3rd meeting of the UK Fluid Network Special Interest Group on Non-Equilibrium Molecular Dynamics

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June 13-14, 2024 Imperial College London

About

This is the book of abstracts for the 3rd UK Fluid Network Special Interest Group on Non-Equilibrium Molecular Dynamics (NEMD) meeting, held at Imperial College London on the 13th and 14th of June 2024. The conference is organised into 30 minute invited talks and 20 minute contributed talks, grouped into themes (e.g. multiscale modelling, thermal, solid-liquid interfaces, liquid-vapour interfaces, tribology, boiling, droplets and dilute gas methods), with a discussion session led by the 3 speakers afterwards, in which the audience could ask detailed questions on the work (in a Faraday like style) as well as discussions on the wider topic of the session.

Any questions please contact the conference organisation committee:

- Edward Smith, Brunel University London
- James Ewen, Imperial College London
- Rohit Pillai, University of Edinburgh

Cover image credit: Edward Smith.

Description: Moving contact line between two walls, fitted with by an intrinsic surface using Chebyshev Polynomials.

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Conference Schedule

IT: Invited Talk, CT: Contributed Talk

Day 1: Thursday, 13 June

10:00-10:20	Coffee and Reception		
10:20-10:30	Welcome remarks		
10:30-11:00	IT	Daniele Dini Imperial	NEMD Simulations as a Powerful Modelling Tool in Tribology
11:00-11:20	СТ	Antonio Buffo Politecnico di Torino	Coupling Dissipative Particle Dynamics and Computational Fluid Dynamics for an industrial mixing process
11:20-11:40	СТ	Dmitry Nerukh Aston University	Hybridising molecular dynamics with hydrodynamics
11:40-12:00	Discussion		
12:00-13:00	Lunch		
13:00-13:30	IT	Fernando Bresme Imperial	Taming Complex Fluids with thermal fields: a non-equilibrium molecular dynamics journey
13:30-13:50	СТ	Gota Kikugawa Tohoku University	Molecular-scale picture on heat transfer characteristics of organic interfaces and polymeric materials
13:50-14:10	СТ	Laurent Joly Université Lyon 1	Molecular views on thermo-osmotic transport
14:10-14:30	Discussion		
14:30-14:50	Coffee Break		
14:50-15:20	IT	Marcello Sega UCL	Structural and transport properties at the liquid/vapor interface of water and simple liquids
15:20-15:40	СТ	Muhammad Rizwanur Rahman Imperial	Thin Films: Formation, Frustration and Fragmentation
15:40-16:00	СТ	Donatas Surblys Tohoku University	Heat Transfer at Solid-Liquid Interfaces and beyond via Molecular Dynamics: Various Insights
16:00-16:20	Discussion		
16:20-16:40	Coffee Break		

16:40-17:10	IT	Yasutaka Yamaguchi Osaka University	Mechanical and Thermodynamic Features of Liquid-Related Interfaces and Wetting by Molecular Dynamics
17:10-17:30	СТ	Takeshi Omori Osaka Metropolitan University	Measuring dynamic contact angles by computational fluid dynamics and molecular dynamics
17:30-17:50	СТ	Alex Lukyanov University of Reading	Non-locality of the contact line in dynamic wetting phenomena - a MD study
17:50-18:10	СТ	Hiroki Kusudo Tohoku University	Heat transport phenomenon during dynamic wetting: insight from molecular dynamics
18:10-18:30	Discussion		
18:30-19:30	Poster session		
19:30-	Conference Dinner		

Posters

Name	Affiliation and Poster title		
Shukai Cheng	Tohoku University	Study on solid-liquid phase change properties of sugar alcohols via molecular dynamics	
Matthew Val	University of	Data Driven Models for Accurate Prediction of	
Meyers	Manchester	Nucleate Boiling on Oxidised Surfaces	
Hiroki Imai	University of Tokyo	Analysis of the non-equilibrium gas flows in the	
		Knudsen layer above porous membranes	
Sritay Mistry	Brunel University	Small nanobubbles through high frequency	
Sintay winstry		vibrations	
Pengxu Chen	University of	Icequakes: Vibrating Supercooled Water at the	
religitu chen	Edinburgh	Nanoscale	
Saikat Datta	University of	Impact of Surface Wettability on Nanopore	
Jaikat Datta	Edinburgh	Evaporation	
	Brunel University	Nanobubbles Formation and Their Impacts on	
Hamidreza		the Inherent Properties of Graphene-Reinforced	
Hassanloo		Polar and Alcoholic Host Liquids: A Molecular	
		Dynamics Investigation	

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8:30-9:00			Coffee
9:00-9:30	IT	Shin-ichi Tsuda Kyushu University	A multi-scale study on hydrogen cavitating flow
9:30-9:50	СТ	Patrick Sullivan Durham University	Nanoscale Surface Effects on Vapour Bubble Nucleation
9:50-10:10	СТ	Sritay Mistry Brunel University	Hydrogen nanobubbles in ammonia
10:10-10:30	Discussion		
10:30-10:50	Coffee Break		
10:50-11:20	IT	Peter Daivis RMIT	Can a mesoscopic model describe stick-slip flow?
11:20-11:40	СТ	Takuya Kuwahara Osaka Metropolitan University	In situ synthesis of superlubric interfaces via mechanochemistry: learning molecular mechanisms from computer simulations
11:40-12:00	СТ	Zhaoran Zhu Imperial	Effect of Electric Fields on the Decomposition of Nanoconfined Phosphate Esters
12:00-12:20	Discussion		
12:20-13:20			Lunch
13:20-13:50	IT	Billy Todd Swinburne University of Technology	Interfacial Transport for Tribological Applications: Equilibrium and Nonequilibrium Molecular Dynamics Methods
13:50-14:10	СТ	Samy Merabia CNRS and Université Lyon 1	Thermal transport at solid-liquid interfaces: colloidal metallic nanoparticles and nanostructured gold-water interfaces coated with graphene
14:10-14:30	СТ	Davide Sarpa University of Southampton	Exploring Lubricant Chemistry: From Molecular Dynamics to Linear-scaling DFT
14:30-14:50	Discussion		
14:50-15:10	Coffee		
15:10-15:40	IT	Kazumichi Kobayashi Hokkaido University	Molecular fluid dynamics approach to boundary conditions at vapor-liquid interfaces for the Boltzmann equation
15:40-16:00	СТ	Ikuya Kinefuchi University of Tokyo	Non-Markovian dissipative particle dynamics
16:00-16:20	СТ	Carlos Corral-Casas Imperial	Velocity Slip in Fluids under Molecular Confinement
16:20-16:40	Discussion		
16:40			End of event

Day 2: Friday, 14 June

Invited Talk Abstracts

Daniele Dini

Imperial College London d.dini@imperial.ac.uk

NEMD Simulations as a Powerful Modelling Tool in Tribology

This talk will cover recent advances in modeling aspects of a variety of problems where the behaviour of tribological interfaces controls the performance of engineering systems. These are centred around the use of NEMD simulations of systems in confinement and will demonstrate how the use of models at the molecular scales is key to shed light on the mechanisms that control friction and performance of components and systems.

The talk will start with an overview of the modeling tools developed to study interfacial phenomena across the scales and will then move onto demonstrating how in-silico experiments can be used to shed light on various physical, chemical and mechanical phenomena that affect frictional interactions and engineering performance in several applications in the energy sector, including electric vehicles (EVs) and triboelectric nanogenerators (TENGs), manufacturing, biomedical applications, consumer goods, as well as functionalized and hierarchical materials and surfaces.

The main themes discussed are the study of the influence of molecular processes on frictional, rheological and material response, the potential breakdown of continuum theories at the nanoand microscales, as well as important aspects linked to the development of computational models which are twinned with relevant applications.

The presentation will conclude with highlighting the current limitations of existing models and techniques and an outlook at future trends and examples of how to change current engineering practice and place tribological interfaces at the centre of design strategy using a bottom-up approach. This will enable to directly use the insight gained from simulations at the smallest scales for the development of new disruptive solutions and to accelerate screening of e.g. new material and lubricant formulations.

Fernando Bresme

Imperial College London fbresme@imperial.ac.uk

Taming Complex Fluids with thermal fields: a non-equilibrium molecular dynamics journey

Thermal fields induce a range of non-equilibrium effects in complex fluids consisting of nanoparticle suspensions (e.g., Soret, Seebeck, Peltier effects), which can potentially be exploited in energy conversion (thermoelectrics), analytical devices for detection of biomolecules, or nanoparticle transport and assembly. The combination of non-equilibrium multiscale simulations and non-equilibrium theory has paved the way to elucidate the physical behaviour of complex fluids under external fields, showing that their response is much richer than previously anticipated. I will discuss the use of these techniques to predict and observe novel non-equilibrium effects in complex fluids that emerge from the coupling of heat fluxes and internal degrees of freedom of nanoparticles and molecules.

Marcello Sega

Department of Chemical Engineering, University College London m.sega@ucl.ac.uk

Structural and transport properties at the liquid/vapor interface of water and simple liquids

The interfacial region at the liquid/vapor interface of small molecular fluids like water is characterized by a marked inhomogeneity and anisotropy. Our understanding of the interfacial region has significantly evolved over the past two decades, also thanks to the perspectives opened by recent advances in computational methods. In this contribution, I will present recent results on structural, dynamics, and transport properties, discussing enhanced mobility and the appearance of a reduced surface shear viscosity.

Yasutaka Yamaguchi

Osaka University yamaguchi@mech.eng.osaka-u.ac.jp

Mechanical and Thermodynamic Features of Liquid-Related Interfaces and Wetting by Molecular Dynamics

Connection between the macroscopic fluid and heat flow and microscopic molecular motion by using MD and related methods is one of the main topics to be focus of the workshop. At a liquidvapor (LV) interface, Bakker's equation, which relates the macroscopic LV interfacial tension to the anisotropy of the microscopic local stress near the interface existing is known. For a quasi-1D LV coexistence system with a flat LV-interface, by integrating the stress difference between the diagonal stress components tangential and normal to the interface between the bulk positions of the liquid and vapor phases, the LV interfacial tension is obtained. We have extended Bakker's equation to flat solid-liquid (SL) and solid-vapor (SV) interfaces. Through a careful choice of the SL and SV interface positions, the microscopic interpretation of Young's equation was clarified as the force balance exerted on the fluid molecules in a finite region surrounding the contact line. In addition, the SL and SV interfacial tensions were calculated as the free energy per unit area based on the thermodynamic integration methods, where the solid-fluid (SF) work of adhesion was calculated by quasi-statically isolating the solid and fluid sandwiching a depletion layer by using a virtual wall interacting only with the fluid, or by gradually reducing the SF interaction strength. As a result, it was shown that the mechanically obtained SL and SV interfacial tensions and thermodynamically obtained works of adhesion agreed well for a Lennard-Jones (LJ) fluid on a simple crystal surface. Furthermore, we also showed that the apparent contact angle of a hemi-cylindrical droplet corresponded well with that predicted by Young's equation using the interfacial tensions or the work of adhesion. In this talk, these topics as well as recent results about line tension and LL interfaces will be introduced.

Shin-ichi Tsuda

Kyushu University tsudashin@mech.kyushu-u.ac.jp

A multi-scale study on hydrogen cavitating flow

Recently, an appropriate prediction technique of hydrogen cavitating flow has been required due to a rapid increase of the demand for designing turbomachinery such as high-speed rotating pumps using liquid hydrogen as an efficient transport method of the clean energy source. However, it is currently difficult due to few knowledge of the liquid-vapor phase change of hydrogen as well as the few experimental data. Particularly, we must understand the multi-scale structure of the phase change for developing an appropriate cavitation model implemented in CFD simulations because liquid hydrogen will contain few bubble nuclei different from water, and cavitation may start from a molecular scale like homogeneous bubble nucleation. In this study, we have tackled to construct a multi-scale CFD simulation method for hydrogen cavitating flows employing Multi-Process (MP) model as a cavitation model developed by our group, in which the main elementary processes of cavitation such as a spherical bubble expansion as a macroscopic scale and bubble inception or evaporation as a microscopic scale can be simultaneously incorporated. As an analysis for the former macroscopic scale, we conducted a bubble dynamics analysis using Rayleigh-Plesset equation for a single bubble motion coupled to Plesset-Zwick equation focusing on the thermal transfer in liquid hydrogen for a deeper understanding of the macroscopic behavior. Also, for the microscopic process of bubble inception or evaporation, some theoretical studies and path-integral Centroid Molecular Dynamics (CMD) simulations, in which the quantum nature special to liquid hydrogen can be included in the same framework as the classical mechanics, were conducted focusing on the two microscopic elementary processes. Finally, we are going to summarize both of the macroscopic and microscopic acknowledgment into the MP model applied in the turbulent cavitation CFD, i.e. Large Eddy Simulation (LES) analysis.

Peter Daivis

RMIT peter.daivis@rmit.edu.au

Can a mesoscopic model describe stick-slip flow?

Stick-slip flow is observed when the rheological properties of a lubricating fluid between two very closely spaced surfaces intermittently undergo a dramatic change. This phenomenon has been studied experimentally using the highly sophisticated surface force apparatus, and also by molecular dynamics simulations. Comparisons between experiment and simulation have been controversial. As the detail and realism of the molecular dynamics simulations has progressively improved, a better understanding of the subtlety of this effect has been achieved. However, this has also resulted in a loss of simplicity in the physical explanation for stick-slip flow. An alternative approach that may provide more insight is to construct a mesoscopic continuum model to describe stick-slip flow. While simple models that qualitatively reproduce the observed behaviour have been proposed before, little work has been done to test them quantitatively. In this presentation, I will describe our progress towards the goal of arriving at a quantitatively accurate and conceptually simple mesoscopic model of stick-slip flow with the capacity to incorporate the subtlety of the results obtained by experiment and molecular simulation.

Billy Todd

Swinburne University of Technology btodd@swin.edu.au

Interfacial Transport for Tribological Applications: Equilibrium and Nonequilibrium Molecular Dynamics Methods

In MD simulation there are two approaches to calculate transport properties of fluids, namely either equilibrium (EMD) or nonequilibrium (NEMD) methods. The former is limited to the linear response regime and provides a zero-field limiting value for a transport property. The latter is more general and can be used to compute transport properties at arbitrarily large fields which are typically orders of magnitude larger than those experimentally accessible.

We present developments made in both these branches of MD by our group and collaborators over recent years. An accurate and reliable EMD approach to compute the linear-regime friction coefficient and thermal (Kapitza) resistance for highly confined fluids is presented and compared to direct NEMD simulations. Comparisons are made to alternative linear response methods and various limitations are discussed.

Next, we demonstrate that nonlinear response theory in the form of the transient-time correlation function technique (TTCF) enables accurate calculations of transport properties under experimentally accessible strain rates. We compute the friction coefficient, slip velocity and shear pressure at laboratory values of strain rate for a simplistic confined atomic fluid and a realistic lubrication system consisting of squalane confined to surfactant-enabled iron oxide walls at strain rates between 10^5 and 10^8 s⁻¹. Our TTCF calculations make the former strain rate simulations possible, whereas we show it is impossible to obtain statistically significant measurements via direct NEMD simulations alone.

The potential of these new calculations is made more expansive by our recent publication [1] and associated public domain software, which interfaces with the LAMMPS software package to allow anyone to set up their own tribological systems and perform calculations at experimentally accessible strain rates.

References:

[1] L. Maffioli, et. al., Comput. Phys. Commun. 300, 109205 (2024).

Kazumichi Kobayashi

Hokkaido University kobakazu@eng.hokudai.ac.jp

Molecular fluid dynamics approach to boundary conditions at vapor-liquid interfaces for the Boltzmann equation

Heat and mass transport processes at the vapor-liquid interface are essentially nonequilibrium phenomena. Therefore, the Boltzmann equation is useful for analyzing such phenomena. The boundary conditions of the vapor-liquid interface for the Boltzmann equation include various coefficients such as the evaporation and condensation coefficients, which mean the evaporation and condensation probabilities of vapor molecules, and the accommodation coefficient, which defines the momentum transport at the interface. In this presentation, we report the results of obtaining the values of these coefficients using molecular dynamics and kinetic theory of gases.

Contributed Talk Abstracts

Davide Sarpa

University of Southampton d.sarpa@soton.ac.uk

Exploring Lubricant Chemistry: From Molecular Dynamics to Linear-scaling DFT

Lubricants are essential tools in enhancing efficiency and reducing machinery wear and tear. Their complexity often leads to a trial-and-error approach in development. Computational simulations offer a promising avenue to unravel the intricate chemistry involved, ultimately enabling the design of superior lubricants. In this study, we employ a spectrum of simulations, starting with molecular dynamics simulations of a bulk mixture of di(2-ethylhexyl) sebacate (DEHS) and di(2-ethylhexyl) adipate (DEHA) esters and of a confined hydrocarbon, 9,10-dimethyloctadecane, a significant component of the industrially important PAO2 lubricant. These simulations are conducted between Hematite [001] slabs, investigating various operational conditions using two distinct force fields, LOPLS-AA and ReaxFF. Subsequently, we delve into more precise yet computationally intensive quantum mechanical simulations to probe the interaction between Zinc dialkyldithiophosphates (ZDDP), a common class of lubricant additives, and a [001] Hematite surface. Our approach includes density functional methods including linear scaling DFT with ONETEP to explore phase space. Our primary objective is to gain insights into the chemical behavior of this complex mixture, with a particular focus on the impact of confinement on lubricant rheological properties and the degradation patterns of ZDDP. Our findings reveal good agreement between L-OPLS-AA molecular dynamics simulations and experimental data for both bulk and confined systems. In contrast, ReaxFF tends to overestimate viscosities but provides superior descriptions of Hematite structure and density. We posit that the computational methods and workflow outlined here hold promise for simulating combinations of lubricants, additives, and surfaces, shedding light on the intricate microscopic behavior of these technologically important yet poorly understood challenging systems.

Laurent Joly

Institut Lumière Matière / Université Lyon 1 laurent.joly@univ-lyon1.fr

Molecular views on thermo-osmotic transport

Thermo-osmotic flows are generated at interfaces by thermal gradients. They represent powerful tools to manipulate liquids in micro and nanofluidic systems, and can play a key role in living systems, in sustainable energies, or in water treatment and desalination processes. During this talk I will illustrate with recent work how molecular dynamics simulations challenge the standard description of thermo-osmotic flows. I will in particular discuss the critical role of interfacial hydrodynamics, the usually neglected role of water, and the complex effect of surface charge. These theoretical results open many perspectives for the efficient harvesting of waste heat.

Samy Merabia

CNRS and Université Lyon 1 samy.merabia@univ-lyon1.fr

Thermal transport at solid-liquid interfaces: colloidal metallic nanoparticles and nanostructured gold-water interfaces coated with graphene

In this contribution, we will discuss two examples of thermal transport at solid-liquid interfaces. The first example concerns heat transfer from metallic nanoparticles to their aqueous environments. We show using molecular dynamics simulations that the thermal boundary (Kapitza) conductance of metallic nanoparticles in water increases with the nanoparticle curvature [1]. This behavior is interpreted based on a generalized acoustic mismatch model. We also report a significant (300%) increase of the conductance for charged nanoparticles immersed in an electrolyte. We interpret the increase of the Kapitza conductance as a combined result of the shift of the water density distribution toward the charged nanoparticle and an accumulation of the counterions around the nanoparticle surface [2]. Finally, we discuss the fate of metallic nanoparticles heated to very high temperatures and show how the onset of water cavitation depends on the wetting properties of the nanoparticle [3].

The second example to be discussed concerns heat transfer at nanostructured gold-water interfaces. We present an innovative solution to increase the corresponding interfacial resistance: we insert graphene layers between the nanostructure and water [4]. The presence of graphene permits to stabilize a so-called Fakir state between water and the gold nanostructure thus minimizing the contact between them. We discuss also the effect of intercalating few graphene layers on the overall thermal conductance [4].

N.B : work in collaboration with C. Herrero, O. Gutiérrez, R. Rabani, A. Rajabpour, L. Joly, R. Santamaria

References:

[1] O. Gutiérrez-Varela, S. Merabia and R. Santamaria, J. Chem. Phys. 157 (2022) 084702

[2] O. Gutiérrez-Varela, J. Lombard, T. Biben, R. Santamaria and S. Merabia, Langmuir 39 (2023), 18263-18275

[3] R Rabani, MH Saidi, A Rajabpour, L Joly, S Merabia, Langmuir 39 (2023), 15222-15230

[4] C. Herrero, L. Joly and S. Merabia, Appl. Phys. Lett. 120 (2022) 171620

Takuya Kuwahara

Osaka Metropolitan University kuwa@omu.ac.jp

In situ synthesis of superlubric interfaces via mechanochemistry: learning molecular mechanisms from computer simulations

Boundary lubrication is a regime of lubrication in which the friction between two materials in relative motion is determined by properties of the surfaces and interactions between lubricants and surfaces. During running-in, surfaces undergo severe plastic deformation and chemical reactions with lubricant molecules, resulting in the formation of tribolayers on top of asperities and thus establishment of superlubric interfaces. These processes are dominated by atomic-scale phenomena but they are not accessible experimentally, which has hindered understanding of the underlying mechanisms. Here we employ computer simulations to gain the atomic-scale insights into the in situ synthesis of superlubric nanostructures and design principles for controlling interfacial phenomena and chemical structures. An example is boundary lubrication of tetrahedral amorphous carbon with organic friction modifiers such as oleic acid and glycerol (Kuwahara et al., Nat. Commun. 10, 151, 2019). Decomposition of lubricants is driven by the normal pressure and shear stress, producing chemical fragments which are able to passivate surface dangling bonds of carbon atoms. The decomposition rates of lubricants are dominated by the number of reactive sites in the lubricants. Multiple reactive centers are necessary to make chemical bonds bridging across the interface. This is the case for oleic acid but not for stearic acid. Another example is in situ synthesis of graphene nitride on a ceramic surface lubricated with glycerol. The low-friction carbon nanolayer can form via mechanochemical decomposition of glycerol on the non-carbonaceous surface. As a result, we paved the way for the in situ formation of superlubric carbon nanostructures on both carbon and non-carbon surfaces by utilizing interfacial mechanochemistry.

Takeshi Omori

Osaka Metropolitan University t.omori@omu.ac.jp

Measuring dynamic contact angles by computational fluid dynamics and molecular dynamics

The prediction of dynamic wetting is of significant practical interest: it plays a vital role in the design of many industrial processes and devices in different fields. It is also scientifically interesting because the phenomena are governed by multi-scale physics - molecular scale physics near the interfaces and continuum mechanics in the bulk – and the construction of a model to cover the whole system is challenging. In this talk, the application of the continuum mechanics to the molecular scale is first discussed, and the scale dependence of dynamic contact angles simulated both by computational fluid dynamics and molecular dynamics are presented to give ideas how to interpret experimentally obtained dynamic contact angles.

Gota Kikugawa

Tohoku University kikugawa@tohoku.ac.jp

Molecular-scale picture on heat transfer characteristics of organic interfaces and polymeric materials

Recently, heat conduction through the organic materials draws a great attention due to the capability of controlling thermal conductance by molecular chain alignment or molecular organization. Therefore, soft matters comprised of organic molecules and polymeric materials are promising candidates for heat transfer materials applied particularly to nanoscale devices. In our study, we performed molecular dynamics (MD) simulations on heat conduction in two situations of organic substances: interface modified by an organic self-assembled monolayer (SAM) and crosslinked polymeric materials in a bulk state. To analyze thermal energy transfer in detail, we performed the decomposition of energy transfer modes in an interaction-based description from the molecular dynamics perspective, i.e., total heat flux was decomposed into the energy exchange by molecular interactions like covalent-bond interactions and intermolecular interactions. As for the SAM-solvent interface systems, we showed that typical alkanethiolate SAMs and more hydrophilic SAMs having different terminal groups modified on the solid substrate enable to increase (and decrease) the overall thermal boundary conductance (TBC). Furthermore, the detailed energy carriers inside the SAM were examined by using energy decomposition techniques. In the context of energy transfer inside polymer chains, the variation of thermal conductivity with changing internal molecular-scale structure in the amorphous crosslinked polymers was investigated. Here we examined the heat conduction in epoxy thermosetting polymers, for which the crosslinking process was realized by the MD simulations incorporated with chemical kinetic reaction model. Thermal conductivity was compared between different kinds of epoxy materials which have the distinct internal crosslinking structure. In addition, we correlated the thermal conductivity with the simple index representing internal crosslinking structure.

Hiroki Kusudo

Tohoku University kusudo@tohoku.ac.jp

Heat transport phenomenon during dynamic wetting: insight from molecular dynamics

A number of theoretical simulations and experimental studies about the dynamic contact line (DCL) have been conducted; however, the governing principle of the CL motion still remains unclear due to the lack of the detailed information around the DCL. In this study, we give a new insight into the dynamic wetting phenomenon from the viewpoint of the nanoscale heat transport induced in the vicinity of the dynamic contact lines. We employed a NEMD simulation of a quasi-2D Couette-type flow system of a Lennard-Jones liquid confined between two sliding solid walls, which induced the two different DCLs. We found that the difference between the advancing and receding CLs are distinct not only in the contact angle but also in the temperature; the advancing and receding CLs are heating and cooling, respectively. Based on the energy conservation law of continuum mechanics, theoretically, the heat production and absorption originate not only from the stress work term, which corresponds to viscous dissipation in the bulk, but also from the internal energy change along the pathline, and we found that the heat production and absorption around the DCLs were induced mainly by the latter. In the Lagrangian description, the fluid in the vicinity of the DCL changes its interface by moving among the solid-liquid, solid-vapor and liquid-vapor interfaces, which induces the temperature rise/drop at the DCLs in same mechanism as the latent heat of phase change. This heat transport phenomenon, induced by the interface change along the pathline, is not observed only in the present system but also in the system with piston pushing the liquid confined within the nanochannel, i.e., the Poiseuille-flow system with DCLs. While the advancing CL is heating as well as Couette-type flow system with DCLs, the liquid-vapor interface is cooling due to the two pairs of line-symmetrical vortices in liquid, which induce the change of the fluid from the liquid phase to the liquid-vapor interface.

Donatas Surblys

Tohoku University donatas@tohoku.ac.jp

Heat Transfer at Solid-Liquid Interfaces and beyond via Molecular Dynamics: Various Insights

Due to recent advances in semiconductor technology, the heat dissipation of various electronic devices has become an engineering challenge which needs to be tackled in order to avoid malfunctions and shortened component lifetimes. A common thermal management solution is to have thermal interface materials (TIMs) fill the gaps at the cooled component and the heat sink contact area, increasing the heat transfer efficiency. As the electric component size decreases, the thermal resistance between the components and TIMs themselves becomes a significant contributor to the overall thermal resistance, and surface treatments that reduce such interfacial thermal resistance are of great interest. In this presentation, I will go over various work done by our group. There is a wide variety of ways to change the interaction between the component and TIM at the interface. We investigated several such cases to elucidate fundamental heat transfer mechanisms, specifically: effect of crystal lattice orientation on ultra-thin films, effect of surface roughness, small and large surfactant molecules and self-assembled and highly-oriented molecule layers. In addition, to research on topics related to heat transfer, analysis methods are also developed alongside, such as robust estimation of heat flux in complex systems, evaluating of work of adhesion and harmonic chain modeling of solid-liquid interfacial transport. These methods have provided new insight into heat transfer mechanism, paving a way to more efficient thermal management solutions.

Muhammad Rizwanur Rahman

Imperial College London m.rahman20@imperial.ac.uk

Thin Films: Formation, Frustration and Fragmentation

The mechanism governing the rupture dynamics of thin liquid films, from formation to fragmentation, is explored through non-equilibrium molecular dynamics simulations. Our study reveals that, despite the diversity in rupture pathways contingent upon film stability, these processes share a common microscopic origin, and exhibit seamless evolution from one to the other. A crucial finding of this study is the identification of a transient deterministic 'memory window' embedded within the stochastic progression leading to a rupture event. The existence of this brief yet finite window challenges the longstanding perception of such phenomena as inherently random, suggesting a more complex interplay of determinism within the apparent randomness. Following the onset of rupture, our detailed examination of the propagation dynamics of rupture sites assesses the classical Taylor-Culick (TC) theory, specially in the context of nanoscale phenomena. By resolving the surface forces and curvature effects at the molecular level, we successfully bridge the divide between the continuum scale TC theory and atomic-scale observations. This reconciliation clarifies the applicability and constraints of the TC theory at the nanoscale, and provides insight on thin film dynamics across different scales.

Sritay Mistry

Brunel University sritay.mistry@brunel.ac.uk

Hydrogen nanobubbles in ammonia

Addressing climate change has led to a global shift towards green energy, with hydrogen emerging as "the" promising green fuel. Despite its potential, hydrogen presents significant challenges in storage and transport due to its low energy density in its readily available gaseous form. A novel approach to mitigate these issues involves blending hydrogen in the form of nanobubbles with liquid ammonia, which is another prospective green fuel. Adding hydrogen in the form of nanobubbles, as opposed to direct dissolution, would theoretically allow significantly more gas in the fuel blend. However, there is currently no knowledge on whether hydrogen nanobubbles can be stabilized in liquid ammonia. This research specifically investigates the stability of hydrogen nanobubbles within liquid ammonia, using the molecular dynamics (MD) simulation method and complementing it with numerical simulations based on the Epstein-Plesset equations. These simulations study various bubble sizes and concentrations of dissolved gas to determine the conditions for obtaining stable hydrogen nanobubbles. Early findings are promising, indicating the possibility of stable nanobubbles at high dissolved gas or bubble concentrations, establishing at least one route to achieving stable bubbles. The research points towards a potential method for storing and compressing hydrogen without the need for heavy-duty pressurized containers. Should these hydrogen nanobubbles prove to be a stable method for blending with ammonia, it could mark a significant step forward in overcoming the current limitations of hydrogen and ammonia fuels.

Ikuya Kinefuchi

The University of Tokyo kine@fel.t.u-tokyo.ac.jp

Non-Markovian dissipative particle dynamics

In the present study, we derive the equation of motion for non-Markovian dissipative particle dynamics (NMDPD) by introducing the memory effects on the time evolution of the system [Y. Yoshimoto et al., Phys. Rev. E 88, 043305 (2013)]. Our formulation is based on the generalized Langevin equation, which describes the motions of the centers of mass of clusters comprising microscopic particles. The mean, friction, and fluctuating forces in the NMDPD model are directly constructed from an underlying MD system without any scaling procedure. To validate our formulation, we construct NMDPD models from high-density Lennard-Jones systems, in which the typical time scales of the coarse-grained particle motions and the fluctuating forces are not fully separable. The NMDPD models reproduce the temperatures, diffusion coefficients, and viscosities of the corresponding MD systems more accurately than the DPD models based on a Markovian approximation.

Patrick Sullivan

Durham University Patrick.J.Sullivan@durham.ac.uk

Nanoscale Surface Effects on Vapour Bubble Nucleation

It is widely accepted that vapour bubbles form preferentially at imperfections on solid surfaces where the free energy barrier to nucleation is lower. This hypothesis is supported by classical nucleation theory (CNT), which predicts increased nucleation rates at locations with lower wettability or in surface cavities, where gas can become entrapped forming so called "active sites" on the surface. The existing models for the formation of these active sites focus on the geometry of the cavity and the inability of the fluid to displace a non-condensable entrapped gas from the surface, which is linked to the macroscale contact angle.

Using molecular dynamics simulations, we show how the presence of surface roughness can create active sites for nucleation without the requirement of trapping a secondary fluid. This is achieved through the spontaneous dewetting of surface cavities as temperature is increased. We demonstrate that these dewetted cavities have the potential to reduce the temperature at which nucleation occurs on the surface, but that behaviour does not hold in both extremes of wettability. For lyophobic surfaces, where the nucleation barrier is low, it is shown that the cavities must be sufficiently large to offer a reduction in nucleation temperature. For lyophilic surfaces, the formation of a non-evaporating layer of adsorbed molecules causes the contact line at the cavity mouth to de-pin. This allows the cavity to rewet, and there is subsequently no decrease in nucleation temperature compared to a smooth surface.

Dmitry Nerukh

Aston University D.Nerukh@aston.ac.uk

Hybridising molecular dynamics with hydrodynamics

We propose a particle-based methodology that hybridises Newtonian dynamics of atoms at microscale with Landau-Lifshitz Fluctuating Hydrodynamics of hydrodynamic fields at macroscale, valid at all intermediate scales with correct limiting cases. The methodology uses linear interpolation of hydrodynamic fields with stochastic correction matching the fluctuation parameters at corresponding scales. The equations of motion of the hybrid particles are derived from the principle of least action and Gauss's principle of least constraints.

We compare our results with our previously developed hybrid MD/LLFH methodology based on fundamentally different approach. We also present the application of our methodology to Couette flow of nano-confined water and compare our hybrid simulations with all-atom NEMD results. Physical characteristics of the system as well as the computational efficiency of the algorithm are calculated and analysed.

Antonio Buffo

Politecnico di Torino, Italy antonio.buffo@polito.it

Coupling Dissipative Particle Dynamics and Computational Fluid Dynamics for an industrial mixing process

Dissipative Particle Dynamics (DPD) has emerged as an easy and powerful Coarse Graining (CG) technique for understanding the transport properties of complex fluids. DPD operates by simulating particles as interacting entities subject to conservative, dissipative, and random forces, capturing hydrodynamic interactions and thermal fluctuations. This approach allows for the investigation of complex fluid systems, including colloidal suspensions, polymer solutions, and biomolecular assemblies, under various conditions. One significant advantage of DPD lies in its computational efficiency, enabling the simulation of large systems over long time scales compared to Molecular Dynamics (MD). This capability is particularly valuable for studying transport phenomena of complex fluids, such as viscosity, which are crucial for understanding material behavior in industrial processes.

The rheology of these fluids poses a significant challenge due to their non-Newtonian behavior, which is influenced by the local composition. To address this challenge, multiscale approaches have been proposed to integrate rheological insights from non-equilibrium Dissipative Particle Dynamics (DPD) with Computational Fluid Dynamics (CFD) simulations. In this study, we explore an approach utilizing Gaussian Process Regression (GPR), a machine learning-based regression tool, to study an industrial mixing process carried out in a static mixer. Specifically, we investigate a system consisting of a high-concentration solution of a surfactant in water under laminar fluid dynamics conditions. Our findings indicate that the mixture exhibits the expected shear-thinning behavior and demonstrates viscosity values that align well with rheological experiments. While our results demonstrate the feasibility of the coupling approach, further research on DPD is needed to enhance the accuracy and predictive capability of the methodology.

Zhaoran Zhu

Imperial College London zhaoran.zhu22@imperial.ac.uk

Effect of Electric Fields on the Decomposition of Nanoconfined Phosphate Esters

Phosphate esters are important lubricant additives that decompose on metal surfaces and form protective polyphosphate films. For many applications, such as electric vehicles and wind turbines, an understanding of the molecular decomposition of lubricant additives in the presence of electric fields is urgently required. Experimental investigations have yielded contradictory results, with some suggesting that electric fields improve tribological performance, while others report the opposite effect. Here, we use non-equilibrium molecular dynamics (NEMD) simulations to study the decomposition of tri-n-butyl phosphate (TNBP) molecules nanoconfined between ferrous surfaces (iron and iron oxide) under electrostatic fields.

Carlos Corral-Casas

Imperial College London
c.corral-casas@imperial.ac.uk

Velocity Slip in Fluids under Molecular Confinement

The lack of understanding of fluid velocity slip in channels of molecular length scales hinders the development of potentially disruptive technologies (e.g., membranes for enhanced filtration), whose behaviour is influenced by the mechanisms at the fluid-solid interface. In this work, we address two key aspects that remain elusive in confined fluid flows despite extensive research. First, we study the conditions for applying the Navier-Stokes equations with slip boundary conditions, to clarify whether the Knudsen number criterion (introduced for the rarefied gas at the microscale) holds for arbitrary densities and tighter geometries. Second, we assess the dependence of velocity slip on the fluid nominal density, confinement, wall roughness, and curvature, to resolve the discrepancies reported in the literature.

To fill these gaps, we have considered the time evolution of a hard-sphere fluid interacting with walls via the Maxwell scattering kernel. We observed that the slip criterion derived for rarefied conditions also holds for dense gases, as long as the fluid is confined within channels larger than about ten molecular diameters. Moreover, it is found that the velocity slip depends linearly on the peak density. This relationship can be attributed to the fact that the latter directly correlates with the fluid-wall collision frequency, which in turn determines the amount of tangential momentum transferred from the fluid to the walls. This also explains why the velocity slip scales with the Smoluchowski prefactor when the wall roughness is varied by changing the accommodation coefficient. This result is not an artifact of the hard-sphere model, as we also found it in fluids described by Lennard-Jones potentials confined between physical walls.

To sum up, this study provides crucial insights into the complexities that dictate fluid velocity slip in molecularly confined channels, paving the way for a more comprehensive understanding of such phenomena.

Alex Lukyanov

University of Reading a.lukyanov@reading.ac.uk

Non-locality of the contact line in dynamic wetting phenomena - a MD study

The notion of the contact line is fundamental to capillary science, where in a large category of wetting phenomena, it was always regarded as a one-dimensional object involving only microscopic length scales. This prevailing opinion had a strong impact and repercussions on the developing theories and methodologies used to interpret experimental data. It is hypothesised that this is not the case under certain conditions leading to non-local effects and requiring the development of a modified force balance at the contact line.

Poster Abstracts

Shukai Cheng

Institute of Fluid Science, Tohoku University cheng.shukai.p8@dc.tohoku.ac.jp

Study on solid-liquid phase change properties of sugar alcohols via molecular dynamics

Sugar alcohol phase change materials (PCMs) have gained considerable attention in recent years owing to their higher thermal conductivity and larger latent heat when compared to traditional paraffin materials. However, comparative analytical studies of sugar alcohol PCMs remain inadequate. In this study, the local equilibrium non-equilibrium molecular dynamics (LE-NEMD) and equilibrium molecular dynamics (EMD) simulations were employed to investigate the melting process and fusion latent heat of sugar alcohols (glycerol, erythritol, arabinitol, and mannitol). The OPLS-AA force field was used, as it was able to recreate the experimental melting point and latent heat trends. On the other hand, it was observed that melting temperatures varied under different directions of one-dimensional heat flow in glycerol, arabinitol, and mannitol. It was found that the strength of intermolecular interactions within the different molecular layers had a proportional correlation with the anisotropic melting tendencies, which can be more intuitively reflected in the difference in the number of hydrogen bonds within different molecular layers. In addition, the decomposition of the latent heat reveals that the largest contribution is from van der Waals and Coulombic energies, for which the interaction energy between hydroxyl groups accounts for a large portion of it. It was confirmed by hydrogen bond analysis that latent heat is largely influenced by the breakage of hydrogen bonds during the phase transition from solid to liquid and that the differences in the hydrogen bonding lifetimes of different sugar alcohols during the melting process may play a role in determining latent heat. Erythritol and mannitol with stable crystal structure and even number of carbon atoms tend to have higher latent heat and were considered as better candidates for PCMs. These results are hoped to result in better optimization of the design and performance evaluation of future sugar alcohol PCMs.

Matthew Val Meyers

University of Manchester matthew.meyers@postgrad.manchester.ac.uk

Data Driven Models for Accurate Prediction of Nucleate Boiling on Oxidised Surfaces

Nuclear fuel cladding surfaces have oxidised from the harsh conditions that heat transfer surfaces are exposed to over their lifetime. The impact of this change to the material, in the context of boiling and heat transfer, is not well understood especially at the variety of scales these physical processes occur at. This research aims to develop a proof of concept for a multi-scale, multi-fidelity modelling framework for better prediction of nucleate boiling and critical heat flux (CHF) on heat transfer surfaces with complex morphology within nuclear reactors. The research project ultimately aims to contribute to the development of the modelling capabilities needed to understand the small-scale dynamics due to different features involved with corrosion. The first stage of the research involves using molecular dynamics to carry out initial numerical studies of heterogenous nucleation of liquid argon on smooth and rough platinum surfaces.

Hiroki Imai

The University of Tokyo imai@fel.t.u-tokyo.ac.jp

Analysis of the non-equilibrium gas flows in the Knudsen layer above porous membranes

Evaporation from porous membranes is important for understanding both natural phenomena and industrial applications, such as transpiration, micro pumps, and cooling devices. With the ongoing trend of integration, power semiconductor devices are emitting heat flux exceeding 1 kW/cm². To address this challenge, cooling devices utilizing evaporation from porous membranes attract considerable attention, necessitating an understanding of the pore-scale effect on effective mass flux. Initially, we focus on evaporation from two-dimensional porous surfaces and clarify the pore-scale effect on mass flux. For small-pore scale, the surface non-uniformity does not affect the overall flow structure, and flows from two-dimensional porous surfaces can be regarded as the simple superposition of flows from each pore. It leads to that the flow from porous surfaces can be expressed by the flow from a uniform liquid surface with the accommodation coefficients set to the same value as the porosity. For large-pore scales, the gas flow structure just above the liquid surface is similar to evaporation from a uniform liquid surface. By considering a control volume and solving conservation laws, the effective mass flux for the large-pore limit is obtained. Next, in the case of evaporation from porous array membranes, a three-dimensional analysis of non-equilibrium gas flows in the Knudsen layer considering the heat transfer in liquid and solid phases becomes imperative. We propose a simulation method that combines a continuum-based approach that connects the solid- and liquid-phase analyses and the gas-phase analysis by considering mass and energy conservation at the porous membrane surface. Using the coupled-simulation technique, we thoroughly investigate how convection in porous membranes and the pore scale impact on the evaporative mass flux. We clarify the pressure dependence of the mass flux for various pore diameters and construct simple models to predict the evaporation mass flux.

Sritay Mistry

Brunel University sritay.mistry@brunel.ac.uk

Small nanobubbles through high frequency vibrations

Nano- and micro-bubbles have diverse applications in environmental, industrial, and medical fields, such as water treatment, plant growth, gas storage, medical imaging, and surface cleaning. Smaller bubbles are particularly effective in these applications due to increased zeta potential, Laplace pressure and surface-area-to-volume ratio, enhancing their performance in various applications. They can resist buoyancy effects, penetrate biofilms, support aerobic bacteria in anaerobic conditions, facilitate organic matter hydrolysis and diffuse across barrier tissues, among others.

Current technologies, however, face limitations in producing and controlling the size of nanobubbles, particularly those smaller than 50 nm. To overcome these limitations, we propose a novel method for generating nanobubbles using ultrahigh frequency vibrations on nanotube membranes. This technique allows for the creation of uniformly sized nanobubbles by controlling the frequency, amplitude, and duration of vibrations, as well as the pressure in gas and liquid reservoirs.

Our initial studies conducted using the molecular dynamics (MD) simulation method show that applying vibrations to a nanotube membrane aids in nucleation and growth of a stable nanobubble. The vibrational energy helps gas molecules overcome the flow resistance offered by the membrane pore, enabling a high gas flux which leads to the creation and growth of a nanobubble, instead of simply dissolving in the liquid. Adjusting the vibrational parameters allows for precise control over bubble size. This new method could enable the generation of smaller and consistently sized nanobubbles, allowing for enhanced precision in applications where bubble size and consistency are critical.

Pengxu Chen

The University of Edinburgh pengxu.chen@ed.ac.uk

Icequakes: Vibrating Supercooled Water at the Nanoscale

Controlling ice nucleation plays an essential role in various engineering applications, such as food freezing, cryopreservation and developing anti-icing coatings. In recent years, the use of high-frequency surface vibrations has emerged as a promising anti-icing/de-icing technology. However, the effects of such vibrations on nanoscale ice nucleation (i.e. formation of critical ice clusters that precede bulk ice formation) remain poorly-understood. Using molecular dynamics (MD) simulation, this study explores how surface vibrations affect nanoscale ice nucleation from supercooled water. We demonstrate that ice nucleation can be either hindered or enhanced by surface vibrations, depending on setup and vibrational parameters. We observe that, in water nano-films, GHz-order surface vibrations inhibit the formation of large pre-critical ice-like clusters, reducing the ice nucleation probability. Conversely, in confined nano-pores, MHz-order surface vibrations are shown to trigger regions of negative pressure, which enhances the probability of ice nucleation. This study advances our understanding of the interplay between surface vibration dynamics and ice nucleation, which can enable future anti-icing and freezing technologies.

Saikat Datta

University of Edinburgh Saikat.Datta@ed.ac.uk

Impact of Surface Wettability on Nanopore Evaporation

The decrease in transistor size has continually enabled higher performance electronic devices with increased transistor density. Thermal management of integrated circuits (ICs) has increasingly become the main factor preventing performance improvements. To address this issue, there has been growing interest in employing two-phase cooling methods that utilize the latent heat of vaporization of the working fluid, effectively extracting more heat from ICs. Passive evaporation-based cooling devices, such as vapour chambers, offer an alternative approach by leveraging thin-film evaporation directly through porous wicking structures. Recent experimental advancements have achieved the fabrication of few-nanometer-thick pores, demonstrating ultra-high evaporation fluxes that surpass theoretical predictions. However, the underlying physics of "nanopore" evaporation is not fully comprehended due to the extremely small scales involved.

In this study, we conduct non-equilibrium molecular dynamics simulations to investigate the evaporation of water from metal nanopores, and show that evaporative mass flux primarily originates from the near-wall region due to the formation of the adsorbed layer on the inner pore-wall. This contrasts with the uniform mass flux seen in larger pores. Furthermore, we observe that heat flux initially decreases when wettability increases, but then increases with the highest wettabilities. This results from the interplay between the work of adhesion, thermal kinetic energy, and potential energy from bulk molecules. Low wettability causes a low momentum transfer rate between solid and liquid molecules but allows for easy escape of the molecules from the pore wall. On the other hand, high wettability ensures a high momentum transfer rate, but molecules require higher energy to escape. The insights gained provide a valuable understanding of thin-film evaporation in nanopores, with potential applications in the design of thermal management systems.

Hamidreza Hassanloo

Brunel University London Hamidreza.Hassanloo@brunel.ac.uk

Nanobubbles Formation and Their Impacts on the Inherent Properties of Graphene-Reinforced Polar and Alcoholic Host Liquids: A Molecular Dynamics Investigation

Significant efforts have been made to replace conventional thermal fluids with those that have enhanced thermophysical properties, where nanoscale phenomena, particularly the incorporation of nanoparticles such as graphene, play a crucial role. Graphene's outstanding properties make it a promising candidate for altering and improving the inherent properties of working fluids. The existence of dissolved gases, especially in industrial processes like electrochemical reactions, markedly affects fluid behavior and thermophysical properties, potentially leading to the formation of nanobubbles, which further influence the inherent properties of host liquids. This investigation utilizes molecular dynamics simulations to explore the formation, behavior, and effects of nanobubbles on the intrinsic properties of graphene-water and graphene-methanol nanofluids.

Useful Information

Talks will be held at the Royal School of Mines (RSM) Sutton Lecture Theatre - 131 on the 1st floor.

Coffee breaks and lunches will be offered in reception rooms 301D and 301E on the 3rd floor.

The poster session will be held on Thursday evening in room 301D

Wi-Fi will be available during the conference through eduroam, please contact the organisers if you need an alternative solution

The **conference dinner** will be held at the **Ognisko restaurant** (https://www.ogniskorestaurant.co.uk/), at 55 Exhibition Rd, London SW7 2PG at 19:30 on 13th June.

How to get to conference venue



The RSM building (above) is within the South Kensington Campus of Imperial College London, London SW7 2AZ (see red arrow on next page). The Imperial campus is close to the **South Kensington** or **Gloucester Road** tube stations on District and Piccadilly Lines.

