Science Newsletter

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Contents

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Introduction:

There are 3 main elements in the Science Newsletter which is composed. In the first part, we list the most up to date papers about central issues for each discipline in our university, and they are provided with 5 subjects for a time. In the second part, there are papers from the top journals last month, and most of them are from Nature and Science. In the third part, we post information about calling papers for international conferences. Hopefully, some of the information in this manuscript may be useful for those who are dedicating to scientific career. Besides, the journals are also posted on the website of our library, and they are available to be accessed any time at https://lib.jsut.edu.cn/2018/1015/c5474a113860/page.htm . If there are any questions or suggestions, please send e-mails to ccy@jsut.edu.cn in no hesitate.

Ⅰ Topics

The keywords of this month is **Mathematics**:
We post several papers which are related to the top concerned topics in researches on Mathematics. The papers are classified in 5 categories, and they are: **Statistical modeling, Parameter optimization, Time series analysis, Applied mathematics** and **Topology**. Also, the listed papers are all arranged in a descending sort of JCR impact factor. If you want full pages of these papers, please contact us for help.

STATISTICAL MODELING

Proc Natl Acad Sci U S A (impact factor: 9.1) 1 区 TOP

Data-driven Mori-Zwanzig modeling of Lagrangian particle dynamics in turbulent flows.

Xander de Wit, Alessandro Gabbana, et. al

Abstract:
The dynamics of Lagrangian particles in turbulence play a crucial role in mixing, transport, and dispersion in complex flows. Their trajectories exhibit highly nontrivial statistical behavior, motivating the development of surrogate models that can reproduce these trajectories without incurring the high computational cost of direct numerical simulations of the full Eulerian field. This task is particularly challenging because

reduced-order models typically lack access to the full set of interactions with the underlying turbulent field. Novel data-driven machine learning techniques can be powerful in capturing and reproducing complex statistics of the reduced-order/surrogate dynamics. In this work, we show how one can learn a surrogate dynamical system that is able to evolve a turbulent Lagrangian trajectory in a way that is point-wise accurate for short-time predictions (with respect to Kolmogorov time) and stable and statistically accurate at long times. This approach is based on the Mori-Zwanzig formalism, which prescribes a mathematical decomposition of the full dynamical system into resolved dynamics that depend on the current state and the past history of a reduced set of observables, and the unresolved orthogonal dynamics due to unresolved degrees of freedom of the initial state. We show how by training this reduced order model on a point-wise error metric on short time-prediction, we are able to correctly learn the dynamics of Lagrangian turbulence, such that also the long-time statistical behavior is stably recovered at test time. This opens up a range of applications, for example, for the control of active Lagrangian agents in turbulence.

Sci Total Environ (impact factor: 8) 2 区 TOP

QSAR meets ecology: Predictive framework for assessing pesticide toxicity against mayfly using consensus modelling.

Disha Mahapatra, Shubha Das, et. al

Abstract:

The extensive use of pesticides in agriculture holds serious toxicological risks to aquatic and terrestrial ecosystems. Traditional toxicity assessment methods are costly, time-consuming, and ethically constrained due to animal testing requirements. In this context, quantitative structure-activity relationship (QSAR) offers a distinct benefit to forecast the toxicity of substances. The current study builds partial least squares (PLS)-based QSAR models for evaluating the detrimental impacts of chemicals against mayfly (Ephemera vulgata) species, following OECD rules and using LD50 as a specified endpoint. Mayfly is useful in providing food for fish and is designated as a standard species that preserves freshwater habitats, indicating heavy metal contamination. The results from internal and external validation parameters (R2 = 0.684-0.689, Q2(LOO) = 0.648-0.661, R2pred or Q2F1 = 0.665-0.694, and Q2F2 = 0.661-0.690) confirmed that the produced model is stable and robust, as all the statistical parameters are very close to each other. Intelligent consensus prediction (ICP) is used to enhance the external predictivity and reliability of the model (R2pred or Q2F1 = 0.726 and Q2F2 = 0.722). In accordance with the information obtained, the presence of electronegative atoms, large fragments, aliphatic (CHR3) groups, less polar atoms, poisonous phosphate groups, and high number of long carbon chains are the principal biomarkers for pesticide toxicity. This framework was further used to screen the Pesticides Properties Database (PPDB) to evaluate the reliability of

established models. This helps design eco-friendly chemicals, streamlines regulatory decision-making, confirms the external predictability of the established model, and advances the development of a sustainable earth.

Chem Res Toxicol (impact factor: 3.8) 3 ☒

Machine Learning-Based Quantitative Structure Activity Relationship Modeling of Repeated Dose Toxicity: A Data-Driven Approach Following Organisation for Economic Co-operation and Development Test Guidelines 407, 408, and 422 Supported by Experimental Validation.

Souvik Pore, Zsuzsanna Szepesi, et. al

Abstract:

In recent years, the rapid increase in the production and environmental release of synthetic organic chemicals has raised serious concerns about their potential adverse effects on human health and the environment. Repeated exposure to such substances can lead to significant toxicological effects, underscoring the importance of early and reliable hazard assessment. However, experimental determination of repeated-dose toxicity (RDT) is costly, time-consuming, and constrained by ethical considerations. In this study, we developed various classification-based predictive models to evaluate the subchronic RDT potential of chemicals after oral exposure. We compiled data from eChemPortal and J-CHECK databases. The data set contains two study-derived effect levels: NOAEL (no observed adverse effect level) and LOAEL (lowest observed adverse effect level), for which separate models have been developed. A key strength of this data set is that all studies followed standardized OECD test guidelines (407, 408, and 422) and were conducted under good laboratory practice (GLP) conditions, ensuring regulatory relevance and high data reliability. Multiple machine learning algorithms were systematically evaluated, and the best models were selected using a multicriteria analysis based on the sum of ranking differences (SRD) technique. The final selected models achieved accuracies on the training sets ranging from 0.665 to 0.902, while the test sets showed accuracies ranging from 0.642 to 0.682. We also conducted a substructure analysis to identify the key substructures involved in the toxicity. This analysis revealed eight structural motifs, with chlorine- and amine-group-containing aromatic systems being particularly significant. The final developed models were experimentally validated using chemical substances provided by Global Product Compliance (GPC) Europe AB. Additionally, the models were applied to the Pesticides Properties DataBase (PPDB) to screen for pesticides with potential toxicity upon repeated exposure. To facilitate accessibility and regulatory application, the final models have been implemented in both a Python-based tool and a web application. Scientific contribution: this study presents predictive models as alternatives to traditional animal testing for assessing the subchronic oral repeated-dose toxicity (RDT) of chemicals. Our models demonstrate strong statistical performance, indicating their suitability for further application, as supported by experimental validation. These models could be used for preliminary hazard screening or weight-of-evidence evaluations. An additional advantage is that these models were developed using data that were tested in accordance with internationally harmonized test protocols, thereby enhancing their acceptance for regulatory decision-making.

PARAMETER OPTIMIZATION

J Environ Manage (impact factor: 8.4) 2 ☒

Decoding the drivers of global desertification sensitivity from 2005 to 2020.

Qi Wu, Gangte Lin, Min He, et. al

Abstract:

Land desertification threatens ecosystem sustainability and socioeconomic development globally. We assessed global desertification sensitivity from 2005 to 2020 using the Google Earth Engine-Mediterranean Desertification and Land Use (GEE-MEDALUS) model, integrating Climate (CQI), Soil (SQI), Vegetation (VQI), and Management (MQI) Quality Indices. Drivers were quantified with the Optimal Parameters-based Geographical Detector (OPGD) at the global scale, and causality was evaluated in China using the Geographical Convergent Cross Mapping (GCCM) model. Results showed persistent spatial heterogeneity, with high to extreme sensitivity concentrated in arid, semi-arid, and sub-humid margins, particularly across North Africa, the Middle East and Central Asia. Temporally, extreme sensitivity areas remained stable (11.5%-12.0%), while high sensitivity expanded slightly (20.8% to 21.8%). OPGD identified CQI and SQI as dominant drivers (mean q = 0.74 and 0.65), surpassing VQI and MQI (mean q = 0.56 and 0.53). Specifically, the Aridity Index and Soil Organic Matter were the most influential indicators (q = 0.80 and 0.79), and their interaction amplified explanatory power (q = 0.77-0.80). GCCM confirmed causal linkages for all indicators except Depth to Bedrock. These findings highlight a distinct climate-soil co-limitation, and help prioritize interventions to enhance resilience under environmental change.

J Environ Manage (impact factor: 8.4) 2 ☒

A critical review on the removal of heavy metals in aqueous solution through pulse electrochemical processes: Basic principles, system design and environmental applications.

Peidong Su, Meng Su, Haoyang Xiong, et al

Abstract:

Electrochemical methods are considered among the most effective strategies for the removal of heavy metal ions from wastewater. The traditional direct current (DC) electrochemical method mainly targets aqueous solutions containing single metal pollutants, so when multiple competing ions appear, it significantly hinders the effective DC electrodeposition of heavy metal ions. Conversely, pulsed current (PC) electrolysis characterized by periodically varying current or potential has been widely employed in chemical synthesis due to its unique ability to regulate the local

microenvironment surrounding the electrode. This article elaborates on the sources and risks associated with heavy metals, and presents the advantages of pulse electrochemical technology in treating heavy metal ions. And the fundamental principles, experimental methods, optimal operating conditions and parameters, as well as environmental applications of the two primary methods of electrocoagulation and electrodeposition were thoroughly discussed. At the same time, this article also analyzed the reasons why PC method can suppress side reactions such as water splitting reaction. Finally, the most promising avenues and potential opportunities and challenges of pulse electrochemical technology in heavy metal recovery were proposed. The finding in this review will provide useful implications in guiding the application of pulse electrochemistry in heavy metals removal from wastewater.

ISA Trans (impact factor: 6.5) 2 ☒

New results of vehicle sway dynamic system via a new LKF lemma and optimization algorithm.

Yunpei Chen, Can Zhao, et. al

Abstract:

In vehicle systems, both information transmission and motor response exhibit non-negligible time-delay characteristics. To make performance predictions more consistent with actual vehicles, this paper focuses on the conservatism of vehicle delay systems. Existing methods involve strict constraints and limitations, and some approaches exhibit stronger conservatism. Therefore, this paper proposes a new slack Lyapunov function lemma to handle time-delay terms in the system by constructing a relaxation matrix. Additionally, a genetic algorithm is employed to optimize the adjustable parameters in the quadratic function negative determination lemma, further reducing the conservatism of the linear matrix inequality. Based on these strategies, stability criteria for the Takagi-Sugeno fuzzy vehicle sway system are developed. Simulation results demonstrate that the proposed method increases the system's maximum time-delay upper bound, reduces conservatism, and verifies the effectiveness and feasibility of the proposed approach.

TIME SERIES ANALYSIS

Water Res (impact factor: 12.4) 1 ☒ TOP

An attention fusion of Fourier-analysis-based transformer and CNN-BiLSTM for coastal inorganic nitrogen concentration forecasts.

Abstract:
Accurate forecasting of coastal inorganic nitrogen is critical for mitigating harmful algal blooms but remains challenging due to prevalent data gaps and skewed concentration distributions. This study proposes AFTB, a novel deep learning architecture that integrates a Fourier-enhanced Transformer with a CNN-BiLSTM network via dedicated attention mechanisms for robust multi-step forecasting. A logarithmic transformation is introduced to address severe right-skewness with a modified loss function balancing error weighting. Extreme-value oversampling strategy also improves the performance. Comprehensive evaluation across nine buoy stations in Guangxi, China demonstrates AFTB's superior accuracy over strong baselines (ChloroFormer, CNN-Transformer, Informer). Crucially, controlled Missing-Completely-at-Random experiments provide direct evidence of its exceptional robustness to training data incompleteness, showing minimal mean performance variance as missingness increases. Analysis of internal attention weights reveals interpretable forecasting patterns and validates the design of the fusion mechanisms. With competitive inference speed, AFTB presents a practical and resilient solution for operational water quality forecasting systems.

Med Phys (impact factor: 3.2) 3 区

Real-time energy measurement of clinical carbon ion beams using a cross-correlation time-of-flight method with parallel-plate chambers.

Na Kwon, Sung Choi, Soorim Han, et. al

Abstract:
In carbon-ion radiotherapy (CIRT), the beam energy determines both the particle range and the overall dosimetric quality. Range-verification QA devices such as Zebra and Giraffe, which are based on multilayer ionization chambers (MLICs), can verify the range but only under dedicated QA conditions, leaving any energy deviations introduced by nozzle components undetected in real time. In particular, nozzle structures such as ridge filters can broaden or modulate the energy spectrum, causing the effective energy delivered to the patient to differ from the nominal accelerator setting. These limitations highlight the need for a real-time method capable of verifying the beam energy under actual clinical operating conditions.We proposed a TOF-based beam-energy measurement concept that leverages a cross-correlation analysis of full detector waveforms. Compact and radiation-hard parallel-plate chambers (PPCs) were developed and evaluated, in contrast to prior TOF systems based on semiconductor detectors.PPCs (2.5 cm diameter active area, 0.4 mm gas gap) were operated in CO2. Two detectors were mounted coaxially with detector separations of 22.5 and 46.3 cm.

Experiments were performed at Yonsei Heavy-ion Therapy Center (HITC) using four nominal energies (102.6, 140.4, 250.3, 430 MeV/nucleon) and three intensities, covering the clinically interesting ranges. Signals were digitized with a 1 GHz bandwidth oscilloscope. For each spill, paired waveforms were cross-correlated, and peak times were refined by parabolic interpolation to determine TOF. Precision and accuracy were evaluated across energies, intensities, and detector separations.The PPCs operated stably for all beam conditions. Under pencil-beam delivery and normalized to 1 s acquisitions, the timing precision of the mean TOF (standard error) remained within 1 ps for both detector separations, scaling with 1 / N $1/\sqrt N $ (N: number of TOF samples per acquisition) and not representing the single-particle TOF resolution. Residuals between measured and theoretical TOF remained within 80 ps across energies and distances. After relativistic conversion from TOF to kinetic energy and then to water-equivalent range, all deviations were within a 1 mm range shift, meeting the recommended clinical criteria for range verification.We demonstrated that compact CO2-filled PPCs, operated as a TOF pair, can measure carbon-ion beam energy across the clinically relevant range of energies (≈ 100-430 MeV/u) and intensities used in routine treatment delivery. We achieved sub-picosecond timing precision on the TOF mean (standard error) per 1 s acquisition and submillimeter water-equivalent range accuracy using a robust cross-correlation analysis method. These results open the way to the integration of PPC-based TOF monitoring to tighten beam-delivery tolerances and improve the reliability and safety of carbon-ion radiotherapy.

PLoS One (impact factor: 2.6) 3 ☒

Modeling the seasonal epidemic of human brucellosis in China: A comparative time series analysis.

Yuqi Jiang, Jinhua Zhao, et. al

Abstract:

While time-series models have been applied to forecast brucellosis incidence in China, systematic comparisons of multiple models remain relatively limited. This study aimed to elucidate the epidemic characteristics of human brucellosis and to provide a comparative assessment of several time-series prediction models, in order to identify a suitable predictive framework for future incidence forecasting.Monthly and annual incidence rates (per 100,000 population) of brucellosis in China from January 2011 to December 2020 were used as raw data. Seven time-series models were developed and compared using R software (version 4.3.1): Seasonal Autoregressive Integrated Moving Average (SARIMA), Holt-Winters additive model, Holt-Winters multiplicative model, Neural Network Autoregressive (NNAR) model, Exponential Smoothing State Space (ETS) model, TBATS model, and Prophet model. A rolling-window cross-validation was applied to assess model stability. Model performance was

evaluated using root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE), and mean absolute scaled error (MASE).Among the seven models evaluated, the Holt-Winters multiplicative model demonstrated the most stable and superior predictive performance on the test set (MAE = 0.034, RMSE = 0.040, MAPE = 14.881%, MASE = 0.891), which serves as strong evidence for its best generalization capability among the compared models.Given its stable and superior performance in the test set, the Holt-Winters multiplicative model is recommended for short-term brucellosis forecasting in China. It captures the characteristic spring-summer peak, and its integration into surveillance systems could enhance early warning and targeted interventions.

APPLIED MATHEMATICS

Proc Natl Acad Sci U S A (impact factor: 9.1) 1 区 TOP

Controlled propagation of soliton bullets in an engineered strain field.

Alexis de la Cotte, Xingzhou Tang, et. al

Abstract

Predicting and controlling the propagation of nonlinear responses in materials is critical to a range of fields, from the manipulation of single electrons in quantum optics to the understanding of crack propagation and failure of quasi-brittle materials. Solitons, which are highly localized strain patterns that propagate and persist due to nonlinear feedback mechanisms, can be produced in liquid crystal (LC) films under high-frequency AC electric fields. In previous work using uniformly oriented films of LC, soliton bullets propagated in one preset direction perpendicular to the far-field orientation of the LC director. Here, we show that confinement of the LC between asymmetric surfaces and the introduction of strain can provide a versatile mechanism to modulate the propagation direction of solitons. Specifically, we find that soliton bullets propagate along two oblique axes, where the angle can be dynamically modulated with the electric field frequency. The origins of this behavior are understood through theory and simulations, where the forces driving soliton motion are analyzed. Importantly, asymmetric flexoelectric torques lead to frequency-dependent oblique trajectories in the presence of hybrid LC anchoring, with numerical simulations predicting asynchronous out-of-plane fluctuations that are verified in experiments. Overall, our results highlight the interplay between the nonlinear action of external fields and the far-field strain on soliton propagation. They also show that

confinement can be used to control the direction of propagation of nonlinear signals and demonstrate how LCs can be used as model systems to test and predict the effects of nonlinear excitations in new material designs.

Proc Natl Acad Sci U S A (impact factor: 9.1) 1 ☒ TOP

VIBES: A multiscale modeling approach integrating within-host and between-hosts dynamics in epidemics.

Paulo Ventura, Yong Dam Jeong, et. al

Abstract

Infectious disease spread is a multiscale process composed of within-host (biological) and between-host (social) drivers and disentangling them from each other is a central challenge in epidemiology. Here, we introduce VIBES, a multiscale modeling framework that explicitly integrates viral dynamics based on patient-level data with population-level transmission on a data-driven network of social contacts. Using SARS-CoV-2 as a case study, we analyze three emergent epidemic properties, namely the generation time, serial interval, and presymptomatic transmission. First, we established a purely biological baseline, thus independent of the reproduction number (R), from the within-host model, estimating a generation time of 6.3 d for symptomatic individuals and 43.1% presymptomatic transmission. Then, using the full model incorporating social contacts, we found a shorter generation time (5.4 d at R = 3.0) and an increase in presymptomatic transmission (52.8% at R = 3.0), disentangling the impact of social drivers from a purely biological baseline. We further show that as pathogen transmissibility increases (R from 1.3 to 6), competition among infectious individuals shortens the generation time and serial interval by up to 21% and 13%, respectively. Conversely, a social intervention, like isolation, increases the proportion of presymptomatic transmission by about 30%. Our framework also estimates metrics that are challenging to obtain empirically, such as the generation time for asymptomatic individuals (5.6 d; 95%CI: 5.1 to 6.0 at R = 1.3). Our findings establish multiscale modeling as a powerful tool for mechanistically quantifying how pathogen biology and human social behavior shape epidemic dynamics as well as for assessing public health interventions.

JHEP Rep (impact factor: 7.5) 1 ☒

Deep Learning-Based Generation of Synthetic Multiphasic MRI In Hepatocellular Carcinoma and Cirrhosis.

Sara Abosabie, Salma Abosabie, et. al

Abstract

There is a growing interest in reducing contrast medium use and the lengthy scan duration in liver imaging. This proof-of-concept study aimed to evaluate the feasibility

of deep learning-based generation of synthetic three-dimensional liver contrast-enhanced multiphasic MRI exams that are similar to ground-truth exams in hepatocellular carcinoma and cirrhosis.MRI exams from hepatocellular carcinoma or cirrhosis patients at a single academic center were retrospectively collected. A three-dimensional cycle-consistent generative adversarial network was trained to generate synthetic three-dimensional T1-weighted contrast-enhanced multiphasic liver MRI exams, including arterial, portal venous, delayed, and hepatobiliary phases, using two precontrast T1-weighted and T2-weighted input phases. Quantitative performance evaluated similarity, error, and overlap metrics between synthetic and ground-truth exams. For the qualitative multi-reader study, three blinded radiologists assessed the ground-truth and synthetic MRI exams using a comprehensive questionnaire. Questionnaire tasks 1-5: visual Turing test (ground-truth vs synthetic nature), image quality, anatomic accuracy, disease diagnosability, artifacts, task 6: Liver Imaging Reporting and Data System features.The study included 3,198 MRI phases from 533 MRI exams from 185 hepatocellular carcinoma (mean age, 62.1 years±9.7[SD]; 141 males) and 182 cirrhosis patients (54.4 years±10.0; 111 males). Synthetic MRI exams achieved high quantitative and qualitative similarity to ground-truth exams. Quantitative analysis demonstrated high structural similarity index (0.86±0.03), overlap (0.97±0.05), and low symmetric mean absolute percent error (0.63%±0.23%). Qualitative multi-reader study showed no significant difference in tasks 1-5 (p=0.06-0.50) and high performance metrics in task 6 (accuracy:0.76-0.86; precision:0.96-1.00) with moderate to perfect Fleiss's kappa interrater agreement (0.58-1.00, p<0.001).Deep learning enabled generation of synthetic three-dimensional liver contrast-enhanced multiphasic MRI exams from precontrast sequences, achieving high quantitative and qualitative similarity to ground-truth images.This work demonstrates the early feasibility of generating high-quality, three-dimensional contrast-enhanced multiphasic liver MRI exams from precontrast sequences, with synthetic exams showing strong agreement with ground truth across quantitative metrics and key qualitative criteria, including the visual Turing test, image quality, disease diagnosability, anatomic accuracy, artifact severity, and hepatocellular carcinoma Liver Imaging Reporting and Data System features. Despite the model currently representing a proof of concept based on a moderate single-center dataset, with a need for larger multicenter studies and external validation, the results highlight the potential to transform liver MRI workflows by reducing contrast media costs and potential side effects, significantly shortening acquisition time-especially the prolonged 20-minute hepatobiliary phase-and improving accessibility for patients unable to tolerate contrast-enhanced MRI due to renal impairment, contrast agent allergy, or claustrophobia.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

TOPOLOGY

Science (impact factor: 45.8) 1 区 TOP

High-dimensional topological photonic entanglement.

M Zakeri, Armando Perez-Leija, et. al

Abstract

The generation and manipulation of high-dimensional quantum states lies at the heart of modern quantum computation. The use of topology to resiliently encode and transport quantum information has been widely investigated in condensed matter and has recently penetrated quantum photonics. However, a route to scale up to a large number of entangled topological photonic modes has been missing. In this work, we demonstrate a method to generate high-dimensional topological photonic entanglement. Our platform relies on designed silicon photonic waveguide topological superlattices, which support nonlinear generation of energy-time-entangled photon pairs on a superposition of multiple topological modes. We show strong signatures of entanglement of up to five topological modes with resilience to nanofabrication imperfections, providing a route toward scalable, fault-tolerant quantum photonic states.

J Am Chem Soc (impact factor: 15.6) 1 区 TOP

Stabilizing Structural Transitional States between 1- and 2-Dimensional Topologies via Hydrogen Bond-Mediated Crystal Engineering.

Mariya Aleksich, Adriana Ladera, et. al

Abstract:

Metal-organic chalcogenolates (MOChas) are hybrid materials composed of metal-chalcogenide networks coordinated by organic ligands, offering a versatile platform for structural and electronic tunability. The use of molecular ligand design to steer material formation represents a powerful strategy for accessing new solid-state topologies. In this work, we report two new silver benzenethiolate MOChas incorporating protic meta-functionalized ligands — hydroxy (-OH) and amine (-NH2) — which exhibit hydrogen-bond-driven supramolecular organization and novel inorganic connectivities. Rather than modifying existing materials, we contextualize these compounds as distinct outcomes within a structural continuum. Silver para- and meta-methoxy-benzenethiolates (p-OCH3 and m-OCH3) serve as control points for known 2D and 1D topologies, respectively. The new materials, m-OH and m-NH2, were structurally characterized using small molecule serial femtosecond crystallography (smSFX), and their intermediate energetic and electronic properties were confirmed through density functional theory (DFT) calculations. We introduce the concept of supramolecular distortion to describe how ligand-driven intermolecular interactions reshape inorganic

topology—not as deviations from a fixed state, but as distinct, kinetically accessible ground-state architectures. This work establishes a design paradigm linking organic ligand identity to predictable shifts in inorganic dimensionality in MOChas.

IEEE Trans Neural Netw Learn Syst (impact factor: 8.9) 1 区 TOP

Toward Robust End-to-End Delay Prediction: A GNN Approach With Routing-Aware Attention and Masked Subgraph Sampling.

Zichen Wang, Yiqi Chen, Dongwei Liu, et. al

Abstract:

The end-to-end delay prediction is critical for intelligent network management, particularly in latency-sensitive and dynamic environments. While recent deep learning (DL) models have shown promising results, their reliance on sequential encoding of routing paths limits generalization to unseen routing schemes. In this article, we propose a robust graph neural network (GNN)-based delay prediction model that overcomes this limitation by introducing a global routing representation and a routing-aware attention mechanism. The model queries flow-relevant features from a unified topology-routing map without relying on routing sequences. In addition, a mask-based subgraph sampling strategy enables the model to infer global routing correlations from partial flow interactions, further enhancing its adaptability. Extensive experiments are conducted on four public datasets-TnCwD, NSFNET, GBN, and GEANT2. The results demonstrate that our model not only outperforms existing methods in prediction accuracy but also exhibits strong generalization across diverse routing configurations. Future work will focus on further validating the model under more complex and dynamic routing scenarios.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Ⅱ Concentration

PHYSICS

Multiparameter estimation with an array of entangled atomic sensors

Yifan Li, Lex Joosten, Youcef Baamara, et al.

Abstract

In quantum metrology, entangled states of many-particle systems are investigated to enhance measurement precision of the most precise clocks and field sensors. Whereas single-parameter quantum metrology is well established, joint multiparameter estimation poses conceptual challenges and has been explored only theoretically. We experimentally demonstrated multiparameter quantum metrology with an array of entangled atomic ensembles. By splitting a spin-squeezed ensemble, we created an atomic sensor array featuring intersensor entanglement that can be flexibly configured to enhance measurement precision of multiple parameters jointly. Using an optimal estimation protocol, we achieved substantial gains over the standard quantum limit in key multiparameter estimation tasks, thus grounding the concept of quantum enhancement of field sensor arrays and imaging devices.

Self-induced Floquet magnons in magnetic vortices

Christopher Heins, Lukas Körber, Joo-Von Kim, et al.

Abstract

Driving condensed matter systems with periodic electromagnetic fields can result in exotic states not found in equilibrium. Termed Floquet engineering, such periodic driving applied to electronic systems can induce topological band structures and control spin interactions. In this study, we present a class of Floquet states in a magnetic vortex that arise from nonlinear interactions between the vortex core and microwave magnons. Floquet bands emerge through the periodic oscillation of the core, which can be initiated by either driving the core directly or pumping azimuthal magnon modes. For the latter, the azimuthal modes induce core gyration through nonlinear interactions, which in turn renormalizes the magnon band structure. This represents a self-induced mechanism for Floquet band engineering and opens avenues to study and control nonlinear magnon dynamics.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

A magnetic massive star has experienced a stellar merger

A. J. Frost, H. Sana, et al.

Abstract

Massive stars (those $\geqslant$8 solar masses at formation) have radiative envelopes that cannot sustain a dynamo, the mechanism that produces magnetic fields in lower-mass stars. Despite this, approximately 7% of massive stars have observed magnetic fields, the origin of which is debated. We used multi-epoch interferometric and spectroscopic observations to characterize HD 148937, a binary system of two massive stars. We found that only one star is magnetic and that it appears younger than its companion. The system properties and a surrounding bipolar nebula can be reproduced with a model in which two stars merged (in a previous triple system) to produce the magnetic massive star. Our results provide observational evidence that magnetic fields form in at least some massive stars through stellar mergers.

MATERIALS

Highly efficient, deep-ultraviolet luminescence in hBN moiré quantum wells

Chengyun Hong, Fangzhou Zhao, et al.

Abstract

Twisted stacking of two-dimensional van der Waals (vdW) semiconductors creates moiré superlattices, which provides unprecedented control over quantum states and their light-matter interactions. We demonstrate that a simple twist interface between two single-crystalline bulks of hexagonal boron nitride (hBN) creates moiré quantum wells (QWs) embedded in a three-dimensional vdW structure. hBN moiré QWs strongly confine charge carriers under both optical excitation and electrical injection. Despite their indirect bandgap, they emit intense deep-ultraviolet luminescence in the extreme wavelength bands from 215 to 240 nanometers, exceeding that of state-of-the-art conventional aluminum gallium nitride (AlGaN) multiple QWs by more than an order of magnitude. Furthermore, the twist angle control allows wide tunability of luminescence energy and efficiency in moiré QWs.

Strong and brittle lithium dendrites

Qing Ai, Boyu Zhang, Xing Liu, et al.

Abstract

The growth and penetration of lithium dendrites through electrolytes and separators remain key challenges to realizing high–energy density lithium-metal batteries. Using mechanically strong electrolytes and separators has been considered a promising strategy based on the commonly believed softness of lithium. However, dendrite formation persists in stiff solid electrolytes, suggesting distinct mechanical behaviors. We measured the mechanical properties of individual lithium dendrites using an air-free protocol. We found that lithium dendrites are unexpectedly strong and brittle, with fracture stress greater than ~150 megapascals, unlike the ductile bulk metal. Cryo–transmission electron microscopy and mechanical modeling showed that this behavior arises from solid electrolyte interface constraints and nanoscale strengthening. These findings provide alternative mechanisms for dendrite penetration and dead lithium formation as well as guidance for design strategies for lithium-metal batteries.

Irregular hierarchical-porous polymer for high-performance soft thermoelectrics

Xiao Zhang, Dongyang Wang, et al.

Abstract

Polymer thermoelectrics offer an inherently soft, cost-effective, and lightweight solution to convert ubiquitous heat sources into sustainable electricity. However, their realistic applications are hindered by insufficient performance and the scaling complexity. We introduce irregular hierarchical-porous thermoelectric polymers, featuring irregularly shaped and distributed pores with diameters that range from less than 10 nanometers to micrometers. This porous structure not only enhances multiple phonon-like scattering, achieving a 72% reduction in lattice thermal conductivity, but also unexpectedly improves charge transport through nanoconfinement-enhanced crystallization. The optimized film yields a benchmark figure-of-merit zT of 1.64 at 343 kelvin. Moreover, this method is compatible with easy-to-process spray-coating techniques.

CHEMISTRY

Organocatalyst-controlled stereoselective head-to-tail macrocyclizations

Jonas W. Rackl, Linus B. Boll, et. al

Abstract

Chiral macrocycles are key to the discovery of new medicines. Their synthesis is, however, challenging and typically requires the often-cumbersome installation of stereochemical features in a linear precursor. In this study, we report a catalyst-controlled stereoselective head-to-tail macrocyclization. The method utilizes a bifunctional peptide catalyst to template the terminal functional groups of the linear precursor, thereby favoring intra- over intermolecular reaction and enabling exquisite control over the stereochemistry of the emerging stereogenic centers. Diverse 12- to 18‐membered macrocyclic lactones and lactams were obtained from achiral linear precursors. The organocatalyst even dictates the stereochemical outcome upon cyclizing a chiral linear precursor. This catalyst-controlled stereoselective head-to-tail macrocyclization provides a practical route to chiral macrocycles with predictable stereochemical outcomes. The utility was highlighted by synthesizing the core of the natural product robotnikinin.

A 36-ring zeolite with intrinsic cylindrical mesopores

Jiazheng Sun, Xudong Tian, et. al

Abstract

Stable extra-large pore zeolites are highly desirable for catalysis and molecular separation, but most remain microporous, limiting their effectiveness for bulky substrates. Among the few extra-large pore zeolites that exhibit mesoporosity, the pores typically form as elongated, non-circular pore aperture. we report NJU120-6, a stable silicate zeolite with an intrinsic cylindrical mesoporous system, have the currently largest 36-ring windows with a free diameter of 25.71 Ångstroms by 19.12 Ångstroms. NJU120-6 exhibits the lowest framework density of 9.39 Si atoms nm−3 and a pore volume of 0.66 cubic centimeters per grams. It remains stable up to 1173 K and can incorporate aluminum and titanium, enabling superior performance in catalytic cracking and in liquid-phase alkene oxidations of bulky molecules, respectively.

Engineered aldehyde dehydrogenases for amide bond formation

Lei Gao, Xiang Qiu, Jun Yang, et. al

Abstract

Amide bond formation is widely used in pharmaceutical synthesis, typically involving stoichiometric coupling reagents to activate carboxylic acid substrates for a condensation reaction. As an alternative approach, we repurposed aldehyde dehydrogenases into oxidative amidases by creating a more hydrophobic and spacious catalytic pocket for amines to capture the thioester intermediate. This biocatalyst efficiently facilitates the formation of amide bonds between diverse aldehydes and amines. We also developed a two-step enzymatic cascade to synthesize amides from

broadly available aliphatic alcohols. This biocatalytic strategy enabled the redesign of synthetic routes for five drug molecules. Our findings highlight the potential of oxidative amidases in advancing the synthesis of structurally diverse drug molecules through efficient amide bond formation.

BIOLOGY

Human DHX29 detects nonoptimal codon usage to regulate mRNA stability

Fabian Hia, Yitong Wu, et al.

Abstract

Synonymous codon usage controls global gene expression in both prokaryotic and eukaryotic species. Nonoptimal codons are known to induce mRNA decay; however, the underlying molecular mechanism remains poorly understood in human cells. Through genome-wide CRISPR screening, we identified the RNA-binding protein DHX29 as a critical regulator of codon-dependent gene expression. Cryogenic electron microscopy and selective ribosome profiling demonstrated that DHX29 directly interacts with the A-site entrance of the translating 80S ribosome, the binding site for the eEF1A•GTP•aminoacyl-tRNA ternary complex, suggesting a role in monitoring aminoacyl-tRNA sampling. Proteomic analysis further revealed that DHX29 recruits the GIGYF2•4EHP complex to mediate global suppression of nonoptimal mRNAs. These findings establish a mechanistic link between synonymous codon usage and the regulation of gene expression.

Genomic approaches to accelerate American chestnut restoration

Jared W. Westbrook, Joanna Malukiewicz, et. al

Abstract

More than a century after two introduced pathogens killed billions of American chestnut trees, introgression of resistance alleles from Chinese chestnuts has contributed to the recovery of self-sustaining populations. However, progress has been slow because of the complex genetic architecture of resistance. To better understand blight resistance, we compared reference genomes, gene expression responses, and stem metabolite profiles of the resistant Chinese and susceptible American chestnut species. To accelerate resistance breeding, we conducted large-scale phenotyping and genotyping in hybrids of these species. Simulation and inoculation experiments suggest

that significant resistance gains are possible through selectively breeding trees with an average of 70 to 85% American chestnut ancestry. The resources developed in this work are foundational for breeding to create diverse restoration populations with sufficient disease resistance and competitive growth.

A non-enzymatic role of Nudix hydrolase 5 in repressing purine de novo synthesis

Tuan-Anh Nguyen, Jung-Ming G. Lin, et. al

Abstract

Folate metabolism is intricately linked to purine de novo synthesis through the incorporation of folate-derived one-carbon units into the purine scaffold. By investigating chemical and genetic dependencies caused by mutations in methylenetetrahydrofolate dehydrogenase, cyclohydrolase, and formyltetrahydrofolate synthetase 1 (MTHFD1), we discovered a key role for Nudix hydrolase 5 (NUDT5) in regulating purine de novo synthesis. Genetic depletion and selective chemical degradation showed that a scaffolding role, rather than NUDT5 enzymatic activity, was causing this phenotype. NUDT5 interacted with phosphoribosyl pyrophosphate amidotransferase (PPAT), the rate-limiting enzyme of purine de novo synthesis, to repress the pathway in response to increased purine abundance. Through this mechanism, loss of NUDT5 mediates resistance to purine analogs in cancer treatment and prevents adenosine toxicity in MTHFD1 deficiency.

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

Ⅲ Calling for papers

ICoMS 2026

Submission deadline:	**Apr 5, 2026**
Conference date:	**Sep 11, 2026 - Sep 13, 2026**
Full name:	**International Conference on Mathematics and Statistics**
Location:	**Paris, France**

ICoMS 2026 is organized to bring together worldwide leading researchers and practitioners interested in advancing the state of the art in Mathematics and Statistics, for exchanging knowledge that encompasses a broad range of disciplines among various distinct communities. It is hoped that researchers and practitioners will bring new prospects for collaboration across disciplines and gain inspiration to facilitate novel breakthroughs. The themes for this conference are thus focused on "Cross-disciplinary Innovation and Applications of Mathematics, Statistics, and Computer Science".

The annually held conference is expected to provide an opportunity for the researchers to meet and discuss the latest solutions, scientific results and methods in solving intriguing problems in the fields of Mathematics and Statistics. The conference programme will include prominent keynote speakers, invited speakers and regular paper presentations in parallel tracks. The General Chairs, along with the entire team cordially invite you to submit your latest research results and to take part in the upcoming conference.

Please identify the official email address and phone number of the conference. Unofficial emails or phone calls do not represent the view of the conference. It may involve fraud in the name of conference. Please feel free to contact us.

Call for papers:

1. Mathematical Modeling and Computer Science Applications: Computational mathematical methods and algorithms; Numerical computation and optimization methods; Application of mathematical models in computer science; Computer-aided proof and verification
2. Data Science and Statistical Computing: Big data analysis and mining; Statistical learning and machine learning; Data visualization and visual analytics; Statistical computing and computational statistics
3. Computational Statistics and Statistical Computing: Computational methods for statistical inference and modeling; High-performance computing in statistics; Statistical software and programming languages; Computer-based statistical methods and experimental design
4. Computer Vision and Image Processing: Image recognition and classification; Object detection and tracking; Image segmentation and reconstruction; Computer vision algorithms and applications
5. Computer Networks and Security: Network analysis and modeling; Network security and privacy protection; Network optimization and performance evaluation; Computer-based network management and control

AMMS 2026

Submission deadline: **Apr 5, 2026**
Conference date: **Sep 11, 2026 - Sep 13, 2026**
Full name: **International Applied Mathematics, Modelling and Simulation Conference**
Location: **Paris, France**

2026 8th International Applied Mathematics, Modelling and Simulation Conference (AMMS 2026) will be jointly held with 2026 9th International Conference on Mathematics and Statistics (ICoMS 2026) from September 11-13, 2026 in Paris, France. This Conference will cover topics on Applied Mathematics, Modelling, Simulation and related fields. It dedicates to providing a platform for exchanging the latest research results and sharing the advanced research methods for researchers, practitioners, and professinals from all over the world.

AMMS is an annually-held conference, which serves to bring experts, scholars and businessmen together to communciate face to face and explore chances for possible cooperation. AMMS 2026 welcomes scholars and researchers working in the field of Applied Mathematics, Modelling and Simulation from all over the world to submit original and not published papers for reviewing of publication and presentation; submit abstract for presentation only or register for participation and listening conference.

Topics of Interest :

Topic 1: Mathematics

Analysis； Algebra； Applied Mathematics； Computational Mathematics； Control Theory and Automation；Data Mining and Soft Computing；Geometry；Mathematical Chemistry and Biology；Optimization and Operational Research； Rough Set and Soft Set Theory； Statistics； Theoretical Computer Science…etc

Topic 2: Statistics

Probability Theory； Stochastic Processes； Simulation, Parametric and Nonparametric Inference；Multivariate； Baysian Inference； Regression Analysis Estimation Theory； Etc

Topic 3: Simulation Tools and Platforms

Enterprise Resource Planning； Petri Nets； Virtual Reality and Graphical Simulations； Discrete-Event Simulation； Security/Emergency Support Tools； Plant Simulation…etc

Topic 4: Complex Systems Modeling and Simulation

Collaborative Systems;Business Process Modeling

Multiscale Simulation;Performance Analysis;Social Systems Simulation…etc

Topic 5: Formal Methods

Security;Planning and Scheduling;Ontologies;Conceptual Modeling;Stochastic Modeling and Simulation;Dynamical Systems Models and Methods…etc

Topic 6: Application Domains

Automotive Industry;Chemical and Petroleum Engineering;Military and Defense;Construction Engineering and Project Management;Telecommunication Systems and Networks;Energy and Power Systems…etc

Editor: Chaoyi Chu（褚朝奕） TEL: 3548 Email: ccy@jsut.edu.cn

MSEA 2026

Submission deadline: **Apr 8, 2026**
Conference date: **May 8, 2026 - May 10, 2026**
Full name: **International Conference on Mathematical Statistics and Economic Analysis**
Location: **Beijing, China**

Mathematical statistics is a branch of mathematics, which is divided into descriptive statistics and inferential statistics. Based on probability theory, it studies the statistical regularity of a large number of random phenomena. The task of descriptive statistics is to collect data, sort and group them, prepare frequency distribution tables, draw frequency distribution curves, and calculate various characteristic indexes to describe the concentration trend, deviation trend and skewness of frequency distribution. Inferential statistics is to infer and predict the whole on the basis of descriptive statistics and the regularity summarized from sample data.

Call for Papers:

◕ Economic Analysis
World economy
Digital economy
Urban economy
Media economy
Public economy
Energy economy
Economic policy
Internet economy
Mathematical finance
Financial Engineering
Experimental economy
Environmental economy
International economy
Finance, taxation, trade
Low carbon development
Business big data analytics
Economic big data analytics
Empirical economic research
National development economy
International Political Economy
Financial marekts and investments
Sustainable economic developmen

◕ Mathematical Statistics
Physics
Statistics
Applied mathematics
Electronic Information engineering
Information and computing science
Probability Theory and Mathematical Statistics

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AI2M4RI 2026

Submission deadline: **Apr 15, 2026**
Conference date: **Feb 18, 2026 - Feb 20, 2026**
Full name: **International Workshop on AI & Mathematical Methods for Real-world Impact**
Location: **Athens, Greece**

Artificial Intelligence and mathematical modeling are increasingly driving breakthroughs in solving complex real-world problems across health, environment, mobility, economics, and social systems. As data grows in scale and complexity, the integration of rigorous mathematical methods with modern AI becomes essential for building reliable, interpretable, and impactful solutions. This workshop brings together researchers, practitioners, and students working at the intersection of AI, machine learning, mathematics, and applied sciences to exchange ideas, present innovative methodologies, and showcase applications that deliver tangible real-world benefits. It aims to foster interdisciplinary dialogue, highlight emerging challenges, and inspire new collaborations that push the boundaries of AI-driven mathematical modeling.

***Call for papers:**
Machine learning and statistical modeling for real-world data
Integrating AI, ABM, and Mathematical Tools for Advances in Mining and Geology
Mathematical modeling, simulation, and dynamical systems
Explainable, interpretable, and trustworthy AI
Optimization, control, and decision-making under uncertainty
Artificial Intelligence and Probabilistic Modeling for Sports Betting
AI for health, environment, climate, and public policy
Spatio-temporal modeling, forecasting, and geospatial analytics
AI and mathematical tools for resource-limited or data-scarce settings
Hybrid AI–mathematics approaches (physics-informed ML, model-driven ML, etc.)
Case studies demonstrating real-world impact
Probabilistic modeling, Bayesian inference, and uncertainty quantification
Numerical methods and scientific computing for AI systems
Graph theory, network science, and graph-based machine learning
AI-Driven Enterprise Management Strategies in Low Income Countries
Reinforcement learning and sequential decision processes
Optimization algorithms for large-scale or complex systems
AI for epidemiology, disease modeling, and public health surveillance
Mathematical foundations of deep learning and representation learning
Fairness, robustness, and bias mitigation in AI models
Data assimilation, sensor fusion, and real-time prediction
AI for sustainable development, agriculture, and natural resource management
Multi-agent systems, game theory, and collective intelligence
AI-driven mathematical modeling for mobility, logistics, and smart cities
Computational social science and socio-economic modeling
Verification, validation, and reliability of AI-based mathematical models

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ICPAM 2026

Submission deadline:	**Apr 25, 2026**
Conference date:	**Jul 15, 2026 - Jul 18, 2026**
Full name:	**International Conference on Pure and Applied Mathematics**
Location:	**London, UK**

The International Conference on Pure and Applied Mathematics has been successfully held for the last thirteen years in various locations: Paris (2012), Moscow (2013), Madrid (2014), Rome (2015), London (2016), Prague (2017), Budapest (2018), Brussels (2019), Online (2020 & 2021), Bratislava (2022), Porto (2023), Zagreb (2024)., Rome (2025) The support and participation of our members and scholars have made it possible for the 15th ICPAM to be held in London, UK, from July 15-18, 2026.

This remarkable event brings together professors, researchers, scholars, and students in the field of Pure and Applied Mathematics, making the conference a perfect platform to share experiences, foster collaborations across industry and academia, and evaluate emerging technologies worldwide.

ICPAM 2026 will feature renowned keynote speakers, oral presentations, poster sessions, and technical conferences related to the topics addressed in the Scientific Program, as well as social events.

We welcome your participation!

Topics of interest

*Applied Mathematics
*Approximation Theory
*Computational Physics
*Image Processing
*Computational Mathematics
*Mathematical Physics

For more information on the call for papers topics, please go to the official conference website

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