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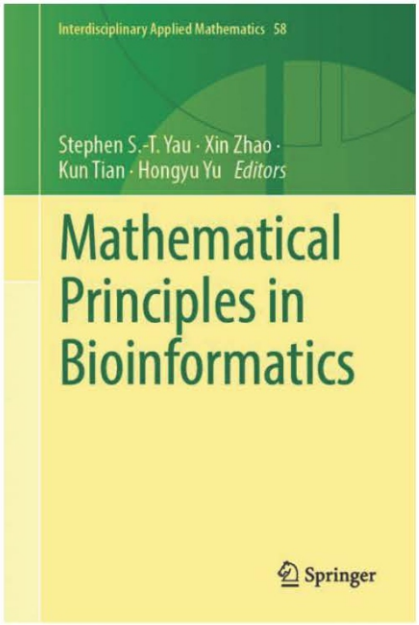
TSIMF
清华三亚国际数学论坛

10th
论坛建成十周年
The 10th Anniversary of TSIMF

第五届生物信息学和生物物理学中的算法和数学TSIMF国际会议

The 5th TSIMF conference on Computational and Mathematical Bioinformatics and Biophysics

December 11-15, 2023



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Interdisciplinary Applied Mathematics

Mathematics and Statistics: Computer and Information Systems Applications, Bioinformatics, Applications of Mathematics

Stephen S.-T. Yau - *Tsinghua University, Beijing, China*, Xin Zhao - *Beijing Electronic Science and Technology Institute, Beijing, China*, Kun Tian - *Renmin University of China, Beijing, China*, Hongyu Yu - *Tsinghua University, Beijing, China*

Mathematical Principles in Bioinformatics

- Focuses on alignment-free methods in sequence comparison, which are neglected in many books on bioinformatics
- Introduces the method to form a practical genome/protein space and proposes the convex hull principle
- Based on the author's research works, bioinformatics from the view of a mathematician

This textbook introduces bioinformatics to students in mathematics with no biology background assumed and it provides solid mathematical tools for biology students along with an understanding of how to implement them in bioinformatics problems. In addition to the basics, the text offers new approaches to understanding biological sequences. The concise presentation distinguishes itself from others on the subject, discussing and providing principles that relate to current open problems in bioinformatics as well as considering a variety of models. The convex hull principle is highlighted, opening a new interdisciplinary research area at the intersection of biology, mathematics, and computer science. Prerequisites include first courses in linear algebra, probability and statistics, and mathematical analysis. Researchers in mathematics, biology, and math-biology, will also find aspects of this text useful. This textbook is written based on the authors' research works that have been published in various journals along with the lecture notes used when teaching bioinformatics courses at the University of Illinois at Chicago and at Tsinghua University. The content may be divided into two parts. The first part includes three chapters, introducing some basic concepts. Chapter 1 provides biological background in molecular biology for mathematicians. Chapter 2 describes biological databases that are commonly used. Chapter 3 is concerned with alignment methods includ...

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Call for paper

Computational and Mathematical Bioinformatics and Biophysics

The 5th Conference on Computational and Mathematical Bioinformatics and Biophysics will take place at the Tsinghua Sanya International Mathematics Forum (TSIMF) in Sanya, China, on December 11 – 15, 2023 (http://www.tsimf.cn/meeting/detail?id=319). To record this event, a special issue with the same title will appear in the journal, Communications in Information & Systems (CIS) https://www.intlpress.com/site/pub/pages/journals/items/cis/_home/_main/index.php.

The purpose of this special issue is to provide a medium for researchers from mathematical and biophysical sciences and other related disciplines to report recent advances and challenges on Computational and Mathematical Bioinformatics and Biophysics. Numerous areas of mathematics, including differential equations, geometry, topology, graph theory, combinatorics, optimization, machine learning, functional analysis, harmonic analysis, stochastic analysis, and statistical inference, underpin bioinformatics and biophysics, will be highlighted in this special issue.

Original papers and high-quality review articles are solicited for this special issue. Potential topics include, but are not limited to:

- ***Analysis of human genome and molecular evaluation***
- ***Single cell sequencing analysis, gene sequencing analysis, single-cell RNA sequence analysis***
- ***Differential geometry based multiscale models***
- ***Topological data analysis of biomolecules***
- ***Computational geometry, spectral geometry, geometric algebra***
- ***Knot theory, geometric topology***
- ***Implicit solvent models and electrostatic analysis***
- ***Biomolecular transport, ion channel***
- ***Quantum mechanics, molecular mechanics, Brownian dynamics***
- ***Mathematical AI for biosciences***
- ***Rational drug design, drug discovery and delivery***
- ***Algorithms and applications of the above topics***

To submit a manuscript, please email the journal manager Jenny Chen at (jenny@ims.cuhk.edu.hk) and copying to the Guest Editors. All manuscripts are subject to the standard peer review process before publication.

Important Dates:
Manuscript Due: ***March 1, 2024***
First Round of Reviews: ***May 1, 2024***
Anticipated Publication Date: ***October 1, 2024***

Guest editors:
Stephen S.-T. Yau, Tsinghua University, China
Guowei Wei, Michigan State University, USA
Shan Zhao, The University of Alabama, USA
Chenglong Yu, Monash University, Australia

The 5th Conference on Computational and Mathematical Bioinformatics and Biophysics, December 11 - 15, 2023

Time&Date	Monday (December 11)	Tuesday (December 12)	Wednesday (December 13)	Thursday (December 14)	Friday (December 15)
7:30-8:30	**Breakfast (60 minutes)**				
Chair	Stephen Yau	Huan-Xiang Zhou	Jie Wu	Yi Xiao	Jingqiao Duan
8:30-9:00			Xiaoqin Zou		
9:00-9:30	John Z.H. Zhang	Yuguang Mu	Xiao He	Shi-Jie Chen	Jie Wu
9:30-10:00	Huan-Xiang Zhou	Xiangyu Luo	Yu Xue	Wenfei Li	Weihua Geng
10:00-10:30	Haiyan Liu	Hongyu Yu	The opening ceremony of the 10th anniversary of TSIMF 10:00-12:00	Minghui Yang	Kelin Xia
10:30-11:00	**Coffee Break (within 30 minutes)**			**Coffee Break (within 30 minutes)**	
Chair	Guowei Wei	Xinqi Cong		Shi-Jie Chen	Jian Jiang
11:00-11:30	Xinqi Gong	Qingchuan Zheng		Lei Zhang	Buyong Ma
11:30-12:00	Changjun Chen	Jian Jiang		Shengyou Huang	Qiantao Wang
12:00-14:00	**Lunch break (120 minutes)**				
Chair	Shan Zhao	Weihua Geng	Group photo 13:00	Lei Zhang	
14:00-14:30	Guowei Wei	Ruohan Ren	Free Discussion 13:30-17:00 南山寺	Jingqiao Duan	
14:30-15:00	Yi Xiao	Xu-Qian Fan		Zhan Chen	
15:00-15:30	Wei Han	Tao Zhou		Shenggao Zhou	
15:30-16:00	**Coffee Break (within 30 minutes)**			**Coffee Break (within 30 minutes)**	
Chair	John Z.H. Zhang	Xiaoqin Zou		Zhan Chen	
16:00-16:30	Chunmei Wang	Dmytro Kozakov		Hao Dong	
16:30-17:00	Ye Mei	Yunxiang Sun		Shixin Xu	
17:00-17:30	Cong Shen	Haifeng Chen		Yuanzhen Shao	
17:30-19:00	**Dinner**		Banquet 18:00-20:00	**Dinner**	

Titles and Abstracts

Mathematics in action: from pandemic to drug discovery

Wei, Guowei (魏国卫)
Michigan State University, USA

Mathematics underpins fundamental theories in physics such as quantum mechanics, general relativity, and quantum field theory. Nonetheless, its success in modern biology, namely cellular biology, molecular biology, chemical biology, genomics, and genetics, has been quite limited. Artificial intelligence (AI) has fundamentally changed the landscape of science, engineering, and technology in the past decade and holds a great future for discovering the rules of life. However, AI-based biological discovery encounters challenges arising from the intricate complexity, high dimensionality, nonlinearity, and multiscale biological systems. We tackle these challenges by a mathematical AI paradigm. We have introduced persistent cohomology, persistent spectral graphs, persistent path Laplacians, persistent sheaf Laplacians, and evolutionary de Rham-Hodge theory to significantly enhance AI's ability to tackle biological challenges. Using our mathematical AI approaches, my team has been the top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design and discovery for years. By further integrating mathematical AI with millions of genomes isolated from patients, we uncovered the mechanisms of SARS-CoV-2 evolution and accurately forecast emerging dominant SARS-CoV-2 variants.

Mathematical AI for molecular data analysis

Xia, Kelin (夏克林)
Nanyang Technological Universit

Artificial intelligence (AI) based molecular data analysis has begun to gain momentum due to the great advancement in experimental data, computational power and learning models. However, a major issue that remains for all AI-based learning models is the efficient molecular representations and featurization. Here we propose advanced mathematics-based molecular representations and featurization (or feature engineering). Molecular structures and their interactions are represented as various simplicial complexes (Rips complex, Neighborhood complex, Dowker complex, and Hom-complex), hypergraphs, and Tor-algebra-based models. Molecular descriptors are systematically generated from various persistent invariants, including persistent homology, persistent Ricci curvature, persistent spectral, and persistent Tor-algebra. These features are combined with machine learning and deep learning models, including random forest, CNN, RNN, GNN, Transformer, BERT, and others. They have demonstrated great advantage over traditional models in drug design and material informatics.

Improving Protein-ligand interaction prediction: OnionNet and Beyond

Mu, Yuguang(慕宇光)
Nanyang Technological University, Singapore

While there has been significant progress in molecular property prediction in computer-aided drug design, there is a critical need to have fast and accurate models. Many of the currently available methods are mostly specialists in predicting specific properties, leading to the use of many models side-by-side that lead to impossibly high computational overheads for the common researcher. Henceforth, the authors propose a single, generalist unified model exploiting graph convolutional variational encoders that can simultaneously predict multiple properties such as absorption, distribution, metabolism, excretion and toxicity (ADMET), target-specific docking score prediction and drug-drug interactions. Considerably, the use of this method allows for state-of-the-art virtual screening with an acceleration advantage of up to two orders of magnitude. The minimisation of a graph variational encoder's latent space also allows for accelerated development of specific drugs for targets with Pareto optimality principles considered, and has the added advantage of explainability.

A New Diffuse-Interface Approach to Ensemble Average Solvation Energy

Shao, Yuanzhen(邵元桢)
The University of Alabama

Variational implicit solvation models (VISM), because of their relatively low computational cost and satisfactory accuracy, are of paramount importance in the solvation analysis of biological and chemical systems at molecular level. Central in the construction of VSIM is an interface separating the solute and the solvent, which is obtained by optimizing a solvation energy functional. However, due to the random conformational changes of macromolecules, the disposition of a separating interface cannot be unique. Further, the idea of using the value of a solvation energy functional computed at a fixed interface to predict experimentally observed solvation energies is undermined by the fact that experimentally observable quantities are ensemble averaged. In this talk, we will introduce two diffuse interface models to calculate the ensemble average solvation energy.

Atomistic Modeling of Residue-Specific Contributions to Protein Liquid-Liquid Phase Separation

Zhou, Huan-Xiang
University of Illinois at Chicago

Liquid-liquid phase separation of protein solutions has regained heightened attention for its biological importance and pathogenic relevance. Coarse-grained models are limited when explaining residue-level effects on phase equilibrium. I will present our atomistic modeling method, FMAP, for determining phase equilibria [1, 2]. Application of FMAP has produced a number of interesting discoveries, including identifying a single amino-acid substitution (S130W) in the eye lens proteins γ-crystallins responsible for a large increase in the critical temperature for phase separation [3] and revealing how cAMP regulates the phase separation of protein kinase A [4] and how pH regulates the phase separation of polySUMO and polySIM.

1. S. Qin and H.-X. Zhou (2016). Fast method for computing chemical potentials and liquid-liquid phase equilibria of macromolecular solutions. J. Phys. Chem. B. 120, 8164-8174.

2. K. Mazarakos, S. Qin, and H.-X. Zhou (2023). Calculating binodals and interfacial tension of phase-separated condensates from molecular simulations with finite-size corrections. Methods Mol. Biol. 2563, 1-35.

3. S. Qin and H.-X. Zhou (2023). Atomistic modeling of liquid-liquid phase equilibrium explains dependence of critical temperature on γ-crystallin sequence. Commun. Biol. 6, 886.

4. S.-H. Ahn, S. Qin, J. Zhang, J. A. McCammon, J. Zhang, J., and H.-X. Zhou (2021). Characterizing protein kinase A (PKA) subunits as macromolecular regulators of PKA RIα liquid-liquid phase separation. J. Chem. Phys. 154, 221101.

Predicting protein-peptide binding: Importance of peptide flexibility and physicochemical environment

Zou, Xiaoqin(邹晓勤)
University of Missouri

Peptides are short polymer chains consisting of amino acids. They exhibit flexibility and often undergo conformational changes when binding to proteins. Protein-peptide interactions play a crucial role in many cellular processes. The in silico prediction of protein-peptide complex structures is highly desirable for mechanistic studies and therapeutic design. However, predicting all-atom structures of protein-peptide complexes proves challenging without prior knowledge of the binding site and the bound peptide conformation due to the system's vast degrees of freedom. In this talk, I will present our recent development in predicting protein-peptide complex structures. The method integrates information-driven modeling with physically chemistry-based computational modeling of flexible interaction modes. The method has been systematically and extensively tested, and the results will be presented.

Kinetic Determinants of CRISPR/Cas9 Gene Editing: Insights from Data Learning and Energy Landscape Analysis

Chen, Shi-Jie(陈世杰)
University of Missouri, USA

Evaluation of CRISPR Cas9 cleavage efficiency and design of strategies to mitigate off-target effect require a mechanistic understanding and accurate modeling for CRISPR genome editing. The conventional perspective on CRISPR genome editing assumes a state of thermal equilibrium, governed by the principles of equilibrium thermodynamics. However, experimental investigations have suggested that the system is not in equilibrium, and, as a result, the process adheres to the principles of nonequilibrium kinetics. To address this, we leverage large-scale genome editing data and combine supervised machine learning with free energy landscape analysis and kinetic simulations. This integrated approach has yielded significant insights: it revealed a direct correlation between CRISPR cleavage efficiency and the rate of R-loop unfolding, identifying it as the key determinant for CRISPR cleavage efficiency. The finding led to the development of a predictive model for CRISPR based on nonequilibrium kinetics. This novel model not only unveils previously unidentified, yet biologically significant intermediates and pathways but also results in a highly accurate predictive model for both on-target and off-target genome editing. Consequently, it provides a new design strategy for maximizing and minimizing on-target and off-target cleavages, respectively

The Role of Electrostatics in Machine Learning Based Protein Property Prediction

Geng, Weihua(耿伟华)
Southern Methodist University

In this talk, we provide a machine learning model and related numerical algorithms to predict protein properties such as solvation energy, binding affinity, etc. In this model, the protein structure and force field information are abstracted as algebraic, geometric, topological, and electrostatics features. Our particular focus is on the generation of uniform and multiscale electrostatic features from Coulombic interaction and reaction field using fast treecode algorithm and boundary integral Poisson-Boltzmann solver.

Mathematical Graph Neural Network for Drug Discovery

Shen Cong (申聪)
NYU

The application of artificial intelligence (AI) technology in drug discovery has developed rapidly, greatly improving the speed and success rate of drug research. Through mining the hidden distribution patterns in existing data, deep learning models can predict key information such as the activity, targets, and metabolic properties of molecules, thereby assisting R&D personnel at each stage in making decisions. In recent years, the development of graph neural networks (GNNs) has alleviated many shortcomings of traditional deep learning models. Therefore, how to effectively play the role of graph neural networks, further shorten the time, and reduce the cost of drug research has become the focus of academic circles. Here, we propose advanced mathematic based graph neural network models for molecular representation and drug interaction prediction. Different from regular GNNs, we utilize Ricci curvature and analytic torsion to further enhance the GNNs model's ability to capture local information in the graph. Experimental results demonstrate that these models have great advantage over traditional models in drug discovery, material informatics and chemical informatics.

The Finite Expression Method: A Symbolic Approach for Scientific Machine Learning

Wang, Chunmei(王春梅)
University of Florida

Nonlinear dynamics is a pervasive phenomenon observed in scientific and engineering disciplines. However, the task of deriving analytical expressions to model nonlinear dynamics from data remains challenging. In this talk, the speaker will present a novel deep symbolic learning method called the "finite expression method" (FEX) to discover governing equations within a function space containing a finite set of analytic expressions, based on observed dynamic data. The key concept is to employ FEX to generate analytic expressions of the governing equations by learning the derivatives of partial differential equation (PDE) solutions through convolutions. The numerical results demonstrate that our FEX surpasses other existing methods (such as PDE-Net, SINDy, GP, and SPL) in terms of numerical performance across a range of problems, including time-dependent PDE problems and nonlinear dynamical systems with time-varying coefficients. Moreover, the results highlight FEX's flexibility and expressive power in accurately approximating symbolic governing equations.

Novel constrained total variation solvation models and the study of solute-solvent diffuse interface.

Chen, Zhan (陈展)
Georgia Southern University

Implicit solvent models are of tremendous importance to the biomolecular modeling community with thousands of exemplary applications in the literature due to their low computational cost and relatively high accuracy. The accuracy of implicit solvent models depends on the geometric description of the solute-solvent interface and the solvent dielectric profile that is defined near the molecules. In this talk, to improve the accuracy and efficiency of implicit solvent models with physically realistic solute-solvent smooth boundaries, we have introduced new constrained variational implicit solvation models (VISM) including two physical constraints: (1) a novel experimental based domain decomposition, and (2) a two-sided obstacle for the characteristic function describing the optimal diffuse solute-solvent boundary. Rigorous mathematical derivation and analysis of proposed models has been conducted. Our proposed solvation models, systematical parameterization approaches, and numerical algorithm implementation have been validated using several common biomolecular modeling tasks.

Bridging Atomic Details and Overall Kinetics: A Multiscale Computational Approach to Understand Peptide Self-Assembly

Wei Han (韩伟)
Georgia Southern University

Peptide/protein self-assembly is a fundamental process with both important implication in biology and practical value in material science. A detailed and quantitative description of this process is of utmost importance but difficult to obtain due to the complexity of peptide/protein self-assembly that involves multiple stages and phase transitions across a wide range of spatial and temporal scales. Molecular simulations cannot be used to explore the full picture of the process without sacrificing accuracy; kinetic models are often derived to understand experimental observations but with assumptions on underlying microscopic mechanisms and approximation on model parameters.

Here I propose an approach that can overcome this challenge and bridge atomic details and overall kinetics. Exploration of the atomic details of self-assembly is enabled by a combination of an efficient hybrid-resolution model and a metadynamics-based sampling method, both designed for peptide self-assembly simulations. The knowledge from these simulations is then used to derive an assumption-free kinetic model of peptide self-assembly with cluster statistical mechanics. I will further show how our approach can be used to interrogate at an atomic level the dependence of self-assembly of model peptide systems on factors like concentration, which is otherwise computationally too expensive to investigate with conventional simulations. These results allow us to re-evaluate previous kinetic models of peptide self-assembly and generate new insights into the key concepts such as reaction order, critical nucleus size and their relationship. Collectively, this approach paves the way toward a more realistic modeling of peptide self-assembly.

Stochastic Dynamics of Tipping in Biological Sciences

Duan, Jingqiao(段金桥)
Great Bay University

A goal of dynamical systems is to explain, quantify and predict complex phenomena in biological sciences, physical sciences and engineering. These phenomena include periodic and oscillatory motions, heteroclinic and homoclinic motions, diffusion, transport, connecting orbits and transitions.
Tipping is a class of phenomena depicting critical or abrupt transitions from one dynamical regime to another. Oftentimes, these transitions have significant consequences or devastating impacts. Thus, early detection and prediction of tipping is crucial for understanding and mitigating these phenomena. Stochastic dynamical systems are suitable frameworks for investigating tipping phenomena.

The speaker will present an overview about recent advances in the study of tipping phenomena in stochastic dynamical systems, including historical background, motivation, definition, techniques, and indicators for early warning or early detection of tipping.

Construction of Solution Landscapes of Complex Biological Systems

Zhang, Lei(张磊)
Peking University

Energy landscape has been widely applied to many physical and biological systems. A long standing problem in computational physics is how to search for the entire family tree of possible stationary stateson the energy landscape without unwanted random guesses? Here we introduce a novel concept “Solution Landscape”, which is a pathway map consisting of all stationary points and their connections. We develop a generic and efficient saddle dynamics 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 illustrations, we apply the solution landscape approach to study two problems: One is construction of the solution landscapes of gene regulatory networks in cell fate decisions, and the other one is to construct the solution landscape of reaction-diffusion systems, which reveals a nonlinear mechanism for pattern formation beyond Turing instability.

A latent space diffusion model for protein structure generation

Liu, Haiyan(刘海燕)
Univ. Science and Technology of China

we developed a model named PVQD (protein vector quantization and diffusion), in which diffusion was not performed in the original structure space but in a latent representation space of residue-wise three-dimensional structural contexts. This representation was learnt through auto-encoding with vector quantization. Compared with DDPMs in the three-dimensional structure space, the main advantage of PVQD is to divide the challenging task of end-to-end modeling of complicated protein structures between an auto-encoder and a diffusion model. We demonstrated that PVQD unified structure design and prediction in a single framework. We demonstrated that in design PVQD generated designable protein structures composed of non-idealized structure elements, while in prediction PVQD reproduced experimentally observed conformational variations for a set of natural protein.

Two-sample comparison without replicates in biological data analysis

Xue, Yu(薛宇)
Huazhong University of Science & Technology

Conventional two-sample comparison, e.g., the t-test, uses multiple replicates to estimate technical and systematic errors for calculating the statistical significance. However, a large diverse number of biological tasks request innovative mathematic methods, due to lack of either biological or technical replicates. Such difficult tasks include but not limited to the estimation of the functional consequence of a biological sequence with or without a single genetic mutation, and profiling of a patient's molecular data without replicates and any references. As a bioinformatician who is not an expert in mathematics, I hope to share our solutions on three important tasks, including identification of individual cancer mutations that change protein chemical modification state, identification of individual cancer mutations that change protein interaction, and identification of tissue-specific protein markers from COVID-19 patients. In the former two studies, we developed a Parzon window-based method, and used a published tool, model-based analysis of proteomic data (MAP) for the last task. The basic idea of the three study is that the changes of all data points are first ranked, and then data points in a short window are assumed to follow the same distribution, which is used to estimate the technical and systematic errors of each data point. Such a rough method facilitate the discovery of STBD1, a glycophagy receptor, as a new tumor suppressor, as well as finding of S100A8/A9 as lung-specific marker proteins in COVID-19 patients. A general and more rigorous method for addressing such tasks is yet to be developed.

Identification of Cell-Type-Specific Spatially Variable Genes Accounting for Excess Zeros

Luo, Xiangyu(罗翔宇)
Renmin University of China

Spatial transcriptomic techniques can profile gene expressions while retaining the spatial information, thus offering unprecedented opportunities to explore the relationship between gene expression and spatial locations. The spatial relationship may vary across cell types, but there is a lack of statistical methods to identify cell-type-specific spatially variable (SV) genes by simultaneously modeling excess zeros and cell-type proportions. We develop a statistical approach CTSV to detect cell-type-specific SV genes. CTSV directly models spatial raw count data and considers zero-inflation as well as overdispersion using a zero-inflated negative binomial distribution. It then incorporates cell-type proportions and spatial effect functions in the zero-inflated negative binomial regression framework. For robustness, a Cauchy combination rule is applied to integrate p-values from multiple choices of spatial effect functions. Simulation studies show that CTSV not only outperforms competing methods at the aggregated level but also achieves more power at the cell-type level. By analyzing pancreatic ductal adenocarcinoma spatial transcriptomic data, SV genes identified by CTSV reveal biological insights at the cell-type level.

Pain related drug addiction learning

Jiang, Jian(江健)
Wuhan Textile University

Pain is a significant global health issue, and the current treatment options for pain management have limitations in terms of effectiveness, side effects, and potential for addiction. There is a pressing need for improved pain treatments and the development of new drugs. Voltage-gated sodium channels, particularly Nav1.3, Nav1.7, Nav1.8, and Nav1.9, play a crucial role in neuronal excitability and are predominantly expressed in the peripheral nervous system. Targeting these channels may provide a means to treat pain while minimizing central and cardiac adverse effects. In this study, we construct protein-protein interaction (PPI) networks based on pain-related sodium channels and develop a corresponding drug-target interaction (DTI) network to identify potential lead compounds for pain management. To ensure reliable machine learning predictions, we carefully select 111 inhibitor datasets from a pool of over 1000 targets in the PPI network. We employ three distinct machine learning algorithms combined with advanced natural language processing (NLP)-based embeddings, specifically pre-trained transformer and autoencoder representations. Through a systematic screening process, we evaluate the side effects and repurposing potential of over 150000 drug candidates targeting Nav1.7 and Nav1.8 sodium channels. Additionally, we assess the ADMET (absorption, distribution, metabolism, excretion, and toxicity) properties of these candidates to identify leads with near-optimal characteristics. Our strategy provides an innovative platform for the pharmacological development of pain treatments, offering the potential for improved efficacy and reduced side effects.

Computational study of protein interaction systems

John Z.H. Zhang(张增辉)
East China Normal University

We will discuss computational approaches to studying protein interaction systems, from the perspective of quantum calculation of interaction energies, machine learing force field, protein-protein binding predicitons, and the design and optimization of proteins.

Performing enhanced sampling and electrostatic calculation for biomolecules

Chen, Changjun(陈长军)
HZUST

Molecular dynamics simulation is widely used in the study of life science. In this talk, I will give a detailed introduction to our recently developed program FSATOOL (short for fast sampling and analysis tool). FSATOOL contains four functional modules: molecular dynamics simulation module ("sim"), Markov state model module ("msm"), trajectory analysis module ("analysis") and electrostatic calculation module ("surfpb"). It supports the GPU-accelerated molecular dynamics simulation in the implicit and explicit solvent. It can also do many popular calculations like normal modes analysis, structure clustering, dimensional reduction, enhanced sampling and most importantly, the electrostatic potential and binding free energy calculation. A lot of examples are presented in the talk to illustrate the actual performance of FSATOOL.

Matrix Transformation Enhanced Large Model for Predicting the Structure and Dynamics of Multibody Protein Complexes

Gong, Xinqi(龚新奇)
Renmin University

Biomolecules participate in important tasks such as signal transduction and functional execution in the system, and experimental methods are constantly developing to obtain more and more static structures of protein molecules. However, how to efficiently obtain the structure and dynamic signals of multi body protein complexes is a challenging problem. By using adjacency matrices to represent commonly used symbol sequences and tree representations of biomolecules, and considering methods such as elastic networks, graph repair, and triangular multiplication, novel matrix transformations and fills can be further integrated into deep learning large models to calculate important signals such as functional dynamics and multi body protein complex structures that are difficult to obtain in prediction experiments. I will explain four calculation examples of our research group in this area and introduce the validation results of the experimenters. The calculation methods are published in NeuroIPS and IEEE International conferences such as BIBM, and the validation results were published in Nature and Nature Communications journals. Additionally, if time permits, I will also discuss our recent exploration in accelerating matrix calculations.

Diffuse interface model for cell interaction and aggregation with Lennard-Jones type potential

Xu, Shixin(徐士鑫)
Duke Kunshan University

This study introduces a phase-field model designed to simulate the interaction and aggregation of multicellular systems under flow conditions within a bounded spatial domain. The model incorporates a multi-dimensional Lennard-Jones potential to account for short-range repulsion and adhesive bonding between cells. To solve the governing equations while preserving energy law, a second-order accurate C0 finite element method is employed. The validity of the model is established through numerical tests, and experimental data from cell stretch tests is utilized for model calibration and validation. Additionally, the study investigates the impact of varying adhesion properties in red blood cells. Overall, this work presents a thermodynamically consistent and computationally efficient framework for simulating cell–cell and cell–wall interactions under flow conditions. The work is collaborated with Dr. Lingyue Shen, Dr. Ping Lin, and Dr. Zhiliang Xu.

3dRNA/DNA: 3D Structure Prediction from RNA to DNA

Xiao, Yi(肖奕)
Huazhong University Science and Technology

There is an increasing need for determining 3D structures of DNAs. For example, in DNA aptamer selection, the number of possible candidates is very large, and so it is a hard work to determine the best one from the candidates through experiments. It is expected that computational methods of predicting 3D structures of the candidates will be very helpful for increasing the efficiency of aptamer selection. However, no such methods are available, although those for RNAs have been widely developed. Recently, we have extended our computational method of 3D structure prediction of RNAs, 3dRNA, to include DNAs and the web server is now named as 3dRNA/DNA.

3dRNA/DNA is a template-based method, which combines both DNA and RNA 3D template libraries to predict DNA 3D structures. For a target DNA, its sequence and secondary structure are taken as inputs. 3dRNA/DNA decomposes the target RNA into secondary structure elements (SSEs) and finds a 3D template for each of them from a combined SSE 3D template library of DNA and RNA or the bi-residue algorithm. Using the templates of each SSE, the candidates of the 3D structure of the target DNA can be assembled. The benchmarks on three test sets with different numbers of chains show that the mean lowest-RMSD of the built 3D DNA structures is about 2.36 Å for those with one or two chains and about 4 Å with three or more chains. In this talk, I shall report the latest advance in 3dRNA/DNA.

Structure-preserving discretization for the Poisson —Nernst—Planck equations

Zhou Shenggao(周圣高)
Shanghai Jiao Tong University

The Poisson—Nernst—Planck (PNP) equations have been widely used in the simulations of biomolecular systems. This talk proposes novel second-order discretization in time and finite volume discretization in space for modified PNP equations that incorporate effects arising from ionic steric interactions and dielectric inhomogeneity. A multislope method on unstructured meshes is proposed to reconstruct positive, accurate approximations of mobilities on faces of control volumes. Numerical analysis proves that the proposed numerical schemes are able to unconditionally ensure the existence of positive numerical solutions, original energy dissipation, mass conservation, and preservation of steady states at discrete level. Extensive numerical simulations are conducted to demonstrate numerical accuracy and performance in preserving properties of physical significance. Applications in ion permeation through a 3D nanopore show that the modified PNP model, equipped with the proposed schemes, has promising applications in the investigation of ion selectivity and rectification. The proposed second-order discretization can be extended to design temporal second-order schemes with original energy dissipation for a type of gradient flow problems with entropy.

A Hybrid CPU/GPU Method for Hartree-Fock Self-Consistent-Field Calculation

Yang, Minghui(杨明晖)
WIPM, China

We present the progress of WESP (Wuhan Electronic Structure Package), a quantum chemistry software designed for high-throughput computing in the fields of drug and material discovery. The calculation of two-electron repulsion integrals (ERIs) is a hot-pot of Hartree-Fock (HF) calculations. In computing the ERIs of varying angular momentum, both CPU and GPU have their respective advantages. To accelerate the ERI evaluation and Fock matrix generation, a hybrid CPU/GPU method has been proposed to maximize the computational power of both CPU and GPU, while overlapping the CPU and GPU computations. The testing calculations showed that the hybrid CPU/GPU algorithm is more efficient than "GPU-only" when using a single GPU. However, as more GPUs are involved, the advantage diminishes or disappears. Scaling exponents of the hybrid method were slightly higher than "GPU-only," but the pre-exponent factor was significantly lower, making the hybrid method more effective overall, Furthermore, WESP is compared with widely-used quantum chemistry software on the Intel-nVidia platform and some domestic computing platforms.

A geometric characterization of DNA sequence, and beyond

Fan, Xu-Qian (范旭乾)
Jinan University

We will present two common geometric quantities, area and curvature, to DNA sequence analysis based on the graphical representation method introduced by Yau et al. in 2003. If time permits, we will also discuss a geometric algorithm for path planning. This is a joint work with Gong Wenyong.

A topological framework for high-order interactions

Wu, Jie(吴杰)
BIMSA

The high-order interaction structures of complex networks pose a challenging scientific problem. Compared to pairwise interaction networks, where a wealth of mature mathematical tools and theoretical methods are available, mathematical approaches for high-order interaction complex networks are currently quite limited and have not yet formed a mature theoretical framework. In this report, I will introduce our recent proposed mathematical definition of high-order interactions using a binary tree structure, along with its corresponding topological quantitative representation, like the homology. At the same time, I will provide some specific examples of microbial interactions to demonstrate how the proposed theory can be applied to decipher high-order interactions.

Exploring Disease-Related and Functional Amyloid Proteins Self-Assembly through Computational Simulations

Yunxiang Sun(孙运祥)
Ningbo University

The self-assembly of proteins into amyloid fibrils has attracted considerable attention due to their association with various human degenerative diseases, physiological functions, and potential applications in biomedicine and bio-nanotechnology. Despite differences in biological functions, amino acid sequences, and tertiary structures among these amyloid peptides, they share common cross-β architectures in their fibrils. However, oligomers formed during the assembly process are usually heterogeneous and unstable, making their isolation, quantification, and structural determination experimentally challenging. The characterization of these oligomeric intermediates is crucial for understanding pathogenesis, designing anti-amyloidosis drugs, and facilitating the design of functional amyloid peptides. In my presentation, I will discuss the self-assembly mechanism of disease-related polypeptides and functional amyloid peptides based on our systematic computational investigation of the aggregation of amyloid-β, amylin, suckerin, and β-endorphin peptides.

CF22D: Chemistry Functional 2022 with Damped Dispersion

Xiao He (何晓)
East China Normal University

We developed a new density functional named CF22D, which is universally applicable to various types of molecular systems, by building accurate and diverse chemical property databases, introducing new physical descriptors, and utilizing a supervised learning scheme. We chose a flexible functional form that combines a global hybrid meta nonseparable gradient approximation that depends on density and occupied orbitals with a damped dispersion term that depends on geometry. This enabled the CF22D functional to provide universally reliable predictions for molecular energetics, barrier heights, and noncovalent interactions, including the properties of large molecules where the additive effect of many noncovalent interactions is not negligible. The energy functional was optimized by using a new performance-triggered iterative supervised training strategy involving a new, high-precision, diverse chemical property database, named DDB22, and this yielded a universal chemistry functional with higher across-the-board accuracy for both main-group and transition-metal chemistry. The CF22D functional has higher prediction accuracy than most other popular density functionals, and it even performs better than some doubly-hybrid functionals, which are more computationally demanding.

Protein dynamics: energy frustration and allosteric regulation

Wenfei Li(李文飞)
Nanjing University

With the breakthroughs in predicting the three-dimensional static structure of proteins in recent years, the study of protein dynamics has received increasing attention. Enzyme molecules have been widely used as model systems to study protein dynamics, because their catalytic activitiescritically rely on the conformational motions. Enzymes in nature usually have amazing catalytic efficiency. What physical strategies do enzyme molecules adopt to overcome rate-limiting step in catalytic cycle and achieve efficient catalysis is a basic but not fully understood question. In this talk, I will introduce our recent efforts in understanding this issue. By constructing a computational model capable of describing the interplaybetween conformational motions and catalytic activity, we showed that enzymes can utilize energy frustration to realize high catalytic efficiency. We further investigated the allosteric regulation of enzyme dynamics and the prediction of protein dynamic strutures by employing this strategy.

Inductive Learning of Protein-Protein Interaction from Antibody-Antigen Recognition using GraphSAGE

Buyong Ma(马步勇)
Shanghai Jiao Tong University

Antibody is one of the most important immunological molecules and can be engineered as effective biological drugs. We have studied the signal transduction of antibody-antigen recognition, antibody receptor binding, and transmembrane allosteric correlation using molecular dynamic simulations. Antibody- protein antigen interaction is a subset of general protein-protein interaction, sharing similar mechanisms but with distinct special characteristics. Various deep learning approaches were used to predict antibody-antigen interactions. We have shown that an inductive learning model can be demonstrated by learning overall Protein-Protein Interactions from smaller Antibody-Antigen Recognition subset.

Protein Design Based on Deep Learning and Function Validation

Haifeng Chen(陈海峰)
Shanghai Jiao Tong University

Protein design is central to nearly all protein engineering problems, as it can enable the creation of proteins with new biological function, such as improving the catalytic efficiency of enzymes. One key facet of protein design, fixed-backbone protein sequence design, seeks to engineer new sequences that will conform to a prescribed protein backbone structure. Nonetheless, existing sequence design methods present limitations, such as reduced sequence diversity and shortcomings in experimental validation of the designed protein function, inadequacies that obstruct the goal of functional protein design. To improve these limitations, we initially developed the Graphormer-based Protein Design (GPD) model. This model deploys the Transformer on a graph-based representation of 3D protein structures and supplements it with Gaussian noise and a sequence random mask applied to node features, thereby enhancing sequence recovery and diversity. The performance of GPD model was significantly better than that of state-of-the-art model for ProteinMPNN on multiple independent tests, especially for sequence diversity. CalB hydrolase as model system was used to validate the performance of GPD. The results show significant improvement in the catalytic activity and substrate selectivity with 1.7 times increase compared to the CalB wild type and strong substrate selectivity on p-Nitrophenyl acetate with different carbon chain lengths (C2–C16). Thus, GPD method could be used for the de novo design of industrial enzymes and protein drugs with specific functions.

CF22D: Chemistry Functional 2022 with Damped Dispersion

Shengyou Huang(黄胜友)
Huazhong University of Science and Technology

Accurate prediction of drug-protein interactions is crucial for drug discovery. Due to the bottleneck of traditional scoring functions, many machine learning scoring functions (MLSFs) have been proposed for structure-based drug screening. However, existing MLSFs face two challenges: small data limitations and poor interpretability. To address these challenges, we have proposed a physics-based small data machine learning framework for interpretable and generalizable prediction of drug-protein interactions on the target with scarce positive data through a strategy of three training phases with three (Score, Weight, and Ranking) loss functions, named DrugBaiter. DrugBaiter was extensively evaluated on the 102 targets of DUD-E and 81 targets of DEKOIS 2.0 for drug screening, and compared with 18 other scoring functions. It is shown that our DrugBaiter model can significantly improve the drug screening performance even if few actives are known for a target. In addition, DrugBaiter is interpretable in describing the interactions at the atomic level. The power of DrugBaiter is also confirmed by a drug screening application on the SARS-Cov-2 main protease target. It is anticipated that DrugBaiter will serve as a general machine learning scoring model for screening novel drugs on new targets with scarce known actives. DrugBaiter is freely available at http://huanglab.phys.hust.edu.cn/DrugBaiter.

Drug Discovery Driven by Molecular Dynamics Simulation

Qiantao Wang(王乾韬)
Sichuan University

With the rapid development in high performance computing, molecular dynamics (MD) simulation as an accurate physics-based method is becoming more and more accessible for large scale protein-protein and protein-ligand calculations that are of fundamental interests in drug discovery. In this talk, we discuss our recent progress and challenges in applying MD simulation to real world drug discovery projects and the development in next-generation force field.

Mechanism of midazolam metabolism mediated by cytochrome P450 3A4

细胞色素P450 3A4介导的咪达唑仑代谢机制

Qingchuan Zheng(郑清川)
Jilin University

Cytochrome P450 3A4 (CYP3A4) is the most important P450 enzyme in drug metabolism and drug-drug interactions. A large cavity and plasticity of the active site of CYP3A4 allow it to bind multiple drug molecules with multiple binding modes, or even to bind multiple drug molecules in one pocket. Thus, CYP3A4 is capable to metabolize about 50% of the drugs in clinical with relatively complex metabolism processes. The regioselective metabolism of multiple drugs by CYP3A4 is because of the regulation of substrate concentration and the allosteric regulation of other drug molecules, and the metabolism process exhibits complex atypical kinetic features. Understanding the complex microscopic processes of drug metabolism mediated by CYP3A4 and its regulatory mechanisms is important to relevant drug discovery and development, rational utilization of drugs, and disease treatment. In this work, midazolam (MDZ) was used as a probe to reveal the mechanism of CYP3A4 regioselective oxidation through a in silico study integrated multiple computational methods, including homologous modeling, molecular docking, classical molecular dynamics simulations, accelerated molecular dynamics simulations, umbrella sampling and Well-Tempered Metadynamics simulations. Three interaction modes and the key factors between CYP3A4 and MDZ were clarified. Two peripheral allosteric sites of CYP3A4 were predicted. The law of the influence of allosteric effect on the metabolic regioselectivity was summarized in terms of both homologous and heterologous allosteric regulation. The result can provide valuable information on the study of CYP3A4 structure and function, and is significance for the prediction of drug-drug interaction and lead compound optimization.

细胞色素P450 3A4(CYP3A4)是药物代谢和药物-药物相互作用中最为重要的P450酶。CYP3A4的活性位点具有空腔体积较大且可塑性较强的结构特征，可结合多种结构不同的药物分子，甚至可多分子同时结合，故CYP3A4能够代谢临床中大约50%的药物，并且代谢过程相对复杂。CYP3A4对多种药物的代谢因受底物浓度和其它药物分子的别构调控，而具有区域选择性，且代谢过程表现出复杂的非典型动力学特征。理解CYP3A4介导的药物代谢复杂的微观过程及其调控机制，对于相关的药物研发、药物合理使用及疾病治疗都具有重要的指导意义。我们以咪达唑仑(MDZ)分子为探针，采用同源模建、分子对接、经典分子动力学模拟、加速分子动力学模拟、伞形取样和Well-Tempered Metadynamics模拟方法，系统考察了CYP3A4与MDZ的相互作用情况，明确了CYP3A4与MDZ的三种作用模式及作用过程中的关键因素，预测了CYP3A4的两个外周别构位点，从同源和异源别构调控两个方面总结了别构效应对代谢区域选择性的影响规律。该项研究可为研究CYP3A4的结构和功能提供有价值的参考信息，能够促进对药物复杂代谢机制的理解，对药物-药物相互作用预测和先导化合物优化也具有重要意义。

Reference-Potential Methods for the Computation of Free Energy at ab initio QM/MM Level

Ye Mei(梅晔)
East China Normal University

Calculations of thermodynamics properties such as state free energy differences and free energy profile at an ab initio QM/MM level are a daunting challenge, due that extensive phase space sampling is always indispensable before convergence can be reached and for most cases many intermediate states are required to make the conversion between two states smooth enough. Recently, we proposed a reference-potential method for the calculations of thermodynamics properties at high QM/MM levels using phase space sampling under low-level Hamiltonians followed by (extended) free energy perturbation to the high-level Hamiltonian. Although this method is statistically sound, quality of the result is often impaired by the slow convergence when applying these methods. Remedies that can increase the reliability are presented.

Development and Application of Enhanced Sampling Methods Based on Feature Space

Hao Dong(董昊)
Nanjing University

Protein folding and conformational changes are important properties of proteins, and they directly affect protein function and activity. In recent years, we have proposed an enhanced conformational sampling scheme within the framework of the feature space for adaptive updating of protein structures, and successively developed the DAta-Driven Accelerated (DA2) sampling method [1] and the two-ended DA2 (teDA2) sampling method: DA2 is designed to search for biological macromolecules from the known structure of the new functional states, while teDA2 is designed to identify possible paths between two available states of a biomolecule. However, the current scheme uses traditional molecular dynamics simulations for sampling local conformations, which still suffers from insufficient sampling. Therefore, we further developed the MC-DA2 method. This method introduces the idea of Monte Carlo in the DA2 method, which accelerates the driving of conformational changes by randomly adding perturbations in the direction of its principal components to generate new structures for the sampled conformations in the feature space. Using the MC-DA2 method, we have realized the kinetic transition process of common small proteins, such as chignolin (10 residues) and WW-domain (35 residues), from the stretched state to the folded state in solution in hundred-nanosecond simulations.

The optimal genome metric from an alignment-free perspective

Yu, Hongyu(余泓谕)
Tsinghua University

As the number of known genomes rockets, alignment-free methods have gained considerable attention for their high efficiency. However, the abundance of alignment-free features that can be extracted from sequences poses a challenge – how to effectively aggregate this diverse information. We adopt the natural vector framework, which utilizes statistical moments of sequence kmers as feature information, and employ optimization theory to determine the optimal approach for aggregating information within this framework. This method has yielded impressive results in the classification of viral reference sequences.

Deep Learning-Based Predictive Modeling of Prokaryotic Promoter Strength Using Coevolutionary Information

Ren, Ruohan(任若寒)
Tsinghua University

In the field of synthetic biology, precise characterization and optimization of regulatory elements, particularly promoters, are fundamental in designing synthetic gene circuits. Experimental methods for promoter engineering often involve high unpredictability and labor intensiveness. To address these challenges, we present a coevolution-infused deep learning model that accurately predicts the strength of prokaryotic promoters. Our model, validated through fluorescence protein experiments, significantly outperforms existing approaches, achieving a Pearson correlation coefficient (PCC) of 0.56, surpassing the prior benchmark of 0.3. Leveraging coevolutionary information extracted from promoter sequences, our model demonstrates its effectiveness in simulating directed promoter evolution, offering a robust tool for in silico analysis. Additionally, by applying transfer learning, our model displays adaptability, achieving superior performance (R-squared value of 0.77, better than 0.53) in predicting specific promoter strengths (e.g. trc promoter). The results underscore the model's considerable advantage over existing methods, marking a substantial stride in the precise prediction and optimization of prokaryotic promoter strengths, vital in advancing synthetic biology applications.

Exploring geometry of the genome space via Grassman manifolds: the FCGR-SD method

Zhou,Tao(周涛)
Tsinghua University

Genome space is the entire set of genomes of all living organisms, which can be used to gain a comprehensive understanding of the dynamic genomic evolutionary process. Mathematically, the genome space can be regarded as a moduli space of genomes, where each point in the space represents a unique genome, and the distance between two points corresponds to the biological distance between those corresponding genomes.

We aim to explore the manifold structure hidden behind genome sequences by referring to the experience in some biological fields like neuroscience and single-cell genomics. We will start with the chaos game representation of sequences, introduce how the k-mer fragment information in genome sequences is constructed into a matrix, and then embed the sequences into Grassman manifold by extracting the information in the column space.

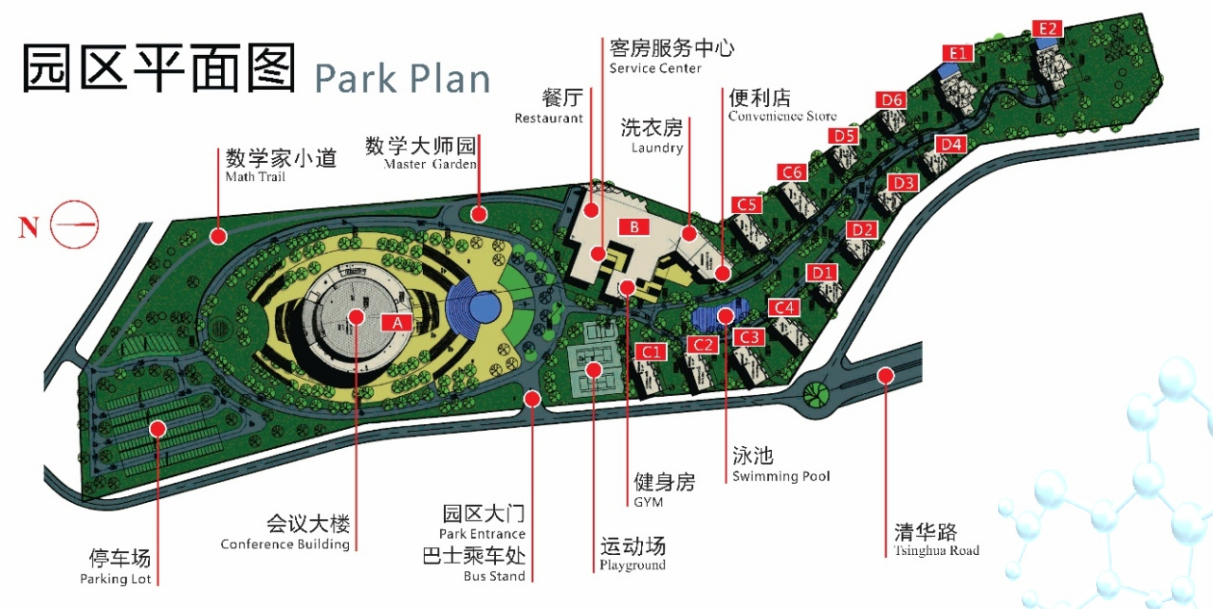
Due to the differences in the information extracted from different sequences in the column space, the dimensions of the manifolds embedded by these sequences may vary. However, we can use a mathematical result to define a unified geodesic distance to characterize the similarity between sequences, and then use this as a basis for downstream analysis such as phylogenetic analysis.

Welcome to TSIMF

The facilities of TSIMF are built on a 23-acre land surrounded by pristine environment at Phoenix Hill of Phoenix Township. The total square footage of all the facilities is over 29,000 square meter that includes state-of-the-art conference facilities (over 10,000 square meter) to hold many international workshops simultaneously, two reading rooms of library, a guest house (over 10,000 square meter) and the associated catering facilities, a large swimming pool, gym and sports court and other recreational facilities.

Management Center of Tsinghua Sanya International Forum is responsible for the construction, operation, management and service of TSIMF. The mission of TSIMF is to become a base for scientific innovations, and for nurturing of innovative human resource; through the interaction between leading mathematicians and core research groups in pure mathematics, applied mathematics, statistics, theoretical physics, applied physics, theoretical biology and other relating disciplines, TSIMF will provide a platform for exploring new directions, developing new methods, nurturing mathematical talents, and working to raise the level of mathematical research in China.

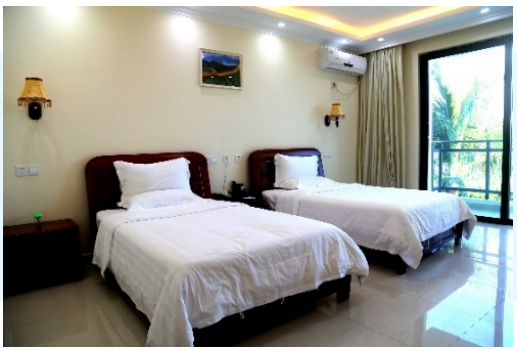
About Facilities



Registration

Conference booklets, room keys and name badges for all participants will be distributed at the front desk. Please take good care of your name badge. It is also your meal card and entrance ticket for all events.

Guest Room



All the rooms are equipped with: free Wi-Fi (no password), TV, air conditioning and other utilities.

Family rooms are also equipped with kitchen and refrigerator.

Library

Opening Hours: 09:00am-22:00pm

TSIMF library is available during the conference and can be accessed by using your room card. There is no need to sign out books but we ask that you kindly return any borrowed books to the book cart in library before your departure.

In order to give readers a better understanding of the contributions made by the Fields Medalists, the library of Tsinghua Sanya International Mathematics Forum (TSIMF) instituted the Special Collection of Fields Medalists as permanent collection of the library to serve the mathematical researchers and readers.
So far, there are 234 books from 47 authors in the Special Collection of Fields Medalists of TSIMF library. They are on display in room A220. The participants are welcome to visit.

Restaurant

All the meals are provided in the restaurant (Building B1) according to the time schedule.

Breakfast	**07:30-08:30**
Lunch	**12:00-13:30**
Dinner	**17:30-19:00**

Laundry

Opening Hours: 24 hours

The self-service laundry room is located in the Building 1 (B1).

Gym

The gym is located in the Building 1 (B1), opposite to the reception hall. The gym provides various fitness equipment, as well as pool tables, tennis tables etc.

Playground

Playground is located on the east of the central gate. There you can play basketball, tennis and badminton. Meanwhile, you can borrow table tennis, basketball, tennis balls and badminton at the reception desk.

Swimming Pool

Please note that there are no lifeguards. We will not be responsible for any accidents or injuries. In case of any injury or any other emergency, please call the reception hall at +86-898-38882828.

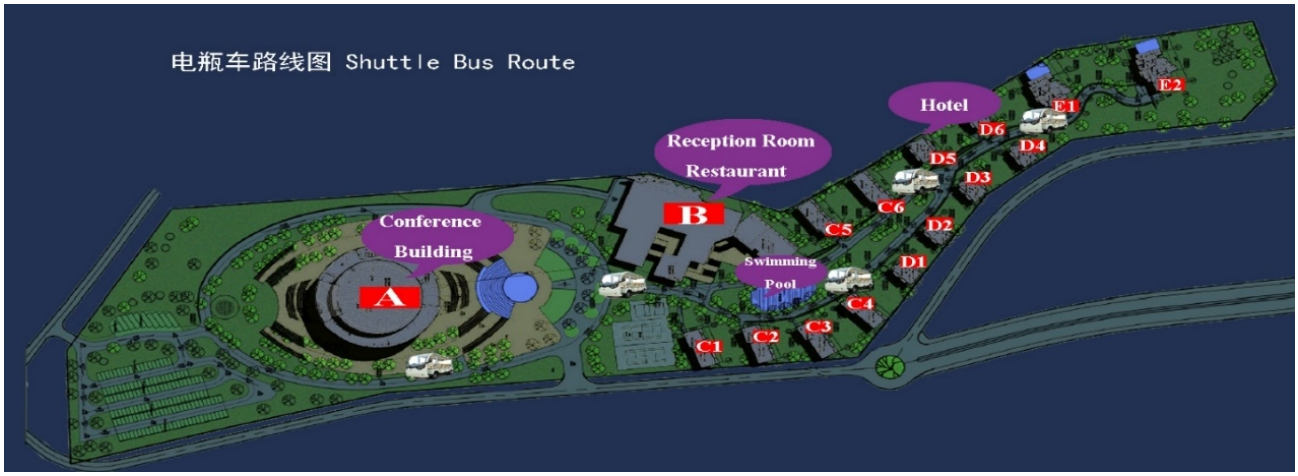
Outside Shuttle Service

We have shuttle bus to take participants to the airport for your departure service. Also, we would provide transportation at the Haihong Square (海虹广场) of Howard Johnson for the participants who will stay outside TSIMF. If you have any questions about transportation arrangement, please feel free to contact Ms. Li Ye (叶莉)at (0086)139-7679-8300.

Free Shuttle Bus Service at TSIMF

We provide free shuttle bus for participants and you are always welcome to take our shuttle bus, all you need to do is wave your hands to stop the bus.

Destinations: Conference Building, Reception Room, Restaurant, Swimming Pool, Hotel etc.



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