Structural databases in the exascale era

Tuesday, April 1, 2025
Lady Margaret Hall, University of Oxford, Oxford, United Kingdom

Aim: 'Discuss integration of MD data with already existing biological data repositories and standards (structural and bioinformatics repositories)'

Expected outcomes: 'Identify additional value-added annotations for deposited data from existing repositories; identify requirements for interoperability between simulation data and accepted standards for biological data repositories'

9:00-9:30	Arrival and coffee
9:30-10:00	**Introduction to MDDB**, our aims, node infrastructure etc.
10:00-11:00	**Participant 5-min presentations, slides optional.** Objective: Introduction of existing databases and their included resources/annotations.
11:00-11:30	Coffee break
11:30-12:00	**Continuation of participant 5-min presentations.**
12:00-13:00	**Discussion.** Objectives: List possible/existing annotations and data types, discuss what to implement in Phase 1 or 2 of the MDDB project, form a working group on the scientific side of data integration.
13:00-14:00	Lunch
14:00-15:00	**APIs – presentations from IRB (MDDB nodes), EBI (PDBe-KB), and discussion.** Objective: what is currently implemented and what could be implemented?
15:00-15:30	Coffee break
15:30-16:30	**Discussion on infrastructure for data integration.** Objectives: what changes need to be made to current infrastructures, establish a working group on the technical/developer side of data integration.
16:30-17:00	**Concluding remarks.** Objectives: summarise which annotations should be included in 'phase 1', API details and potential updates, and annotation/integration long-term goals.
18.00	Dinner at The Cherwell Boat House (https://cherwellboathouse.co.uk/)

* All meals in the programme are provided by MDDB.