Xu               |
| 7:30 PM  | 1:00 | Dinner Break                                      |                                   |
| 8:30 PM  | 2:00 | Data Collection                                   | David / Qingping Xu               |

Day 3 (Wed June 25): Data Processing and Experimental Phasing

|          |      |                                                                        |                          |
|----------|------|------------------------------------------------------------------------|--------------------------|
| 8:30 AM  | 1:00 | Symmetry                                                               | Charles                  |
| 9:30 AM  | 1:00 | Twinning and Other Pathologies lecture + demo                          | Andrey Lebedev (Virtual) |
| 10:30 AM | 0:15 | Break                                                                  |                          |
| 10:45 AM | 0:30 | Tutorial in Dealing with Twinning                                      | Andrey Lebedev (Virtual) |
| 11:15 AM | 1:15 | Phase Problem + EP                                                     | Ed Lowe                  |
| 12:30 PM | 1:00 | Lunch Break                                                            |                          |
| 1:30 PM  | 0:30 | Phasing Demo EP                                                        | Ed Lowe                  |
| 2:00 PM  | 5:30 | Processing Data (coffee available from 4pm)                            |                          |
| 7:30 PM  | 1:00 | Dinner Break                                                           |                          |
| 8:30 PM  | 1:00 | Experimental Phasing: Long Wavelength, Soaks, Identification of Metals | Kamel El'Omari           |
| 9:30 PM  | 0:30 | Dataset of the Day and Practical Session                               |                          |

Day 4 (Thu June 26): Molecular Replacement

|          |      |                                                  |                               |
|----------|------|--------------------------------------------------|-------------------------------|
| 8:30 AM  | 1:00 | Molecular Replacement - basics                   | Randy Read (Virtual) / Airlie |
| 9:30 AM  | 1:00 | Phaser, model prep, docking into CryoEM lectures | Randy Read (Virtual) /Airlie  |
| 10:30 AM | 0:15 | Break                                            |                               |
| 10:45 AM | 0:45 | TBA                                              |                               |
| 11:30 AM | 1:00 | Arcimboldo, Shelx for MR                         | Josep Triviño                 |
| 12:30 PM | 1:00 | Lunch Break                                      |                               |
| 1:30 PM  | 1:00 | Phasing in Phenix                                | Dorothee Liebschner           |
| 2:30 AM  | 1:00 | MR in CCP4 Talk/Demo                             | Adam Simpkin (Virtual)        |
| 3:30 PM  | 4:00 | Practical Session (coffee available from 4pm)    |                               |
| 7:30 PM  | 1:00 | Dinner Break                                     |                               |
| 8:30 PM  | 1:30 | Dataset of the Day and Practical Session         |                               |

Day 5 (Fri June 27): Model Building

|          |      |                                                               |                                |
|----------|------|---------------------------------------------------------------|--------------------------------|
| 8:30 AM  | 1:30 | Introduction to model building and model building in COOT     | Paul Emsley/<br>Lucrecia/Berni |
| 10:00 AM | 0:30 | Model Building in Phenix (1)                                  | Dorothee Liebschner            |
| 10:30 AM | 0:15 | Break                                                         |                                |
| 10:45    | 0:45 | Model Building in Phenix (2)                                  | Dorothee Liebschner            |
| 11:30 PM | 1:00 | Automatic model building in CCP4: Modelcraft + Nautilus + DNA | Paul Bond                      |
| 12:30 PM | 1:00 | Lunch                                                         |                                |
| 1:30 PM  |      | Free time (afternoon and evening)                             |                                |

Day 6 (Sat June 28): Refinement and Ligands

|          |      |                                               |                                          |
|----------|------|-----------------------------------------------|------------------------------------------|
| 8:30 AM  | 1:00 | Introduction to Refinement with CCP4          | Rob Nicholls                             |
| 9:30 AM  | 1:00 | Model-building errors, the quiz               | Robbie Joosten                           |
| 10:30 AM | 0:15 | Break                                         |                                          |
| 10:45 AM | 0:45 | Modelling ligands in CCP4                     | Rob Nicholls                             |
| 11:30 AM | 1:00 | Refinement against cryoEM reconstructions     | Rob Nicholls                             |
| 12:30 PM | 1:00 | Lunch Break                                   |                                          |
| 1:30 PM  | 1:00 | CryoEM: model building and validation         | Genki Terashi/Daisuke<br>Kihara - Purdue |
| 2:30 PM  | 1:30 | Phenix-refine                                 | Pavel Afonine                            |
| 4:00 PM  | 0:15 | Break                                         |                                          |
| 4:15 PM  | 3:15 | Practical Session (coffee available from 4pm) |                                          |
| 7:30 PM  | 1:00 | Dinner Break                                  |                                          |
| 8:30 PM  | 1:30 | Dataset of the Day and Practical Session      |                                          |

Day 7 (Sun June 29): Other Macromolecules, Ligands, Validation

|          |      |                                                             |                           |
|----------|------|-------------------------------------------------------------|---------------------------|
| 8:30 AM  | 1:00 | Carbohydrates                                               | Jon Agirre (Virtual)      |
| 9:30 AM  | 1:00 | Metals / Check my metal; Model completion and Validation -1 | Robbie Joosten            |
| 10:30 AM | 0:15 | Break                                                       |                           |
| 10:45 AM | 0:45 | Model completion and Validation -2                          | Robbie Joosten            |
| 11:30 AM | 1:00 | Coot advanced including DNA/RNA and ligands                 | Paul Emsley               |
| 12:30 PM | 1:00 | Lunch Break                                                 |                           |
| 1:30 PM  | 1:00 | Validation in Phenix                                        | Pavel Afonine             |
| 2:30PM   | 0:45 | Raddam                                                      | Kathryn Shelley (Virtual) |
| 3:15 PM  | 4:15 | Practical Session (coffee available from 4pm)               |                           |
| 7:30 PM  | 1:00 | Dinner Break                                                |                           |
| 8:30 PM  | 1:30 | Dataset of the Day and Practical Session                    |                           |

Day 8 (Mon June 30): Structure Analysis and Deposition

|          |       |                                                              |                            |
|----------|-------|--------------------------------------------------------------|----------------------------|
| 8:00 AM  | 1:00  | Use of PDB                                                   | Stephen Burley (Virtual)   |
| 9:00 AM  | 0:45  | CryoEM: Tools in Phenix (to swap with Brian?)                | Pavel Afonine              |
| 9:45 AM  | 0:45  | RCSB PDB deposition and development, tools (PDB 101 etc) - 1 | Brian Hudson (Virtual)     |
| 10:30 PM | 0:15  | Break                                                        |                            |
| 10:45 AM | 0:45  | RCSB PDB deposition and development, tools (PDB 101 etc) - 2 | Brian Hudson (Virtual)     |
| 11:30 AM | 1:00  | Structural Analysis & Macromolecular Complexes               | Eugene Krissinel (Virtual) |
| 12:30 PM | 1:00  | Lunch Break                                                  |                            |
| 1:30 PM  | 2:00+ | The last hands on and backup                                 |                            |
|          |       | Au revoir                                                    |                            |