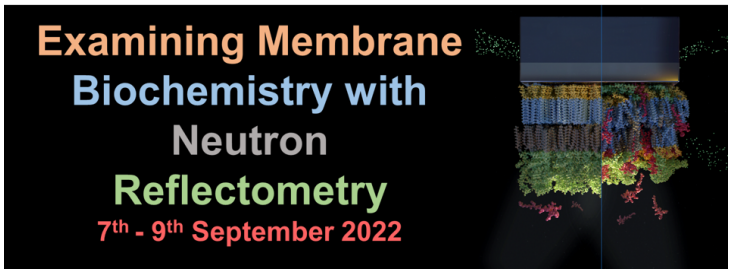


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# Molecular Simulation of Model Biological Membranes

*Friday, 9 September 2022 12:00 (20 minutes)*

Classical molecular dynamics (MD) provides atomic level detail on the structure and dynamics of biological molecules, as well as allowing *in silico* experiments on the system of interest. In particular, MD has been applied to biological membranes where historically there has been a lack of high resolution experimental probes. There are now increasing efforts to combine the level of detail available from MD with reflectivity scattering curves from real samples. In this talk, I will cover our work to develop a computational pipeline at ISIS that allows the inclusion of MD trajectory data into the reflectivity analysis provided by Rascal/RAT. An innovative part of this pipeline is feedback from the fit to experimental data back to the molecular modelling via applied restraints. The pipeline will be made available through an iDAaaS environment.
This work is part of a wider effort in Scientific Computing to develop molecular simulation methods, to elucidate biological structures, and to support the large facilities at Harwell. I will also summarise some of this other work, in order to provide some of the wider context.

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