MD standards, formats, and data interoperability

October 16, 2023 - October 17, 2023
Lady Margaret Hall, University of Oxford, Oxford, United Kingdom

Aim: 'Discuss standards, metadata, formats and reproducibility across MD engines'

Expected outcomes: 'Agreement on standard formats, reproducibility packages (minimum set of files to reproduce a simulation), perspective paper'

Monday 16th October 2023 - Day 1

Time	Activity
10:00 - 10:30	Arrival & coffee
Session 1 - MD databases: Why, how, needs, possibilities	
10:30 - 11:00	Welcome and background to the project - What is MDDB about and for?
11:00 - 11:30	What do we need from/in MD engines to enable this?
11:30 - 12:00	What are the technical requirements/needs from MD/analysis/viz codes?
12:00 - 12:30	Open discussion and interactive report editing
12:30 - 14:00	Lunch
Session 2 - Prototypes, use cases, stress tests, MD collections	
14:00 - 15:00	Examples of MD databases within MDDB consortium
15:00 - 15:30	Open discussion and interactive report editing
15:30 - 16:00	Tea & coffee
Session 3 - FAIR, storage, sharing, metadata, provenance, reproducibility, checking	
16:00 - 17:30	Discussion - Things to facilitate upload/download/remote analysis/participation?
17:30 - 18:30	Break
18:30 - 19:30	Drinks at the Old Library
19:30 - 22:00	Dinner in the Jerwood Room

Tuesday 17th October 2023 - Day 2

Session 4 - Persistent IDs, distributed/federated DB, community, dissemination	
09:30 - 10:00	Links between MD data repositories
10:00 - 11:00	Links to AI/AF2 and other databases
11:00 - 11:30	Tea & coffee
Session 5 - Standards, formats, interoperability, ontologies	
11:30 - 12:00	Molecular descriptors and topology formats
12:00 - 12:30	Open discussion and interactive report editing
12:30 - 14:00	Lunch
Session 6 - Roadmap	
14:00 - 15:30	Goals and action plans
15:30 - 16:00	Wrap up

* *All meals in the programme are provided by MDDB.*