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Advances in Theory and Simulation of Non-equilibrium Systems – Foreword

Over the last few years we have witnessed a growing interest in nonequilibrium research, largely driven by an increasing use of computational and theoretical tools to study materials of relevance in energy or thermophysical applications. Nonequilibrium algorithms are now incorporated into software packages such as LAMMPS and DL POLY which are available free within the academic community, significantly broadening the user base. The ground breaking contributions of the 1970s, 1980s, and 1990s of Evans, Hoover, Morriss and others in developing nonequilibrium methodology paved the way for their widespread uptake.

The application of traditional techniques to new problems prompts many questions that need to be addressed. Fundamental questions concerned with the application of continuum approaches at small scales, the correct implementation of nonequilibrium simulation techniques, and the extension of these to bridge molecular and continuum length scales have given rise to the current growth of interest in nonequilibrium research.

Driven by these changes, we felt it was timely to create a series of conferences on computer simulations and the theory of nonequilibrium systems. The first meeting, NESC'13, took place over two days at Imperial College London, September 2013. The success of that meeting encouraged us to keep faith with the format and so in July 2016, the second conference in the series took place at Halifax Hall, University of Sheffield.

The Sheffield meeting gathered over 50 delegates from 12 countries, including Europe, the USA, Japan and Australia and was held over three days. The meeting incorporated a Festschrift for Bill Hoover, celebrating his 80th birthday and honoring his seminal contributions to computational physics and nonequilibrium simulation. We were especially honored to welcome our keynote speaker, Professor Berni Alder, the founding father of the molecular dynamics simulation method and pioneer in many related fields. Altogether there were 39 oral presentations including 11 invited talks and 10 posters.

The keynote speech delivered by Berni gave a career retrospective on the evolution of molecular dynamics. Divided into three epochs, the talk began with the development of MD shortly after World War 2 when it was used to answer the question of whether or not hard spheres would form a solid phase despite a lack of attractive forces and to study the mechanism of melting, particularly in two dimensions. In the second epoch, MD was used to study transport in fluids. Major findings included the discovery that hydrodynamics applies at the molecular scale, the existence of a long-time tail in the stress autocorrelation function, the usefulness of mode coupling theory, and the non-existence of the Burnett coefficients. The third epoch covered hydrodynamics accompanied by new understandings of boundary conditions and the conditions needed for turbulent flow.

Bill and Carol Hoover jointly gave a two-part talk looking back on Bill's long and illustrious career. Part one of the talk began by Bill relating his earliest childhood memories and his fascination with science and mathematics continuing to graduate school and ending with his and Carol's sabbaticals in Japan. The second part of the historical perspective included his collaborations with Tony de Groot, Harald Posch and Shuichi Nosé, marriage to Carol and their subsequent retirement, which she described as a long-term working vacation!

Several talks focused on the Fluctuation Theory and its applications. It was argued that dissipation, rather than entropy, provides the key to understanding the foundations of statistical mechanics. A local version of the theory can be applied to inhomogeneous systems such as fluids confined between walls. The sufficient condition for a steady state fluctuation relation to hold was discussed and it was argued that the dynamical system must be mixing rather than chaotic.

Discussions during the meeting exposed areas of research for further development where both theory and computer simulations should play an important role. Invited presentations included illuminating discussions of NEMD approaches investigating lubrication processes mediated by hydrated layers in polymers, or by chemisorbed monolayer coatings and thin films under high pressure. These NEMD techniques allow us to advance our microscopic understanding of wear and lubricant degradation. Nonequilibrium theory and continuum numerical simulations can be extended to investigate the complex dynamic behavior of catalytic micropumps, as well as activated processes far from equilibrium conditions, typically when the systems of interest are subjected to external driving forces.

Shockwaves and diffusion provide challenging problems where computational methods can provide much needed insight, for example by combining theoretical analyses of the Maxwell-Cattaneo model with Monte Carlo solutions of the Boltzmann equation or by using the Lorentz gas model, which has attracted considerable interest in statistical mechanics and in the study of ergodic processes. Newton's law of shear viscosity breaks down when the length and timescales over which the strain rate applies become comparable to molecular dimensions. NEMD is ideal for testing generalisations of this linear law. The sinusoidal longitudinal force algorithm has provided unambiguous evidence supporting a non-Markovian generalization of Newton's law.

Coarse graining provides an approach to studying phoretic processes in dilute colloidal suspensions by fluctuating hydrodynamics, or to studying polymer solutions under confinement and away from equilibrium, allowing us to identify the limitations of linear continuum approaches - Navier-Stokes-Fourier – at small confined scales.

Computer simulations are particularly helpful in studying phase transitions and nucleation processes. Extension of these techniques to investigate nonequilibrium phase transitions is a worthwhile objective.

Thermostats are key "devices" in NEMD simulations. They can be used to generate thermal gradients or to enable the temperature relaxation of fluids under shear. The generalized Langevin equation has proven helpful to the study heat transport in nanoscale systems, the simulation of quantum open systems and the handling of quantum fluctuations. The best/correct choice of thermostat used in NEMD is still an open question. Simulations of Fourier heat conduction in one-dimensional chains illustrated the differences between kinetic and configurational thermostats.

A final oral session included contributions from younger researchers. Intrinsic sampling approaches can be used to eliminate the averaging effect of thermal capillary waves at interface. When combined with NEMD they open a promising route to compute interfacial chemical potentials and thermal conductance. NEMD approaches also provide robust tools for the study of radiation damage and structural properties of colloidal suspensions.

The conference included an lively poster session. Contributions included nonequilibrium molecular dynamics (NEMD) methods to study thermal transport across interfaces, aqueous solutions and biological molecules, as well as simulations of the Joule-Thompson effect. Smooth-particle methods were also discussed in the context of mass transfer, applied mechanics modelling in materials and the study of shock waves.

NESC'16 was a very enjoyable event, both scientifically and socially. We would like to thank the personnel at Halifax Hall who provided technical support and took care of all practical aspects. We would also like to acknowledge the sponsors of the conference: The University of Sheffield, Imperial College, the Statistical Mechanics and Thermodynamics Group of the RSC and the CCP5 all provided valuable support in different forms.

Participants at NESC'16 were invited to contribute a manuscript to a special volume of CMST dedicated to the meeting and celebrating Bill Hoover's 80th birthday. The current issue is the result of this call and contains an excellent collection of new results and ideas as well as review material from leaders in the field of nonequilibrium theory and nonequilibrium simulations. We hope you enjoy reading this special issue.

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Guest Editors

Participants at the NESC'16 Conference held at Halifax Hall July 25-27, University of Sheffield, UK, 2016.