UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

Dipartimento di Scienze Fisiche, Informatiche e Matematiche

Interdisciplinary Seminar

Coupling Molecular Dynamics to the Continuum for Fluid Dynamics Simulation

May 21, 2019—14:30

Room L1.5, First Floor, **Physics Building**, FIM Department

Speaker

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Abstract

Fluid dynamics simulation, known as computational fluid dynamics (CFD) is essential in many aspects of engineering design. CFD is reliant on the continuum assumption, modelling the fluid behaviour as a mean field with no molecular detail. However, modelling the molecular nature of reality becomes essential in many problems of interest; wall-fluid interaction, the origins of nucleation, insight into the smallest scales of turbulence and the dynamics of chemicals and biomolecules. As molecular dynamics (MD) modelling is often prohibitively expensive for engineering applications, multi-scale coupling aims to combine continuum and discrete models to include molecular detail only where it is essential. Often this is done by directly linking an MD and CFD simulation together along an interface, with real-time information exchange between the two.

In order to do this correctly, the discrete and continuum paradigms must be combined. In the 1950s, a mathematical framework was developed by Irving & Kirkwood which provides the link between discrete and continuum equations. As in quantum mechanics, the Dirac delta functional is the key to this linking of field and particle descriptions of reality. For fluid dynamics, it is more convenient to work with the integral or control volume form of the equation of motion. We present the process of obtaining equivalent integrated or

control volume equations in the molecular system. This involves integrating the Dirac delta function, which provides a useful operator for linking continuum and discrete systems for coupled fluid simulation. This can be shown to measure exact conservation for a single molecular system trajectory. The mathematical operator can also be used to derive constraint algorithms localised to an arbitrary volume in space, a useful tool for non-equilibrium molecular dynamics (NEMD). The link to NEMD techniques like SLLOD and the resulting phase space compressibility of localised constraints are discussed.

We present a number of application of coupled molecular-continuum simulation of fluid dynamics. This will include a discussion of software and computing considerations, outlining efforts to develop open-source software to lower the barrier to entry in the field of coupling.

Short Bio

Edward Smith (www.edwardsmith.co.uk) is a researcher working on multi-scale methods combining particle and continuum simulation. He earned his PhD at Imperial College London, developing theoretical and computational techniques for the coupled simulation of molecular dynamics (MD) and computational fluid dynamics (CFD). After his PhD, he was awarded the post-doctoral excellence fellowship and published the first ever molecular dynamics simulation of near-wall turbulence. He spent time in Swinburne Australia working with experts in non-equilibrium molecular dynamics and statistical mechanics, before moving to Chemical Engineering at Imperial to work on multi-phase flow and the moving contact line. His next move was to Civil Engineering at Imperial to develop software (www.cpl-library.org), linking particles and continuum flows for granular systems. He recently took up a position at Brunel University London as a lecturer in fluid dynamics.