



Introduction about Duke Kunshan University

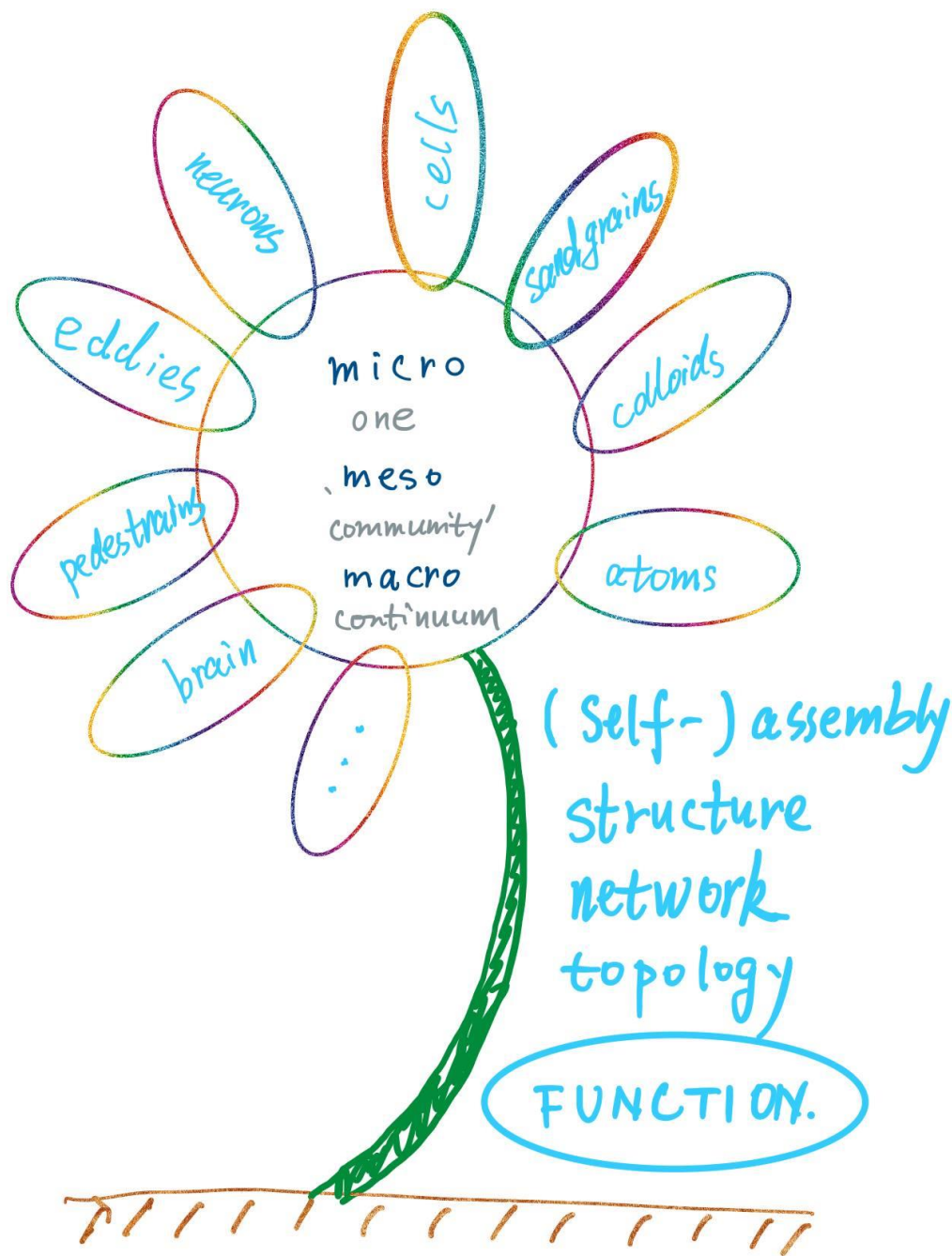
Duke Kunshan is a world-class liberal arts university based in Kunshan, China, that offers a range of high quality, innovative academic programs for students from around the world. It was established in September 2013 as a U.S.-China partnership between Duke University and Wuhan University.

Duke Kunshan welcomed its first students in August 2014. The university began by offering Duke graduate degrees as well as a Global Learning Semester program for undergraduate students from Duke and top-tier Chinese and international universities.

In August 2018, the university welcomed its first undergraduate degree students. The four-year bachelor's degree program follows the liberal arts and sciences tradition, with emphasis on critical thinking, creativity, collaboration and self-exploration.

Our vibrant, high-tech campus covers 200 acres in Kunshan's Yangcheng Lake Science and Technology Park. Take a virtual tour to see our advanced classrooms, conference facilities and library, as well as student and faculty housing, and multiple dining and recreational areas. We also have multipurpose meeting spaces, break rooms and study rooms that allow students to work individually or in groups to review course materials and complete assignments.

The city of Kunshan, in Jiangsu province, is one of China's fastest-growing economies and is a hub for high-tech research and manufacturing. The city is surrounded by picturesque forests and water towns, and is also connected by high-speed rail and subway to Shanghai and Suzhou, two of China's most dynamic cities.



Organizers

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Campus map



2020 DKU Soft Matter Symposium

Symposium Agenda

Venue: IB2050(Zoom Meeting ID:715 337 7467)

Kunshan, Jiangsu Province, China

Time: Dec 17, 2020 to Dec 20, 2020

Sponsors

Zu Chongzhi Center for Mathematics and Computational Sciences

Division of Nature and Applied Science

DKU Association for Science and Technology

Conference Agenda

* Displayed in Beijing time& Eastern Standard Time

Day 1-Thursday, 17 December 2020

Venue: IB2050(Zoom Meeting ID:715 337 7467)

Chair: Shixin Xu

UTC+8	EST
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15:00	2:00*	Reception and Registration(Lobby, CC Building)
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17:30	4:30	Welcome dinner
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20:00	7:00	Masao Doi	The Onsager principle in polymer dynamics
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*: It refers to Dec.17 (EST Time)

Day 2-Friday, 18 December 2020

* Displayed in Beijing time& Eastern Standard Time

Venue: IB2050(Zoom Meeting ID:715 337 7467)

Chair: Kai Huang (Morning Session)+Kai Zhang(Afternoon Session)+ Myung-Joong Hwang (Evening Session)

UTC+8	EST
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8:15	19:15*	Opening speech	1.Welcome speech by Kai Huang, Division chair, Duke Kunshan University
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			2. Welcome speech by Xin Li, Associate Dean for Research, Duke Kunshan University
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8:30	19:30	Patrick Charbonneau	Toward a microscopic understanding of the dynamics of simple glass-forming liquids
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9:30	20:30	Ding Ma	Quantifying the Eddy-Jet Feedback Strength of the Atmospheric Annular Modes Using a Linear Response Function Approach
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10:00	21:00	<i>Mark Shattuck</i>	The City College of New York Deformable Particles
10:30	21:30	Coffee Break	
10:45	21:45	<i>Habib Rahbari</i>	Active microrheology of a bulk metallic glass
11:15	22:15	<i>Ning Xu</i>	Connecting glass forming ability of binary mixtures to melting temperatures
12:00	23:00	Lunch Break	
13:30	0:30**	<i>Ho-Kei Chan</i>	Confinement-induced Columnar Crystals: A Route to New Architecture in the Scientific World
14:00	1:00	<i>Duanduan Wan</i>	Entropy induced photonic band gaps in self-assembled colloidal crystals
14:30	1:30	Coffee Break	
14:45	1:45	<i>Litang Yan</i>	Transport of nanoscale objects on cell membrane: from passive to active particles
15:15	2:15	<i>Joshua Dijksman</i>	Twisting and turning particles
15:45	2:45	<i>Meiying Hou</i>	Experimental evidence of pressure-sensitive intrusion rheology in grains
17:30	4:30	Group Dinner-Executive Dining Room	
20:00	7:00	<i>Stefan Luding</i>	From particle simulations towards a universal continuum theory and applications
21:00	8:00	<i>Matthias Schröter</i>	Different ways of getting into contact in the granular world
21:30	8:30	<i>Matthias Sperl</i>	Dynamics in Granular Matter

*: It refers to Dec.17 (EST Time)

**: It refers to Dec.18(EST Time)

Day 3-Saturday, 19 December 2020

* Displayed in Beijing time& Eastern Standard Time

Venue:IB2050(Zoom Meeting ID:715 337 7467)

Chair: Sze Chai Kwok(Morning Session)+Chang Chung(Afternoon Session)+ Kai Huang(Evening Session)

UTC+8 EST

8:30	19:30*	Brian Salzberg	Extrinsic and Intrinsic Optical Changes in Mammalian Nerve Terminals and a Mechanical Spike
9:30	20:30	<i>John Weisel</i>	Multiscale studies of blood clotting
10:00	21:00	<i>Zhiliang Xu</i>	Mathematical and computational Modeling Blood Clot Formation
10:30	21:30	Coffee Break	
10:45	21:45	<i>Fredric Cohen</i>	Cells maintain their cholesterol content by quickly adjusting the cholesterol chemical potential of their plasma membranes
11:15	22:45	<i>Lei Zhang</i>	Construction of Solution Landscape on the energy landscape
12:00	23:00	Lunch Break	
13:30	0:30**	<i>Yuliang Jin</i>	Machine learning a Gardner transition
14:00	1:00	<i>Xinpeng Xu</i>	Onsager's variational principle in active soft matter
14:30	1:30	Coffee Break	
14:45	1:45	<i>Sze Chai Kwok</i>	Window into cognition: bridging electrophysiology, neuroimaging and neuromodulation
15:15	2:15	<i>Zheng Wang</i>	The pursuit of MRI-based diagnostic and predictive biomarkers in neuropsychiatric disorders
15:45	2:45	<i>Yao Li</i>	Multimodal Brain Imaging from Structure, Function to Metabolism
16:30	4:10	Group Picture	
17:00	4:00	Group Dinner	
20:00	7:00	Rafi Blumenfeld	Structural evolution of dense granular systems: Theory and non-equilibrium detailed balance
21:00	8:00	<i>Raúl Cruz Hidalgo</i>	On the rheological response of nonspherical granular flows
21:30	8:30	<i>Iñaki Echeverría</i>	Estimating density limits for walking pedestrians keeping a safe interpersonal distancing

*: It refers to Dec.18 (EST Time)

**: It refers to Dec.19(EST Time)

Day 4-Sunday, 20 December 2020

* Displayed in Beijing time& Eastern Standard Time

Venue:IB2050(Zoom Meeting ID:715 337 7467)

Chair: Kai Zhang(Morning Session)

UTC+8	EST		
8:30	19:30*	Corey O'Hern	Dense Packing in Protein Cores
9:30	20:30	<i>Weiqing Ren</i>	Interface Profile Near the contact line in electro-wetting on dielectric
10:00	21:00	<i>Yuan Gao</i>	Contact line dynamics for droplets: merging, splitting and variational inequality
10:30	21:30	Coffee Break	
10:45	21:45	<i>Joshua Socolar</i>	Shear jammed states and clogging dynamics in dry granular matter
11:15	22:15	<i>Xiaobo Gong</i>	Numerical modeling of mass transfer over deformable membrane in low Renolds number flow
12:00	23:00	Lunch Break	

Departure

*: It refers to Dec.19(EST Time)

2020 DKU Soft Matter Symposium

Abstract set of papers

Venue: IB2050(Zoom Meeting ID:715 337 7467)

Kunshan, Jiangsu Province, China

Time: Dec 17, 2020 to Dec 20, 2020

Sponsors

Zu Chongzhi Center for Mathematics and Computational Sciences

Division of Nature and Applied Science

DKU Association for Science and Technology

DKU Soft Matter Symposium(Dec.17-20)

Day 1-Thursday, 17 December 2020

Dec.17 20:00pm(Beijing time)//Dec.17 7:00am (Eastern Standard Time)

Speaker: Masao Doi

Title: The Onsager principle in polymer dynamics

The Onsager principle is a variational principle proposed by Lars Onsager in 1931 in his celebrated paper on the reciprocal relation in non-equilibrium thermodynamics. The principle is important in the physics of polymer and soft matter. Almost all kinetic equations which have been used to describe the dynamics of polymer and soft matter systems are derived from this principle. The Onsager principle is also useful in solving these equations. Since it is a principle of minimization, it can be used to get approximate solutions of the equations. Here I review the principle from an application point of view. I take examples from capillary hydrodynamics, gel dynamics and flow of viscoelastic fluids.

Day 2-Friday, 18 December 2020

Dec.18 8:30am (Beijing time)//Dec.17 19:30pm (Eastern Standard Time)

Speaker: Patrick Charbonneau

Title: Toward a microscopic understanding of the dynamics of simple glass-forming liquids

The dynamical arrest predicted by mode-coupling theory and the entropy crisis at the random first-order transition are both exact descriptions of simple glass-forming liquids, albeit only in abstract, infinite-dimensional systems. What survives of these features and what other processes come into play in three-dimensional glass formers are questions that remain largely unanswered. In this talk, I present our recent advances toward a microscopic understanding of the finite-dimensional echo of the infinite-dimensional transitions, and of some of the activated processes that affect the dynamical slowdown of simple yet realistic glass formers.

Dec.18 9:30am (Beijing time)//Dec.17 20:30pm(Eastern Standard Time)

Speaker: Ding Ma

Title: Quantifying the Eddy-Jet Feedback Strength of the Atmospheric Annular Modes Using a Linear Response Function Approach

The annular modes in the atmosphere, which correspond to the leading empirical orthogonal function of zonal wind in both hemispheres, represent meridional shifts of the midlatitude jet. The annular modes are characterized by temporal persistence. It has been argued that a positive feedback between the global-scale jet and synoptic-scale atmospheric eddy is responsible for the persistence of the annular modes. To be specific, the anomalous jet organizes the eddies in such way that the eddy momentum flux tends to reinforce the original jet anomaly. Quantifying the strength of the eddy-jet feedback has significant implications for understanding climate variability. Statistical methods have been proposed to estimate the feedback strength. However, the stochastic nature of eddies sparks a debate over this feedback, as it is indeed impossible to separate the jet-dependent eddy flux from the jet-independent eddy flux and infer causality in a coupled system using pure statistical methods. Here, I adopt a linear response function (LRF) approach, which provides a “ground truth” in an idealized global climate model (GCM). The LRF is constructed from a set of Green’s functions forcing, and accurately represents the collective behavior of eddies in response to jet anomaly. The result unequivocally confirms the presence of a positive eddy-jet feedback in the annular mode dynamics, with a feedback strength of 0.14 day⁻¹ in this idealized GCM. Statistical methods proposed by earlier studies to quantify the feedback strength are evaluated against results from the LRF. It is shown that the jet-independent eddy forcing is quasi-oscillatory, rather than white noise assumed with the statistical methods. Consequently, all these statistical methods underestimate the strength of the feedback.

The present study offers a framework to untangle the multi-scale interactions in a coupled system. In particular, LRF may be used to quantify the collective effects of small-scale stochastic processes in response to large-scale forcing.

Dec.18 10:00am (Beijing time)//Dec.17 21:00pm(Eastern Standard Time)

Speaker: Mark D. Shattuck

Title: Deformable Particles

We introduce a new computational model for deformable particles, appropriate for cells, foams, emulsions, and other soft particulate materials, which adds to the benefits and eliminates

deficiencies of existing models. The model combines the ability to model individual soft particles with the shape-energy function of the vertex model, and adds arbitrary particle deformations. We focus on 2D deformable polygons with a shape-energy function that is minimized for area and perimeter and repulsive interparticle forces. We study the onset of jamming, and find that the packing fraction grows with perimeter to area ratio until reaching the critical value of the underlying Voronoi cells at confluence. We find that deformable packings above and below the critical value are solidlike, which helps explain the solid-to-fluid transition in the vertex model as a transition from tension- to compression-dominated regimes.

Dec.18 10:45am (Beijing time)//Dec.17 21:45pm(Eastern Standard Time)

Speaker: Habib Rahbari

Title: Title: Active microrheology of a bulk metallic glass

Abstract: The glass transition remains unclarified in condensed matter physics. Investigating the mechanical properties of glass is challenging because any global deformation that might result in shear rejuvenation would require a prohibitively long relaxation time. Moreover, glass is well known to be heterogeneous, and a global perturbation would prevent exploration of local mechanical/transport properties. However, investigation based on a local probe, i.e., microrheology, may overcome these problems. Here, we establish active microrheology of a bulk metallic glass, via a probe particle driven into host medium glass. This technique is amenable to experimental investigations via nanoindentation tests. We provide distinct evidence of a strong relationship between the microscopic dynamics of the probe particle and the macroscopic properties of the host medium glass. These findings establish active microrheology as a promising technique for investigating the local properties of bulk metallic glass. "

Dec.18 11:15am (Beijing time)//Dec.17 22:15pm(Eastern Standard Time)

Speaker: Ning Xu

Title: Connecting glass forming ability of binary mixtures to melting temperatures

Abstract: Binary mixtures are usually employed to form glasses. By studying the glass formation of binary mixtures of soft spherical particles with the variation of interaction, particle size, particle stiffness, and pressure, we reveal that the glass-forming ability of binary mixtures of soft particles is related to the equilibrium melting temperatures. In binary mixtures, the two particle species are distinct in their size or stiffness. Due to such distinctions, the two components in a mixture effectively feel different melting temperatures, leading to a melting temperature gap. By varying the particle size, stiffness, and composition over a wide range of pressures, we establish a comprehensive picture for the glass-forming ability, based on our finding of the direct link between the glass-forming ability and the melting temperature gap. Using this link, we explain

the different pressure dependence of the glass-forming ability between Lennard-Jones and harmonic potentials observed in our study. Our results also suggest some strategies to optimize the glass-forming ability via the manipulation of particle interactions.

Dec.18 13:30pm (Beijing time)//Dec.18 0:30am(Eastern Standard Time)

Speaker: Ho-Kei Chan (School of Science, Harbin Institute of Technology)

Title: Confinement-induced Columnar Crystals: A Route to New Architecture in the Scientific World

Abstract: Identical spheres in cylindrical confinement exhibit a complex variety of densest-packed columnar structures. Such densest-packed structures can serve as theoretical models for the structures of a variety of physical systems, such as nanotube-confined fullerenes, nanochannel-confined copolymers, colloidal crystal wires, capillary-tube-confined thermoresponsive microspheres, capillary-tube-confined microbubbles, and fluid-driven self-assemblies of polymer beads. On the other hand, there have been comparatively few studies of this kind for shape-anisotropic particles. Thanks to their rotational degrees of freedom, shape-anisotropic particles in columnar confinement exhibit densest-packed structures with specific orientational order and therefore demonstrate a greater variety of densest-packed crystal structures than their spherical counterparts.

In this talk, I will present a historical overview of research on the densest-packed structures of identical hard spheres in cylindrical confinement, and then present our recent extensions of such research to shape-anisotropic particles. For packings of spheres, I will introduce a variety of columnar crystals as discovered computationally in the past two decades, and explain how a wide range of such structures can be obtained through a method of sequential deposition. I will also discuss how some ordered but non-densest crystal structures can be discovered through this specific method of sequential deposition. For packings of shape-anisotropic particles, I will present a variety of densest-packed columnar crystals as discovered recently for identical spheroids in cylindrical confinement and for identical ellipses within a parallel strip. For the case of spheroids, I will explain how the corresponding densest-packed structures arise from a competition between confinement-induced chiral ordering and shape-anisotropy-induced orientational ordering. For the case of ellipses, I will explain why the corresponding densest-packed structures are all affine transformations of particular densest-packed structures of circular disks. It is believed that the confinement-induced crystal structures presented in this talk would constitute a theoretical basis for the development of novel low-dimensional materials with tailored translational or orientational order.

Dec.18 14:00pm (Beijing time)//Dec.18 1:00am(Eastern Standard Time)

Speaker: Duanduan Wan(Wuhan University)

Title: Entropy induced photonic band gaps in self-assembled colloidal crystals

Abstract: We explore how thermal noise-induced randomness in a self-assembled photonic crystal affects its photonic band gaps (PBGs) using computer simulations. We consider a two-dimensional photonic crystal comprised of a self-assembled array of parallel dielectric hard rods of infinite length with circular or square cross section. We find the PBGs can exist over a large range of intermediate packing densities and the largest band gap does not always appear at the packing density where the crystal is most ordered. An interesting and counterintuitive finding is for rods with square cross section at intermediate packing densities, the transverse magnetic (TM) band gap of the self-assembled (i.e. thermal) system can be larger than that of identical rods arranged in a perfect square lattice. By considering hollow rods, we find the band gap of transverse electric (TE) modes can be substantially increased while that of TM modes show no obvious improvement over solid rods. In all, our study suggests that by suitably choosing the packing density, particle shape, and engineering other dimensions such as particle internal structure, self-assembly can indeed be a promising method to make photonic crystals with large band gaps despite the inherent thermal noise (randomness).

Dec.18 14:45pm (Beijing time)//Dec.18 1:45am(Eastern Standard Time)

Speaker: Litang Yan

Title: Transport of nanoscale objects on cell membrane: from passive to active particles

Abstract: Diffusion is the essential and fundamental means of transport of substances on cell membranes, and the dynamics of biomembranes plays a crucial role in the regulation of numerous cellular processes. The understanding of the complex mechanisms and nature of particle diffusion have a bearing on establishing guidelines for the design of efficient transport materials and unique therapeutic approaches. Herein, we report our recent advances in investigating diffusion dynamics of nanoscale objects on biological membranes, focusing on the approaches of tailored computer simulations and theoretical analysis. Due to the presence of the complicated and heterogeneous environment on native cell membranes, the diffusive transport

behaviors of nanoparticles exhibit unique and variable characteristics. In particular, we introduce the general aspect and basic theories of the diffusion transport of various heterogeneous nanoparticles, including charged Janus nanoparticles, two-dimensional nanosheets, and active particles. Our findings might inform approaches to program transport of various nanomaterials at bio-nano interfaces, and suggest design principles for novel composite systems integrating such nanomaterials with biological membranes.

Dec.18 15:15pm (Beijing time)//Dec.18 2:15am(Eastern Standard Time)

Speaker: Joshua Dijksman

Title: Twisting and turning particles

Abstract: Shearing granular materials induces non-affine displacements. Such non-affine displacements have been studied extensively, and are known to correlate with plasticity and other mechanical features of amorphous packings. A well-known example is shear transformation zones as captured by the local deviation from affine deformation, $D2_{min}$. We analyze sheared frictional athermal disk packings and show that there exists at least one additional mesoscopic transport mechanism that superimposes itself on top of local diffusive motion. We evidence this second transport mechanism in a homogeneous system via a diffusion tensor analysis and show that the trace of the diffusion tensor equals the classic $D2_{min}$ when this second mesoscopic transport is corrected for.

The complexity of particle displacements driven by shear stems from the coupling of confinement and forces displacements. Particle rotations, in contrast, are much less sensitive to confinement effects, while still sensitive to the mechanics of the packing. So far, little attention has been paid to connect microscopic rotational motion to mechanics of athermal amorphous packings. In the same packing as studied for displacements, we find that particle packing mechanics can be directly linked to the rotational motion. Our results show that the diffusive nature of rotational dynamics is highly strain sensitive. Additionally, there is substantial spatial correlation in rotation dynamics that is a function of the particle friction and packing density.

Dec.18 15:45pm (Beijing time)//Dec.18 2:45am(Eastern Standard Time)

Speaker: Meiying Hou

Title: Experimental evidence of pressure-sensitive intrusion rheology in grains

Dec.18 20:00pm (Beijing time)//Dec.18 7:00am(Eastern Standard Time)

Speaker: Stefan Luding

Title: From particle simulations towards a universal continuum theory and applications

Abstract: The dynamic and static behavior of particulate and granular matter (like sand, powder, suspended particles or molecules, often with a wide distribution of particle sizes) is of considerable interest in a wide range of industries and research disciplines. They can behave both solid-like and fluid-like. The related mechanisms/processes in particle systems are active at multiple scales (from nano-meters to meters), and finding the reasons for natural disasters like avalanches or plant problems like silo-failure, is a challenge for both academia and industry.

In order to understand the fundamental micro-mechanics and -physics, one can use particle simulation methods, where often the fluid between the particles is important too. However, large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grained models or by continuum theory. In order to bridge the gap between the scales, so-called micro-macro transition methods are necessary, which translate particle positions, velocities and forces into density-, stress-, and strain-fields. These macroscopic quantities must be compatible with the conservation equations for mass and momentum of continuum theory. Furthermore, non-classical fields are needed to describe the micro-structure (fabric, force-chains) or the statistical fluctuations, e.g. of the kinetic energy, before one can reach the ultimate goal of solving application problems based on a universal granular rheology that involves fluid- as well as solid-mechanics, as well as the jamming/un-jamming transitions between the states.

Examples of multi-scale simulations, involving particle- and continuum-methods, are flows of particles/fluids in narrow channels/pores, dosing of cohesive fine powders in vending machines, avalanche flows on inclined slopes, segregation, rheology testing in ring-shear cells, as well as the study of non-linear elasto-plastic material mechanics related to the failure of cohesive, frictional solids [1-4].

Dec.18 21:00pm (Beijing time)//Dec.18 8:00am(Eastern Standard Time)

Speaker: Matthias Schröter

Title: Different ways of getting into contact in the granular world

Abstract: Contacts form the backbone of granular solids by allowing them to form force chains, which then endow those collections of particles with rigidity. The details of contact formation depend on the particle shape and elasticity and the amount of tangential friction at the contacts.

While we have a partly empirical theory which describes the number of contacts in frictional sphere packings in a first approximation, it is less clear how to expand beyond this approach. Machine Learning gives us some first indications which locally defined physical parameters might be relevant in order to do so.

Dec.18 21:30pm (Beijing time)//Dec.18 8:30am(Eastern Standard Time)

Speaker: Matthias Sperl

Title: Dynamics in Granular Matter

Abstract: (1) Under appropriate driving, otherwise dissipative granular systems can achieve a steady state that can be compared with classical gas and liquid states. Upon cessation of driving, specific cooling phenomena can be observed, i.e., energy dissipation at individual particle collision leads to loss of overall energy in the multi-particle system. (2) It is demonstrated how the arguably simplest dynamical states of granular matter can be investigated naturally by experiments in microgravity.

Dec.19 8:30am (Beijing time)//Dec.18 19:30pm(Eastern Standard Time)

Speaker: Brian Salzberg

Title: Extrinsic and Intrinsic Optical Changes in Mammalian Nerve Terminals and a Mechanical Spike

Abstract: Extrinsic optical change in nerve terminals are due to voltage sensitive dyes, calcium sensitive dyes, etc. Intrinsic optical changes, also accompany the action potential, and the consequent secretion of neuropeptides, in mammalian nerve terminals. These include light scattering changes, related to the action potential, action currents, and exocytosis, and, also intrinsic fluorescence changes related to mitochondrial oxidative phosphorylation. The light scattering changes are related to the small volume changes in the terminals that we show can be detected using high bandwidth atomic force microscopy, and the intrinsic fluorescence changes are related to action potential production in the plasma membrane, through multiple intermediates. These will be discussed, including their likely origins.

Dec.19 9:30am (Beijing time)//Dec.18 20:30pm(Eastern Standard Time)

Speaker: John W. Weisel

Title: Multiscale studies of blood clotting

Abstract: The structure and physical properties of clots and thrombi can be understood from a bottom-up approach, starting with the molecular structures of all components, including the entire structures of fibrinogen and Factor XIII beyond only their crystal structures. The structures and composition of platelet-poor plasma clots, platelet-rich plasma clots, whole blood clots, in vivo hemostatic clots, and thrombi will all be described. The mechanical properties of clots and thrombi are important, since these biological and pathological structures essentially fulfill a mechanical function. The fundamental role of fibrin will be emphasized, since it provides a space-spanning structure that resists the forces that clots and thrombi are subject to in the vasculature. In addition, the contributions of platelets and red blood cells will be described, as well as in vivo effects of blood flow and local environmental conditions. Fibrin is a viscoelastic polymer whose properties can only be understood from a multiscale approach, considering the macroscopic, clot network, individual fibers, protofibrils and fibrin molecules. The degree of branching of the clot network is important, with clots made up of thinner fibers with many branch points being stiffer than clots made up of thicker fibers with fewer branchpoints. With stretching of clots, fibrin fibers become aligned in the direction of stress, before elongation causes unfolding without a change in fibrin's axial periodicity. With compression of clots or thrombi, fibrin fibers first bend and buckle, decreasing clot stiffness, then as they touch each other they stick and together increase the stiffness of clots. Next, the molecular structural origins of the mechanical properties of clots will be described. The sequence of events during unfolding are still being defined, but there is stretching of the α C regions, unfolding of the α C regions, and transient conformational change of the α -helical coiled-coil regions to α -sheets. In fact, the structure of fibrinogen likely evolved to unfold with applied forces, and one function of the α -helical coiled-coil appears to be to transiently take up the slack with unfolding of other molecular domains. Furthermore, there exists in clots and thrombi that contain both platelets and erythrocytes a unique structure that arises from platelet-driven clot contraction, which includes the redistribution of fibrin and platelets to the periphery and erythrocytes to the core, where they are compressed by the forces exerted by platelets into polyhedral-shaped cells called polyhedrocytes. The cellular mechanisms involved in this process will be described. The mechanical properties of fibrin are not only an essential part of the biomechanics of hemostasis and thrombosis, but also necessary for a rapidly developing field of bioengineering that uses fibrin as a versatile biomaterial with exceptional and tunable biochemical and mechanical properties.

Dec.19 10:00am (Beijing time)//Dec.18 9:00pm(Eastern Standard Time)

Speaker: Zhiliang Xu

Title: Mathematical and computational Modeling Blood Clot Formation

Abstract: Blood clotting is a multiscale process involving blood cells, fibrinogen polymerization, coagulation reactions, ligand-receptor interactions and blood plasma flow. In this talk, We will discuss models to cover a few aspects of blood clotting. In particular, a continuum model for studying the structural stability of clots utilized the phase field and energetic variational approaches and a discrete model studying fibrin network mechanics will be discussed. Lastly, we will briefly discuss a new machine learning algorithm for simulating PDEs.

Dec.19 10:45am (Beijing time)//Dec.18 21:45pm(Eastern Standard Time)

Speaker: Fredric Cohen

Title: Cells maintain their cholesterol content by quickly adjusting the cholesterol chemical potential of their plasma membranes

Abstract: Cells maintain their cholesterol content by quickly adjusting the cholesterol chemical potential of their plasma membranes. Artem G. Ayuyan and Fredric S. Cohen. Rush University Medical Center, Dept of Physiology and Biophysics. Chicago, IL

Cholesterol is the most abundant molecule in the plasma membrane, typically about 1/3 of the membrane on a mole basis. At high concentrations of a substance, its interactions are abundant. Thus, determining the chemical potential of cholesterol is a necessary measurement in order to properly understand cholesterol's contributions to cellular processes. We have succeeded in developing a method to measure, and controllably alter or clamp the cholesterol chemical potential of plasma membranes (μ_{PM}). Using these methods, we discovered that when challenged with varied cholesterol levels in extracellular solutions, μ_{PM} quickly (< 5 min) became the same value as μ_{EX} , and this occurred without changes in cell cholesterol content. As a result of this equalization between μ_{PM} and μ_{EX} , net flux of cholesterol between the plasma membrane and extracellular solution ceases, resulting in maintenance of cell cholesterol content. We have found that μ_{PM} and some cell signaling pathways are coupled, and it appears that cell signaling pathways feedback to bring μ_{PM} to μ_{EX} .

Dec.19 11:15am (Beijing time)//Dec.18 22:15pm(Eastern Standard Time)

Speaker: Lei Zhang(Beijing International Center for Mathematical Research, Peking University)

Title: Construction of Solution Landscape on the energy landscape

Abstract: Energy landscape has been widely applied to many physical and biological systems. A long standing problem in computational math and physics is how to search for the entire family tree of possible stationary states, without unwanted random guesses, starting from a parent state on the energy landscape all the way down to energy minima? Here we introduce a novel concept “Solution Landscape”, which is a pathway map consisting of all stationary points and their connections. Then we developed a general and efficient numerical method to construct the solution landscape, which not only identifies all possible minima, but also advances our understanding of how a complex system moves on the energy landscape. As an example, we solve the Landau-de Gennes energy to model a liquid crystal confined in square box; we illustrate the basic concepts by examining the multiple stationary solutions and the connected pathway maps of the model. The joint work with Pingwen Zhang (PKU), Jianyuan Yin (PKU), Jeff Z.Y. Chen (Waterloo).

Dec.19 13:30pm (Beijing time)//Dec.19 0:30am(Eastern Standard Time)

Speaker: Yuliang Jin (Institute of Theoretical Physics, Chinese Academy of Sciences)

Title: Machine learning a Gardner transition

Abstract: Apparent critical phenomena, typically indicated by growing correlation lengths and dynamical slowing-down, are ubiquitous in non-equilibrium systems such as supercooled liquids, amorphous solids, active matter and spin glasses. It is often challenging to determine if such observations are related to a true second-order phase transition as in the equilibrium case, or simply a crossover, and even more so to measure the associated critical exponents. We show that the simulation results of a hard-sphere glass in three dimensions, are consistent with the recent theoretical prediction of a Gardner transition, a continuous non-equilibrium phase transition. Using a hybrid molecular simulation-machine learning approach, we obtain scaling laws for both finite-size and aging effects, and determine the critical exponents that traditional methods fail to estimate. This study provides a novel approach that is useful to understand the nature of glass transitions, and can be generalized to analyze other non-equilibrium phase transitions.

Dec.19 14:00pm (Beijing time)//Dec.19 1:00am(Eastern Standard Time)

Speaker: Xinpeng Xu(Physics Program in Guangdong Technion – Institute of Technology)

Title: Onsager's variational principles in active soft matter

Abstract: Onsager's variational principle (OVP) was originally proposed by Lars Onsager in 1931 [L. Onsager, Phys. Rev., 1931, 37, 405]. This fundamental principle provides a very powerful tool for formulating thermodynamically consistent models in nonequilibrium thermodynamics. It can also be employed to find approximate solutions, especially in the study of soft matter dynamics. In this talk, I will show that OVP can be extended and applied to the dynamic modeling of active soft matter such as suspensions of bacteria and aggregates of animal cells. I will start with a brief introduction to the biology and artificial systems that motivate the studies of active soft matter. I will then quickly review the classical OVP and its extension to active matter dynamics where active forces are included as external non-conservative forces. Next, I use OVP to analyze the directional "walk" of an individual molecular motor on a stiff biofilament. After that I will use OVP to formulate a diffuse-interface model for an active polar droplet on a solid substrate. In addition to the generalized hydrodynamic equations for active polar fluids in the bulk region, we have also derived thermodynamically consistent boundary conditions. Particularly, when the active droplet is very thin, the lubrication approximation can be applied. In this case, I will show that a generalized thin film equation can be derived using OVP. Moreover, OVP can also be used as an approximation tool to find the spreading laws for the thin active polar droplet. Finally, I use OVP to analyze the directional locomotion of a toy two-sphere microswimmer, in which nonlinear dissipation function arises that proposes significant challenges to OVP. In summary, the variational method we have proposed by incorporating biochemical activity into OVP will help to deepen our understanding of the emergent structure and dynamic behaviors of real in vivo biological systems such as bacteria suspensions, individual animal cells and cell aggregates (or tissues).

Dec.19 14:45pm (Beijing time)//Dec.19 1:45am(Eastern Standard Time)

Speaker: Sze Chai Kwok(Duke Kunshan University)

Title: Window into cognition: bridging electrophysiology, neuroimaging and neuromodulation

Abstract: Abstract: In this talk, I will make use of an example of how a combination of methods are employed to help us glimpse into the mechanism of mnemonic cognition. I argue that memories of episodes are mediated by the parietal part of neocortex. This argument helps augment and even challenge a long-standing doctrine in the system neuroscience of memory that the medial temporal lobe being the key locus of complex episodic memories. Specifically, I'll report our discovery of episodic memory cells in the macaque medio-posterior parietal cortex, their involvement in processing complex streams of naturalistic information, and how complex

memories might be structured and recalled in the animals. The development of translational neuromodulation techniques could be added to bring forth a causality dimension to this investigation.

Dec.19 15:15pm (Beijing time)//Dec.19 2:15am(Eastern Standard Time)

Speaker: Zheng Wang(Chinese Academy of Sciences)

Title: The pursuit of MRI-based diagnostic and predictive biomarkers in neuropsychiatric disorders

Abstract: Genetic and phenotypic heterogeneities of psychiatric disorders remain a formidable challenge for understanding circuit mechanisms and accurate diagnosis. Despite tremendous progress in the development of modern medical imaging techniques, identification of imaging-based biomarkers that helps to guide diagnosis and treatment for neuropsychiatric disorders remains an active topic of research. Towards this end, we develop novel cross-species comparative paradigms that translate genetic, behavioral and neuroimaging findings from diseased monkey models to psychiatric patients. Through this work, we have taken a reductionist perspective that leverages the genetically-engineered primate models to dissect clinical heterogeneity of psychiatric diseases. We aim to probe the mechanistic links between gene expressions, dysfunction of specific neural networks and symptomatology, thereby identifying a tangible circuit endophenotype that associates aberrant brain connectome with behavioral domains. Such a circuit endophenotype which may cut across multiple categorical diagnoses provides an alternative route to deconstruct inherent heterogeneity and complex comorbidity in mental disorders.

Dec.19 15:45pm (Beijing time)//Dec.19 2:45am(Eastern Standard Time)

Speaker: Yao Li(Shanghai Jiaotong University)

Title: Multimodal Brain Imaging from Structure, Function to Metabolism

Abstract: Brain mapping is one of the most exciting frontiers of contemporary science. It provides this generation of scientists the opportunity to make major advances on a historic question: how the brain works and what goes wrong when it is injured or diseased? Magnetic resonance (MR)-based neuroimaging techniques have been widely used for brain research because of their noninvasiveness and multimodal capabilities. Exploiting the rich information contents of MR signals, we can obtain structural, functional and metabolic information of the

brain. MR spectroscopic imaging (MRSI) is a beautiful integration of MR spectroscopy and MR imaging, which can provide metabolic status of tissues in vivo without exogenous molecular labels. But its clinical applications have been limited due to long scan time and poor spatial resolution. In this talk, I'll show a new capability for rapid high-resolution metabolic imaging by using a recently developed subspace-based imaging technique called SPICE (SPectroscopic Imaging by exploiting spatioSpectral CorRElation). In an 8-min scan, we can acquire metabolic maps from the whole brain at a nominal spatial resolution of $2.0 \times 2.4 \times 2.0 \text{ mm}^3$. Using SPICE, we are also able to simultaneously acquire QSM and myelin water imaging. We have successfully performed SPICE scans on stroke patients, traumatic brain injury (TBI) patients and brain tumor patients. Our experimental study yielded very encouraging results and showed that ultrahigh-resolution MRSI can capture neurometabolic alterations induced by stroke, TBI and brain tumors effectively.

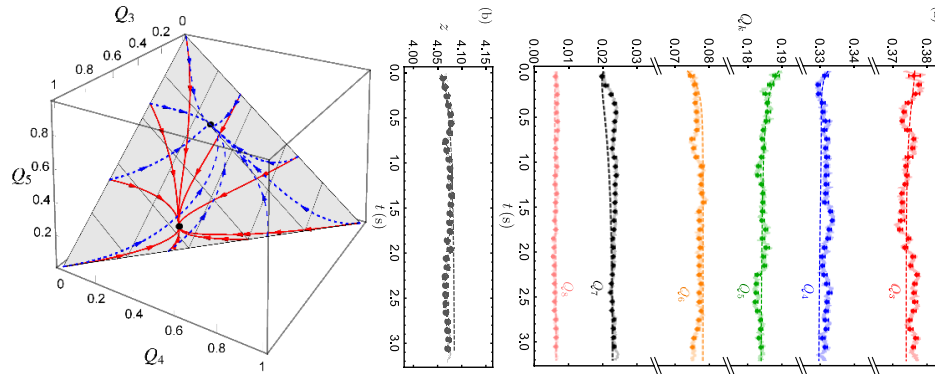
Dec.19 20:00pm (Beijing time)//Dec.19 7:00am(Eastern Standard Time)

Speaker: Rafi Blumenfeld (University of Cambridge)

Title: Structural evolution of dense granular systems: Theory and non-equilibrium detailed balance

Abstract: The large-scale behaviour of granular materials is very sensitive to the grain-scale structure. This structure often depends on the dynamic process generating the system - regarded as history-dependence.

We developed a predictive formalism to model structural organization and evolution of structural properties. Using it, we predict the cell order distribution (COD) and the mean coordination number under any dynamic process. The theory is based on the rates of contact making and breaking events, which determine most of the relevant structural properties. Dynamic equations are constructed for the evolution of structural properties. The steady state, as well as the approach to it are studied analytically. It is found that, for constant breaking / making rates, the steady state of dense systems with cells of order < 7 , is unique and satisfies detailed balance – possibly the first such observation in out-of-equilibrium dynamics. Less dense systems may settle into more than one steady state, none of which satisfies detailed balance. The theoretical analysis is well supported by numerical simulations and initial experimental results.



Dec.19 21:00pm (Beijing time)//Dec.19 8:00am(Eastern Standard Time)

Speaker: Raúl Cruz Hidalgo (Universidad de Navarra)

Title: On the rheological response of nonspherical granular flows

Abstract: We present an extensive numerical and experimental study, investigating a three-dimensional (3D) granular flow of elongated particles down an inclined plane. Similarly to sheared systems, the average particle orientation encloses a small angle with the flow direction. In the bulk, this behavior is independent of the shear rate. However, the particles move in more dilute conditions at the surface, and the average orientation strongly depends on the shear rate. A systematic numerical study, varying the particle aspect ratio and the plane inclination, reveals that the particle size perpendicular to the flow direction, d_{eff} , is an appropriate length scale to define an effective inertial number I_{eff} . It fully captures the impact of the particle shape on the system's rheology. Like for spheres, density and friction result in well-defined functions of the effective inertial number I_{eff} . Thus, we quantify and explain the rheological parameters' dependence on the aspect ratio, based on the micromechanical details.

Dec.19 21:30pm (Beijing time)//Dec.19 8:30am(Eastern Standard Time)

Speaker: Iñaki Echeverría (Universidad de Navarra)

Title: Estimating density limits for walking pedestrians keeping a safe interpersonal distancing

Abstract: With people trying to keep a safe distance from others due to the COVID-19 outbreak, the way in which pedestrians walk has completely changed since the pandemic broke out. Aiming to characterize how people change their behaviour, we have carried out a set of controlled laboratory experiments in which a number of volunteers were asked to roam inside an arena while keeping a prescribed safety distance (PSD). Different conditions of crowd density, walking speed (WS) and prescribed safety distance (PSD) have been tested, showing its impact on other derived magnitudes that have become relevant due to the pandemic: first, d_1 , the distance of each participant to the nearest neighbour (i.e. the closest person); second, v , the velocity of each individual; third, t_{exp} , the time that two pedestrians spend at a distance smaller than 1.5 meters uninterruptedly; and fourth, the persistence of the movement direction O , which characterizes the change in the direction of motion for each pedestrian.

Our results show that, in order to guarantee an interpersonal distance of one meter, the global density of some places should not be higher than 0.16 pedestrians per square meter (around 6 square meters per pedestrian). Besides, we evidence the importance of prescribing a considerable safety distance as some people may underestimate the actual value of the interpersonal distance. Although the extrapolation of our findings to other more realistic scenarios is not straightforward, they can be used as a first approach to inform density restrictions in urban and architectonic spaces based on scientific evidence.

Dec.20 8:30am (Beijing time)//Dec.19 19:30pm(Eastern Standard Time)

Speaker: Corey O'Hern(Yale University)

Title: Using physical features of protein core packing to distinguish real proteins from decoys

Abstract: The ability to consistently distinguish real protein structures from computationally generated model decoys is not yet a solved problem. One route to distinguish real protein structures from decoys is to delineate the important physical features that specify a real protein. For example, it has long been appreciated that the hydrophobic cores of proteins contribute significantly to their stability. We used two sources to obtain datasets of decoys to compare with real protein structures: submissions to the biennial Critical Assessment of protein Structure Prediction competition, in which researchers attempt to predict the structure of a protein only knowing its amino acid sequence, and also decoys generated by 3DRobot, which have user-specified global root-mean-squared deviations from experimentally determined structures. Our analysis revealed that both sets of decoys possess cores that do not recapitulate the key features that define real protein cores. In particular, the model structures appear more densely packed (because of energetically unfavorable atomic overlaps), contain too few residues in the core, and have improper distributions of hydrophobic residues throughout the structure. Based on these observations, we developed a feed-forward neural network, which incorporates key physical features of protein cores, to predict how well a computational model recapitulates the real protein structure without knowledge of the structure of the target sequence. By identifying the important

features of protein structure, our method is able to rank decoy structures with similar accuracy to that obtained by state-of-the-art methods that incorporate many additional features. The small number of physical features makes our model interpretable, emphasizing the importance of protein packing and hydrophobicity in protein structure prediction.

Dec.20 9:30am (Beijing time)//Dec.19 20:30pm(Eastern Standard Time)

Speaker: Weiqing Ren (National University of Singapore)

Title: Interface Profile Near the contact line in electro-wetting on dielectric

Abstract: We consider a charged droplet sitting on a dielectric substrate and study the static profile of the interface near the contact line. We first derive the governing equations using the principle of minimum energy, then discuss the distinguished limit of the model as the dimensionless parameters go to zero. Analysis of the inner problem, which governs the interface profile near the contact line, shows the existence of a well-defined apparent contact angle. The apparent contact angle depends on the applied electrical potential and the thickness of the insulator, and the relation agrees well with the Lippmann-Berge equation.

Dec.20 10:00am (Beijing time)//Dec.19 21:00pm(Eastern Standard Time)

Speaker: Yuan Gao

Title: Contact line dynamics for droplets: merging, splitting and variational inequality

Abstract: The capillary effect caused by the interfacial energy dominates the dynamics of small droplets, particularly the contact lines (where three phases meet).

Via incompressible potential flow, the motion of droplets is purely geometric and is described by the mean curvature flow of the capillary surface coupled with contact line dynamics. This can be formulated as a gradient flow on a Hilbert manifold and leads to effective numerical methods. We propose unconditionally stable first/second order numerical schemes based on explicit moving boundaries and semi-Lagrangian method. To enforce impermeable obstacle constraint, a projection method for a variational inequality is further adapted to simulate the unavoidable merging and splitting of droplets. The phase transition for the emerged contact lines is detected and equipped with contact line mechanism.

Dec.20 10:45am (Beijing time)//Dec.19 21:45pm(Eastern Standard Time)

Speaker: Joshua Soholar(Duke University)

Title: Shear jammed states and clogging dynamics in dry granular matter

Abstract: The formation of elastically stable structures in flowing or slowly sheared granular materials at densities below the jamming threshold is a crucial phenomenon affecting industrial and geophysical processes, yet the fundamental physics underlying such shear jamming or clogging events remains poorly understood. We report on experiments showing the motions of individual grains and stress configurations in monolayers of grains either sheared homogeneously or subjected to an externally forced grain-size intruder. In the sheared system, we apply small-amplitude cyclic shear to jammed states produced by forward shear alone. In some cases, the cyclic shear destroys the stress field, with grains exhibiting diffusive dynamics at long times, while in others the system reaches a stable jammed state with surprisingly strong stiffness. In the intruder experiments, a small disk is driven azimuthally through an annular channel, and we observe features of the clogging dynamics that are significantly different for materials consisting of disks or of pentagonal particles.

Dec.20 11:15am (Beijing time)//Dec.19 22:15pm(Eastern Standard Time)

Speaker: Xiaobo Gong

Title: Numerical modeling of mass transfer over deformable membrane in low Renolds number flow