



YCCSA Seminar Series Summer 2019

An interdisciplinary seminar series hosted by the York Cross-disciplinary Centre for Systems Analysis aimed at researchers from all disciplines

Multiscale multiphysics of liquid solutions of complex molecular systems

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Ron Cooke Hub, RCH/204 at 13:30

Abstract:

Recent experimental and computational advances allow investigations of liquid systems at spatial and temporal scales (nanometers, nanoseconds) where two representations are equally valid and necessary: atomistic and continuous (fluid dynamics). Examples of the former include Molecular Dynamics (MD) simulations of systems composed of tens of millions of atoms or cryo-EM measurements of complete viruses and cell organelles with atomistic resolution. The latter is represented, for example, by the multitude of nano- and micro-fluidic devices including, among others, non-contact liquid atomic force microscopy (NC-AFM) capable of measuring flows of liquids at atomistic scales. Despite comparable quality of theoretical predictions using both atomistic and continuum representations, the physics behind them is fundamentally different, from the basic concepts (discrete atoms vs continuum of matter) to the equations of motion describing the system's structure and dynamics. This disparity becomes particularly obvious if the problem at hand requires transition between the scales or the description of the same system at different scales simultaneously. We will present our recent attempts to develop a unified description of liquid systems such that they are described by the same equations of motion throughout multiple scales, from atomistic to macroscopic hydrodynamic. Two different frameworks will be described each having a set of equations that are valid equations of motion at both limiting scales, MD and hydrodynamic, and at all scales between these extremes. The frameworks are physically consistent, obeying fundamental conservation laws (of mass, momentum, and energy) at all scales. Examples of applying these frameworks to the complete virus in aqueous solution will be given.

The seminar includes a refreshment break to fuel interdisciplinary discussion

***Ron Cooke Hub is on Heslington East Campus – accessible by free bus services
Nos. 66 and UB1 running at frequent intervals from Heslington West.
The YCCSA Seminar room is on the second floor***