ASMaS 2024

The 3rd International Conference on Advanced Smart Materials and Structures 2024

Conference Program

03-05 July 2024

Honorary Chair

- Dr. Tran Trong Dao, Ton Duc Thang University, Vietnam

Conference Chairs

- Chair: Prof. Le Khanh Chau, Ton Duc Thang University, Vietnam
- Co-Chair: Prof. Weihua Li, University of Wollongong, Australia

Keynote Speakers

- Prof. Weihua Li, University of Wollongong, Australia
- Prof. Nguyen Xuan Hung, University of Technology (HUTECH), Vietnam
- Prof. Le Khanh Chau, Ton Duc Thang University, Ho Chi Minh City, Vietnam

Organizing Committee

- Local Committees:

  Dr. Vo Hoang Duy, Ton Duc Thang University, Vietnam

  Dr. Ngo Son Tung, Ton Duc Thang University, Vietnam

  Dr. Thai Hoang Chien, Ton Duc Thang University, Vietnam

  Mr. Tran Cong Thanh, Ton Duc Thang University, Vietnam

  MSc. Nguyen Van Hung, Ton Duc Thang University, Vietnam

  Ms. Tran Thi Hong Tham, Ton Duc Thang University, Vietnam

  MSc. Dang Thi Kim Anh, Ton Duc Thang University, Vietnam

  Dr. Nghiem Quy Hao, Ton Duc Thang University, Vietnam

  Assoc. Prof. Le Duc Hien, Ton Duc Thang University, Vietnam

  Dr. Dinh Hoang Bach, Ton Duc Thang University, Vietnam

- International Committees:

  Prof. Weihua Li, University of Wollongong, Australia

  Prof. Georgievsky, Lomonosov Moscow State University, Russia

  Prof. Seung-Bok Choi, State University of New York, United States

  Prof. Timon Rabczuk, Bauhaus University Weimar, Germany

  Prof. Klaus Hackl, Ruhr University of Bochum, Germany

  Prof. Julius Kaplunov, Keele University, England

  Prof. Sandra Klinge, Technical University of Berlin, Germany

  Prof. J.N. Reddy, Texas A&M University, United States

Scientific Committees:

Prof. Le Khanh Chau, Ton Duc Thang University, Vietnam

Prof. Pham Duc Chinh, Ton Duc Thang University, Vietnam

Prof. Tran Cong Phong, Ton Duc Thang University, Vietnam

Prof. Nguyen Xuan Hung, University of Technology (HUTECH), Vietnam

Prof. Guirong Liu, Cincinnati University, United States.

Prof. Magd Abdel Wahab, Ghent University, Belgium.

Prof. Stephane Bordas, Luxembourg University, Luxembourg.

Prof. I. Kudish, Kettering University, United States.

Prof. Baris Erbas, Eskişehir Technical University, Turkey.

Prof. Tongfei Tian, Sunshine Coast University, Australia.

Prof. Hejun Du, Nanyang Technological University, Singapore.

Assoc. Prof. Jong-Seok Oh, Kongju National University, South Korea.

Prof. Gorbachev Vladimir Ivanovich, Lomonosov Moscow State University, Russia.

Prof. Nikabadze Mikhail Ushangievich, Lomonosov Moscow State University, Russia.

Prof. Zavoychinskaya Eleonora Borisovna, Lomonosov Moscow State University, Russia.

Conference Secretary:

Assoc. Prof. Dang Thuy Dong, Ton Duc Thang University, Vietnam

Dr. Phung Van Phuc, University of Technology (HUTECH), Vietnam

CONFERENCE INFORMATION

I. **Location:**

Tan Phong Campus - Ton Duc Thang University
No. 19, Nguyen Huu Tho St., Tan Phong Ward, District 7, Ho Chi Minh City, Vietnam

II. **Reception Desk:**

The reception desk is located on the Ground floor of Building A.

III. **Language**

All sessions will be presented in English.

IV. **Badges**

Admittance to the venue is restricted to participants wearing their name badges. The wearing of badges is compulsory both inside the venue and at all events organized with its context.

V. **Conference Room's Location**

Conference will be held in the conference rooms of Buildings F, A, and C.

VI. **Conference Room's Equipment**

Each conference room will be equipped with a projector and a notebook computer.

VII. **Guideline for Presentation**

It takes 25 minutes for each presentation. Each paper will be presented orally for 20 minutes followed by 05 minutes discussion. Speakers will be noticed by the service worker 02 minutes before ending.

VIII. **Transportation**

Tan Son Nhat International Airport ⟺ Ton Duc Thang University (TDTU).

– BUS: Take No. 152 air-con airport bus to Ben Thanh Market and then take bus No. 86 to Ton Duc Thang University.

Time required: 60 minutes

Working Time: 06:00 ~ 18:30

Running Frequency: Every 30 minutes

Ticket price is 10.000 VND (approx. US$ 0.44)

Terminal stop - Ben Thanh Market (center of Ho Chi Minh city, bus 152), Ben Thanh market - Ton Duc Thang University (bus 86).

– TAXI: It takes about US$ 8, and about 30 minutes to arrive at Ton Duc Thang University.

IX. **Parking**

Participants with the conference invitation can park their cars at campus parking lots.

X. **Lunch**

Lunch will be served from 11:40 to 13:00 at Building D (11th floor) during the conference.

XI. **Conference Banquet**

The Organizing Committee requests the pleasure of meeting all registered guests at the Conference Dinner on July 03 at 18:30 pm, at D'Maris Phu My Hung (Lotte Mart), 3rd Floor, No 469 Nguyen Huu Tho, Ward Tan Hung, District 7, Ho Chi Minh City.

Note: Please gather at the main hall of building A, there is a university bus to drive you to the Gala dinner.

XII. **Contact**

Dr. Thai Hoang Chien
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Email: thaihoangchien@tdtu.edu.vn

CONFERENCE VENUE

Ton Duc Thang University
No. 19, Nguyen Huu Tho Street, Tan Phong Ward, District 7, Ho Chi Minh City
Telephone: (84-28) 37 755 035

Ton Duc Thang University

"For accomplishment in human development and a society with sustainable, stable growth"

Ton Duc Thang University (TDTU) is a public and autonomous university. Established in 1997, it is situated in the center of Ho Chi Minh City - the commercial hub of Vietnam. The university has six campuses in Ho Chi Minh City (two campuses), Nha Trang City, Lam Dong Province, An Giang Province, and Ca Mau Province. The main campus is located in an area of 265,000 m^2 in Tan Phong Ward, District 7, Ho Chi Minh City, Vietnam.

TDTU is a young and dynamic provider in the higher education sector and is one of the largest universities in Vietnam. The university is committed to Vietnam's sustainable development of human resources. It strives to be a leading research-oriented university regionally and internationally.

The university has been fostering a unique culture that distinguishes itself from the others. Aiming to provide optimal opportunities for quality education, the university is devoted to the promotion of students' learning and research activities. All aspects of the university strive to constantly maintain an effective and efficient academic community for talents to be developed.

After 27 years of development, TDTU has become one of the fastest-growing universities in the country. Currently, the university has 16 faculties. The university offers over 70 programs at the vocational, undergraduate, and postgraduate levels. Approximately 26,000 students are pursuing their studies at the university. According to Times Higher Education (THE) ranking,

TDTU is in the Top 500 world university rankings for 2 consecutive years (2022, 2023) and is in the Top 700 Academic Ranking of World Universities (ARWU) in 2022.

MESSAGE FROM THE HOST UNIVERSITY

Dear our Distinguish Guests;

Ladies, and Gentlemen.

It is a great honor and privilege for Ton Duc Thang University (TDTU) to host the 3rd International Conference on Advanced Smart Materials and Structures (ASMaS 2024). First and foremost, I would like to warmly welcome all participants to this wonderful event.

In accordance with the vision and mission of TDTU to become a world-class research university and broaden international academic cooperation, the annual growth of international conferences is one of our efforts to make this vision and mission come true. Honorably, the ASMaS 2024 conference is co-hosted with the University of Wollongong, Lomonosov Moscow State University, and the Ho Chi Minh Association of Mechanics. This year, the conference has five academic sessions that covering a wide range of fascinating topics such as Mathematical Models and Methods, Smart Materials, Smart and Functionally Graded Structures, Nonlinear Control, Automation, and Robotics, Data driven Computational Mechanics and Machine Learning.

I strongly believe that the participants, researchers, and scholars will find the presented papers interesting, gripping, and informative, which would inspire promising developments and collaborations in the future. Additionally, with the professional and meticulous preparation aimed to satisfying rigorous standards, I also believe that this conference will provide a valuable opportunity for scientists and researchers to disseminate their findings, foster partnerships, and transfer knowledge and technology, thereby promoting community service values worldwide.

On behalf of Ton Duc Thang University, the host of ASMaS 2024, I would like to express my profound appreciation to the universities, co-organizers, and scholars who have contributed to the quality of this conference. I wish great success to ASMaS 2024, and wish all of you good health and happiness.

Dr. Tran Trong Dao
Honorary Chair and President of Ton Duc Thang University

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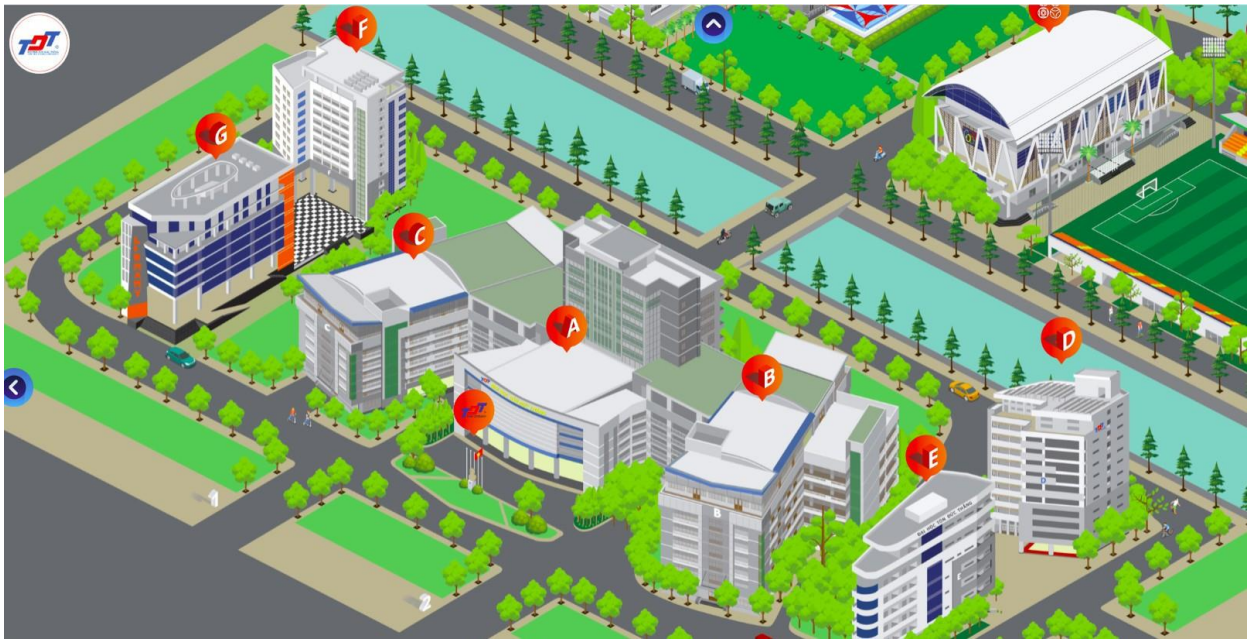
PROGRAM AT A GLANCE

DAY 1: Wednesday, 3rd July 2024	
07:30 ~	Registration
08:30 ~ 09:10	Opening Ceremony
09:10 ~ 10:10	Keynote Speech I: A New Metamaterial Magnetorheological Elastomer Isolator with Tunable Vibration Bandgaps Keynote Speaker: Prof. Weihua Li (University of Wollongong, Australia)
10:10 ~ 10:40	Poster Session Coffee Break
10:40 ~ 11:40	Keynote Speech II: Modeling and 3D-printed fabrication of TPMS-based bioinspired structures Keynote Speaker: Prof. Nguyen Xuan Hung (HUTECH University, Ho Chi Minh City, Viet Nam)
11:40 ~ 13:00	Lunch
13:00 ~ 15:05	Parallel Sessions
15:05 ~ 15:35	Coffee Break
15:35 ~ 17:40	Parallel Sessions
18:30 ~ 21:00	Conference Banquet
DAY 2: Thursday, 4th July 2024	
08:30 ~ 09:30	Keynote Speech III: Data-driven dislocation mediated plasticity Keynote Speaker: Prof. Le Khanh Chau (Ton Duc Thang University, Vietnam)
09:30 ~ 10:00	Coffee Break
10:00 ~ 12:30	Parallel Sessions
12:30 ~ 13:30	Lunch
DAY 3: Friday, 5th July 2024	
Full day	Tour

Notes:

- **Hall F** is inside Building F (you can use any stair around Building F to go to 10th floor, then follow the sign).
- **Room A101** is located at the first floor of Building A. Please use one of 2 stairs at the right side of Building A to access A101.
- **Room A403** is located on the 4th floor of Building A. You can use the elevator or any stair around Building A to access Room A403.
- **Room C010** is located at the ground floor of Building C.



AGENDA IN DETAIL

ASMaS 2024 – 1st day (Stadium Hall 10F)		**Wednesday, 3rd July 2024**
7:30 ~		Registration
08:30 - 09:10		Opening Ceremony
09:10 – 10:10	**K1**	**Keynote Speech 1** – Prof. Weihua Li **Speech title:** *A New Metamaterial Magnetorheological Elastomer Isolator with Tunable Vibration Bandgaps* Chair: Prof. Le Khanh Chau
10:10 – 10:40	**Poster Session (Lobby – 10F)** Chair: Prof. Pham Duc Chinh and Prof. Tran Cong Phong	
	Paper ID	**Paper title and Author(s)**
10:10 – 10:40	ASMAS2024_009	Alpha-glucosidase Inhibitory Activities of Salazinic acid Derivatives from Parmotrema lichen ***Thanh-Hung Do**, Thi-Minh-Dinh Tran*
10:10 – 10:40	ASMAS2024_012	Rational design and simulation of hydrogen storage materials by using first-principles, thermodynamic, and kinetic approaches ***Thong Nguyen-Minh Le**, Amol Deshmukh, Cheng-Chau Chiu, and Jer-Lai Kuo*
10:10 – 10:40	ASMAS2024_015	Globunoids A–D, undescribed bichalconoid and biflavanoids with α-glucosidase and α-amylase inhibitory activities from Knema globularia stems ***Thi-Kim-Dung Le**, Warinthorn Chavasiri*
10:10 – 10:40	ASMAS2024_016	Natural Compounds Inhibit Monkeypox Virus Methyltransferase VP39 *in Silico* Studies ***Quynh Mai Thai**, Huong T. T. Phung, Ngoc Quynh Anh Pham, Jim-Tong Horng, Phuong-Thao Tran, Nguyen Thanh Tung and Son Tung Ngo*
10:10 – 10:40	ASMAS2024_025	α-Glucosidase Inhibitors from the Trunk of *Morus alba* Linn.: Spectroscopy, Molecular Docking and Molecular Dynamics Simulations ***Le-Thuy-Thuy-Trang Hoang** and Van-Kieu Nguyen*
10:10 – 10:40	ASMAS2024_014	Morphology of a Transmembrane Aβ42 Tetramer via REMD Simulations ***Son Tung Ngo**, Trung Hai Nguyen, and Van V. Vu*

10:10 – 10:40	ASMAS2024_021	Synthesis, and characterization of a metal absorbent fabric from polyhydroxyl-nitroso dye applied for heavy metal treatment ***Vu Thi Ngoc Anh***, *Hoang Thuy Ngoc Dung, Nguyen The Hai, Nguyen Van Anh*
10:10 – 10:40	ASMAS2024_039	Nonlinear vibration and dynamic buckling responses of stiffened functionally graded graphene-reinforced cylindrical, parabolic and sinusoid panels using the higher-order shear deformation theory *Tran Quang Minh, Vu Hoai Nam, Vu Minh Duc, Vu Tho Hung, Le Ngoc Ly,* ***Nguyen Thi Phuong***
10:10 – 10:40	ASMAS2024_040	A new analytical approach for nonlinear thermo-mechanical postbuckling of FG-GPLRC circular plates and shallow spherical caps stiffened by spiderweb stiffeners *Vu Hoai Nam, Tran Quang Minh, Pham Thanh Hieu, Vu Tho Hung, Bui Tien Tu, Nguyen Thi Thanh Hoai,* ***Dang Thuy Dong***
10:10 – 10:40	ASMAS2024_001	Absorption coeficient in a gaas/inas/gaas cylindrical semiconductor quantum well with a three level ladder configuration ***Nguyen Tien Dung***, *Tran Cong Phong*
10:10 – 10:40	ASMAS2024_005	Nonlinear optical absorption in hyperbolic quantum wells ***Pham Tuan Vinh***, *Huynh Vinh Phuc, Le Thi Thu Phuong, Tran Cong Phong*
10:10 – 10:40	ASMAS2024_044	Collective excitations in 4-BLG: Inhomogeneity effects ***Vu Dong Duong***, *Nguyen Van Men, and Dong Thi Kim Phuong*
10:10 – 10:40	Coffee Break	
10:40 – 11:40	**K2**	**Keynote Speech 2** – Prof. Nguyen Xuan Hung **Speech title:** *Modeling and 3D-printed fabrication of TPMS-based bioinspired structures* Chair: Prof. Le Khanh Chau
11:40 – 13:00	Lunch	

ASMaS 2024 – 1st day		**Wednesday, 3rd July 2024**
Technical Session (Meeting Room – C010)		
13:00 – 15:05	**Session A-1: Nonlinear Control, Automation, and Robotics** Chair: Prof. Weihua Li	
Time	**Paper ID**	**Paper title and Author(s)**
13:00 – 13:25	ASMAS2024_010	Modeling of Unsteady Vibrations of a Bernoulli-Euler Beam on an Winkler Foundation with Considering Heat and Mass Transfer *Andrei V. Zemskov*, ***Le Van Hao***
13:25 – 13:50	ASMAS2024_004	Two-photon optical absorption in a quantum dot with the Yukawa potential Thai Thi Dang Khuong, Nguyen Bich Thao, Nguyen Van Cong and **Huynh Vinh Phuc**
13:50 – 14:15	ASMAS2024_007	Essential properties of emergent monolayered semiconductors **Duy Khanh Nguyen** and Dang Phuc Dam
14:15 – 14:40	ASMAS2024_035	Implementing Sobol's Global Sensitivity Analysis to SFRC's Flexural Strength Predictive Equation ***Tran T. H. Le***, *Anh-Thang Le*
14:40 – 15:05	ASMAS2024_019	Design and simulation of a novel magnetorheological brake with T-shaped multilayer rotor ***Le Hai Zy Zy***, *Nguyen Van Bien, Diep Bao Tri, Do Quy Duyen and Nguyen Quoc Hung*
15:05 – 15:35	Coffee Break	
15:35 – 17:40	**Session A-2: Nonlinear Control, Automation, and Robotics** Chair: Prof. Sawekchai Tangaramvong	
15:35 – 16:00	ASMAS2024_022	A novel decoupled RBDO approach for structural optimization with probabilistic constraints ***Sawekchai Tangaramvong***, *Arnut Sutha, and Thu Huynh Van*
16:00 – 16:25	ASMAS2024_038	Limit state analysis of structures under cyclic loads using bubble-enriched smoothed finite element method ***Phuc L. H. Ho***, *Changkye Lee, Dung T. Tran, Canh V. Le, Phuong H. Nguyen, Jurng-Jae Yee*

16:25 – 16:50	ASMAS2024_023	Free vibration analysis of functionally graded triply periodic minimal surface nanoplates using meshfree method ***Lieu. B. Nguyen**, Chien H. Thai*
16:50 – 17:15	ASMAS2024_032	Free vibration analysis of magneto electro-elastic plates reinforced with carbon nanotubes: a moving Kriging meshfree approach ***P. T. Hung**, P. Phung-Van, Chien H. Thai*
17:15 – 17:40	ASMAS2024_042	Polytopal composite finite elements for pseudo-lowerbound limit analysis of two dimensional structures ***Hien V. Do** and H. Nguyen-Xuan*
Technical Session (Meeting Room – A101)		
13:00 – 14:40	**Session B-1: Data-driven Computational Mechanics and Machine Learning** Chair: Prof. Klaus Hackl	
Time	**Paper ID**	**Paper title and Author(s)**
13:00 – 13:25	ASMAS2024_011	Model-free data-driven simulation of elasto-plastic materials ***Klaus Hackl**, Kerem Ciftci*
13:25 – 13:50	ASMAS2024_024	Influential Features Analysis and AI-Driven Accuracy Enhancement: A Study Case For DDoS Detection ***Le Ba Nguyen**, Binh Quoc Nguyen, and Ngoc Hong Tran*
13:50 – 14:15	ASMAS2024_026	A Machine Learning Approach fo a Statistical Homogenization Method fo Elastic Two-Phase Materials ***Luzie Schmollack**, Sandra Klinge*
14:15 – 14:40	ASMAS2024_013	Creep and Long-term Strength of High-entropy Alloys ***Saitova R.R.,** Arutyunyan A.R*
14:40 – 15:05	ASMAS2024_041	Synergizing Machine Learning, Molecular Docking, and Dynamics Simulations to Uncover Potent HDAC2 Inhibitors ***Do Thi Mai Dung**, Dao Quang Tung, Pham Thi Kim Anh, Ngo Son Tung, Daniel Baeker, Nguyen Ngoc An*
15:05 – 15:35	Coffee Break	

15:35 – 17:40	**Sessions B-2: Data-driven Computational Mechanics and Machine Learning** Chair: Prof. Joonkyung Jang	
15:35 – 16:00	ASMAS2024_029	Extracting the size distribution of gold nanoparticles from a UV-visible spectrum: an artificial neural network model *Jaeyoung Kim, Seyong Choi, Kiduk Kim, Kisang Byun, and* ***Joonkyung Jang***
16:00 – 16:25	ASMAS2024_027	Analysis of the vibration behavior of continua with physics-informed neural networks ***Stefan Hildebrand*** *and Sandra Klinge*
16:25 – 16:50	ASMAS2024_034	Comparative Study of xLSTM with Conventional Deep Learning Models on Bitcoin Price Trends ***The-Bang Nguyen****, Binh T. H. Duong, Doan-Thao Vo Nguyen, and Quang-Thinh Bui*
16:50 – 17:15	ASMAS2024_030	Analysis of large datasets measured on non-linear oscillators for application in data-driven machine learning ***Nils Gräbner****, Frederik Rentzsch and Utz von Wagner*
17:15 – 17:40	ASMAS2024_043	Ab-initio based Kinetic Modeling of Dissociation Reactions Sodiated Monosaccharides under Collision-induced Dissociation Mass Spectrometry Conditions ***Hai Thi Huynh****, Cheng-Chau Chiu and Jer-Lai Kuo*
18:30 – 21:30	**Conference Banquet**	

ASMaS 2024 – 2nd day (Meeting Room A403)		**Thursday, 4th July 2024**
08:30 – 9:30	**K3**	**Keynote Speech 3** – Prof. Le Khanh Chau **Speech title:** *Data-driven dislocation mediated plasticity* Chair: Prof. Pham Duc Chinh
9:30 – 10:00	Coffee Break	
Technical Session (Meeting Room – A101)		
10:00 – 12:05	**Session C: Smart Materials and Functionally Graded Structures** Chair: Prof. Sandra Klinge	
Time	**Paper ID**	**Paper title and Author(s)**
10:00 – 10:25	ASMAS2024_045	Multiscale modeling of calcified polymer hydrogels *Marc Graham and* ***Sandra Klinge***
10:25 – 10:50	ASMAS2024_036	A locking-free plate element based on asymptotically first order shear deformation theory Hoang-***Giang Bui*** *and Khanh-Chau Le*

10:50 – 11:15	ASMAS2024_008	Dynamic Regimes for Compressing of Thin Plastic Layers D.V. **Georgievskii**
11:15 – 11:40	ASMAS2024_037	Atomistic simulation of high strain rate deformation and shock compression of metal crystals ***Bryukhanov I.A***
11:40 – 12:05	ASMAS2024_033	Unsteady thermoelastic-diffusion vibrations of a Bernoulli-Euler beam on an elastic foundation ***Andrei*** *V. Zemskov,* ***Le Van Hao,*** *and Dmitry O. Serdyuk*
12:05 – 12:30	ASMAS2024_018	NSGA-II, SPEA2+SDE and AMOSA: A comparative study ***Xuan-Binh Lam***
Technical Session (Meeting Room – C010)		
10:00 - 12:05	**Session D: Smart Materials and Functionally Graded Structures** Chair: Prof. Nguyen Quoc Hung	
Time	**Paper ID**	**Paper title and Author(s)**
10:00 – 10:25	ASMAS2024_006	First-principle Calculations of Structural and Electronic Properties of Xenes (X=Si, Ge and Sn) Surfaces with CO or NO2 Adsorption ***Tran Phan Thuy Linh***
10:25 – 10:50	ASMAS2024_031	A Study on Structure Stiffness of 3D Printed Continuous Carbon Fibers Frames ***Tien-Dat Hoang*** *and Nguyen Xuan Hung*
10:50 – 11:15	ASMAS2024_020	A study on velocity profile of magnetorheological Fluid in an annular duct based on finite element analysis ***Nguyen Quoc Hung****, Diep Bao Tri, Bui Quoc Duy, Vo Van cuong, Do Quy Duyen*
11:15 – 11:40	ASMAS2024_017	Study on optimizing the amount of RFCC in high performance concrete (HPC) Nhan ***Vo Hoang****, and Thang Le Anh*
11:40 – 12:05	ASMAS2024_003	The generation of entangled state in a nonlinear coupling coupler pumped in modes is driven by broadband laser ***Doan Quoc Khoa***
12:05 – 13:00	Lunch	

ASMaS 2024 – 3rd day Friday, 5th July 2024	
7:00 – 17:00	Ho Chi Minh City Tour

Collection of the 3rd International Conference on Advanced Smart Materials and Structures (ASMaS-2024)

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A New Metamaterial Magnetorheological Elastomer Isolator with Tunable Vibration Bandgaps

Weihua Li
Advanced Manufacturing Technologies (AMT) research strength
School of Mechanical, Materials, Mechatronic and Biomedical Engineering
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Abstract: Semi-active isolators working with laminated magnetorheological elastomer (MRE) structures have attracted considerable interests in the area of vibration suppression. This work reports the development of a new metamaterial based MRE isolator with enhanced performance suitable for wide frequency ranges, which takes advantage of tunable vibration bandgaps due to the introduction of novel metamaterial structures. Specifically, a metamaterial MRE isolator was designed and prototyped. The mechanism of the formation of vibration bandgaps, for both infinite and finite periodic structures, was theoretically analysed, which details the equivalent negative stiffness of the metamaterial MRE isolator. Experiments were conducted to evaluate bandgaps of the metamaterial MRE isolator and its vibration isolation capacity. Results demonstrate that the new metamaterial MRE isolator is cable of offering enhanced vibration isolation performance with controllable bandgaps. Further research is recommended.

Biography:

Prof. Weihua Li is a Senior Professor and Director of Advanced Manufacturing Technologies Power House at the University of Wollongong. He completed his PhD at Nanyang Technological University (NTU) in 2001. He worked as a Research Fellow at the School of Mechanical and Aerospace Engineering of NTU, before he joined the School of Mechanical, Materials and Mechatronic Engineering as a Lecturer in 2003. His research focuses on Dynamics and Vibration Control, Smart Materials and Structures, Microfluidics and Lab on a Chip. He serves as chief editor or editorial board member for >10 international journals. Professor Li was appointed to the 2023

Australian Research Council (ARC) College of Experts. He is a recipient of Fellow of Engineers Australia, Fellow of the Institute of Physics (UK), JSPS Invitation Fellowship, Australian Endeavour Fellowship, Vice-Chancellor's Award for Excellence in Research Supervision, Vice-Chancellor's Award for Interdisciplinary Research Excellence and numerous Best Paper Awards.

Modeling and 3D-printed fabrication of TPMS-based bioinspired structures

Nguyen Xuan Hung
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Abstract: Bio-inspired structures based on triply periodic minimal surface (TPMS) architectures have been widely known in the literature [1]. These structures represent a significant advancement in the design of novel materials with superior mechanical properties. Inspired by natural geometric forms, TPMS-based designs offer exceptional opportunities to create materials that closely mimic the complex microstructures found in biological systems. These TPMS patterns exhibit key mechanical properties, including lightweight characteristics, high porosity, and impressive energy absorption capabilities, making them highly promising for various engineering applications. This talk devotes a review on modeling and fabrication of bio-inspired TPMS structures, including rotating TPMS-G, IWP, and P types [2,3]. We then discuss their mechanical properties numerically and experimentally. Additionally, several extensive studies on TPMS-based bioinspired structures were addressed [3]. Finally, we provide insights into considerations and recommendations for further advancements.

Keyworks: Triply Periodic Minimal Surfaces, Bioinspired structures, 3D printing, Lattices, Compression Behaviors

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Biography:

Prof. Hung Nguyen Xuan (H. Nguyen-Xuan) is the Director of CIRTech Institute, HUTECH University, Vietnam. He is currently an adjunct professor at China Medical University (Taiwan) and a visiting professor at Sejong University (South Korea). He is the President of Ho Chi Minh City Association for Mechanics. He serves as editorial board member of Composite Structures, Computers & Structures, Engineering Fracture Mechanics and CMC: Computers, Materials & Continua, and editor of CMES: Computer Modeling in Engineering & Sciences, and subject editor (on machine learning) of Underground Space, Associate Editor: Vietnam Journal of Mechanics, International Journal of Hydromechatronics.

Dr. Nguyen-Xuan received his Ph.D. in Computational Mechanics from The University of Liège (Belgium) in 2008. His research focuses on advanced computational methods in engineering, data-driven machine learning modelling, sustainable materials design and 3D printing. He has authored 02 patents, 01 certificate of trademark registration, and published more than 280 peer-reviewed papers indexed in WoS. His remarkable work has earned him recognition for nine consecutive years in the top 1% of highly cited influential scientists of Thomson Reuters and Clarivate: from 2014 to 2021 in the category of Computer Science and 2022 in the field of Cross-Field category.

Dr. Nguyen-Xuan earned several prestigious awards: Alexander von Humboldt Foundation Digital Cooperation Fellowship (2021), outstanding Humboldtian (2019), Georg Forster Research – Alexander von Humboldt (2015), Vietnam National University HCMC (2008 – 2013), and Nguyen Van Dao (2011).

More information found at

http://scholar.google.co.uk/citations?user=3iK9h-gAAAAJ&hl=en

Founder and Director, Deep Additive Manufacturing Lab https://cloud.ht3dprint.com

Data-driven dislocation mediated plasticity

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Abstract: In this paper, a data-driven approach to dislocation-mediated plasticity is presented. Within a dislocation density-based plasticity model incorporating effective disorder temperature, we analyze mechanical test data for various metals under diverse loading conditions and use large scale least squares method to determine the parameters of the theory. This approach enables accurate predictions of stress-strain behavior and temperature evolution for crystals under simple shear, tension/compression, and torsion over a broad range of strain rates and temperatures, where traditional crystal plasticity models fail. Furthermore, it captures size and Bauschinger effects, work hardening, and thermal softening. Next, we model notch-like defects to explore shear band instabilities, with predictions accurately matching Marchand and Duffy's experiments over a broad range of strain rates and temperatures. Finally, we apply this approach to the brittle-ductile transition, predicting fracture toughness in tungsten across a range of temperatures – consistent with the experimental findings of Gumbsch.

Biography:

Prof. Le Khanh Chau is a Senior Researcher at Ton Duc Thang University (Vietnam), with a distinguished academic background from renowned institutions, including Moscow State University and St. Petersburg State University. His research expertise encompasses smart and functionally graded materials, nonlinear vibration, wave propagation, thermodynamic dislocation theory, fracture mechanics, and micromechanics. He is internationally recognized with over 120 publications in leading journals and the authorship of the acclaimed Springer monograph "Vibrations of Shells and Rods". His prior experience includes faculty appointments in Germany and extensive international collaborations. He demonstrated passion for mentorship, having successfully supervised over 50 graduate and postgraduate students.

Alpha-glucosidase Inhibitory Activities of Salazinic acid Derivatives from Parmotrema lichen

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Abstract: Lichens are formed from symbiosis between fungi and algae. They are known as a source of biologically active compounds with a wide range of properties, including antibacterial, antifungal, antioxidant, antivirus, anticancer.

Recent studies have revealed that lichens also contain compounds with potential for treating type 2 diabetes by inhibiting alpha-glucosidase activity in vitro. Furthermore, research suggests that cultivated lichen fungi produce numerous novel compounds with largely unexplored biological activities.

Salazinic acid, isolated from the lichen Parmotrema indicum, along with its synthesized derivatives, demonstrates promising activity against type 2 diabetes. Notably, all derivatives exhibited stronger alpha-glucosidase inhibitory activity compared to the positive control acarbose (IC50 332 μM), with IC50 values below 50 μM. Additionally, the study employed molecular docking simulations to further understand how these compounds interact with alpha-glucosidase.

Rational design and simulation of hydrogen storage materials by using first-principles, thermodynamic, and kinetic approaches

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Abstract: We thoroughly discuss a multiscale modeling scheme to investigate hydrogen storage materials. The structures are engineered and then simulated by first-principles DFT-based calculations. The atomistic thermodynamic model is further employed to reach realistic operating conditions, i.e., at different temperature and pressure ranges. The results obtained with the thermodynamic model could be re-evaluated with a kinetic Monte Carlo simulation, which is also useful for estimating the time scale of the hydrogen adsorption and desorption processes. We demonstrated our approaches by considering hydrogen storage in the Sc-decorated adamantane framework and Sc_2C MXene, which are the porous and layered structures, respectively. Those materials can capture hydrogen with high gravimetric capacities of 5.5-7.2 wt % under cryogenic conditions. At higher temperatures, the uptakes decrease significantly due to weak bonding of molecular hydrogen to the active sites. Particularly on Sc_2C, there are nanosecond time scales to reach thermodynamic equilibriums for hydrogen adsorption/desorption processes. The fast kinetics manifests the influence of kinetic effects in the overall simulation results. The curent approaches pave the way to study gas sorption on a variety of materials relying on the combination of first-principles calculations, and thermodynamic and kinetic models that require less computational effort.

Keyworks: first-principles, thermodynamic, kinetic, hydrogen storage, equilibrium

Globunoids A–D, undescribed bichalconoid and biflavanoids with α-glucosidase and α-amylase inhibitory activities from Knema globularia stems

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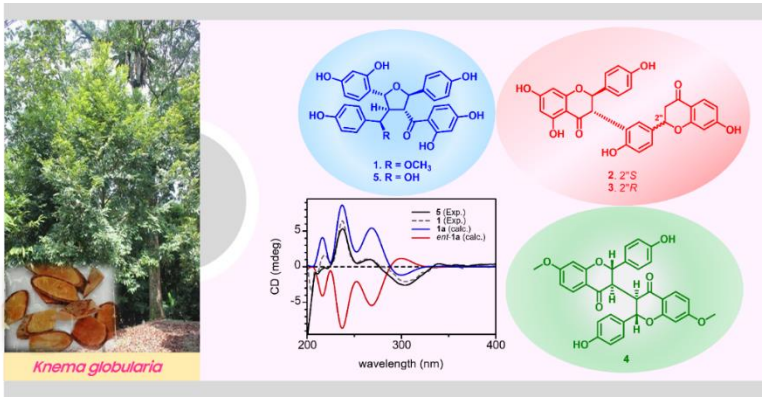
Abstract: A bichalconoid, globunoid A (**1**) and three biflavanones, globunoids B–D (**2**–**4**), previously undescribed, were isolated from the stems of *Knema globularia*, along two known analogues **5**–**6**. The chemical structures of **1**–**4** were elucidated by the comprehensive spectroscopic analysis including UV, IR, HRESIMS, and NMR; the absolute configurations were determined based on their NOESY data, DP4+ statistical analysis, and ECD calculation. Up to now, compounds **2** and **3** represent the first 3,3′′-linked biflavanone structures. Among the isolated compounds, **2**, **3**, and 2,3-dihydrocalodenin B (**6**) potently inhibited *α*-glucosidase and *α*-amylase activities, with IC_{50} values in the range 1.1–7.5 μM. Furthermore, the most active compound **6** was found to be a non-competitive inhibitor against these two enzymes.

Keywords: *Knema globularia* (Lam.) Warb.; Myristicaceae; Biflavonoids; Bichalconoid; *α*-Glucosidase inhibitory activity; *α*-Amylase inhibitory activity



Natural Compounds Inhibit Monkeypox Virus Methyltransferase VP39 *in Silico* Studies

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Abstract: The VP39 enzyme, a crucial 2'-O-RNA methyltransferase identified within the Monkeypox virus (MPXV), plays a vital role in viral RNA replication and transcription. Inhibition of the enzyme may prevent viral replication. Therefore, in this context, we used a combined approach involving atomistic simulations including molecular docking and molecular dynamics simulations, the inhibitory ability of NCI Diversity Set VII natural compounds to VP39 protein was investigated. It should be noted that the computed binding free energy of ligand via molecular docking and linear interaction energy (LIE) approaches are in good agreement with the corresponding experiments with coefficients of R=0.72 and 0.75, respectively. NSC 319990, NSC 196515, NSC 376254 compounds were demonstrated that can inhibit MPVX methyltransferase VP39 protein with the similar affinity compared to available inhibitor sinefungin. Moreover, nine residues involving *Gln39, Gly68, Gly72, Asp95, Arg97, Val116, Asp138, Arg140,* and *Asn156* may be argued that they play an important role in binding process of inhibitors to VP39. target for the development of antiviral drugs against MPXV.

Keywords: MPVX; VP39; LIE; docking; NCI.

α-Glucosidase Inhibitors from the Trunk of *Morus alba* Linn.: Spectroscopy, Molecular Docking and Molecular Dynamics Simulations

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Abstract: The phytochemistry investigation on the trunk of *Morus alba* L. resulted in the isolation of three triterpenoids, including a new gammacerane triterpenoid – morusacerane (1); along with two known compounds of betulinic acid (2) and ursolic acid (3). The structure elucidation was thoroughly conducted based on 1D, 2D-NMR and HRESIMS spectra, followed by a comparison with existing literatures. The evaluation on α-glucosidase inhibitory exhibited the great potential of the application of these isolated compounds in diabetes treatments. The results show that morusacerane (1), betulinic acid (2), and ursolic acid (3) demonstrate the strong inhibitory with the IC_{50} values of 106.1, 11.12, and 7.20 μM, respectively. The results of molecular docking and molecular dynamics simulations suggested that the isolated compounds could generate stable complexes with enzyme α-glucosidase MAL32 through H-bonds and hydrophobic interaction.

Keywords: Molecular docking, molecular dynamics, *Morus alba* L. trunk, Gammacerane, α-glucosidase inhibitory.

Morphology of a Transmembrane Aβ42 Tetramer via REMD Simulations

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Abstract: The folding/misfolding of membrane-permiable Amyloid beta (Aβ) peptides is likely associated with the advancing stage of Alzheimer's disease (AD) by disrupting Ca^{2+} homeostasis. In this context, the aggregation of four transmembrane Aβ_{17-42} peptides was investigated using temperature replica-exchange molecular dynamics (REMD) simulations. The obtained results indicated that the secondary structure of transmembrane Aβ peptides tend to have different propensity compared to those in solution. Interestingly, the residues favorably forming β-structure were interleaved by residues rigidly adopting turn-structure. A combination of β- and turn regions likely forms a pore structure. Six morphologies of 4Aβ were found over the free energy landscape and clustering analysis were performed. Among these, the morphologies include (1) Aβ binding onto the membrane surface and three transmembrane Aβ; (2) three helical and coil transmembrane Aβ; (3) four helical transmembrane Aβ; (4) three helical and one β-hairpin transmembrane Aβ; (5) two helical and two β-strand transmembrane Aβ; and (6) three β-strand and one helical transmembrane Aβ. Although the formation of β-barrel structure was not observed during the 0.28 ms - long MD simulation, the structure is likely to form when the simulation time is further extended.

Keywords: Chemical structure, Conformation, Monomers, Morphology, Peptides and proteins.

Synthesis, and characterization of a metal absorbent fabric from polyhydroxyl-nitroso dye applied for heavy metal treatment

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Abstract

Nowadays, there is a growing trend towards the use of multifunctional dyes, which must possess not only coloristic properties but also other beneficial attributes such as biological, sorption, and electrophysical activity. To enhance these properties, functional groups are incorporated into organic dyes to increase their interaction with materials, broaden their ability to form complexes with various coordination types, and create additional useful characteristics. In this study, a typical polyhydroxyl-nitroso dye based on phloroglucinol and antipyrine was synthesized and thoroughly characterized. The complexation of this compound with heavy metal ions was investigated both in solution and in the solid state using a combination of techniques including ^{1}H NMR, ^{13}C NMR, UV-Vis, IR, EPR spectroscopy, and X-ray structure determination. The results demonstrated that the synthesized compound could precipitate with nearly all heavy metal ions in an acidic solution, rendering it suitable for use as a metal absorbent material. To this end, the ligand was applied to wool fabric, which was then utilized as a metal absorbent material in an acidic aqueous solution. The ability to absorb metallic ions of obtained matterials was evaluated under dynamic and static conditions, revealing that after three cycles of absorption, the concentrations of Cu^{2+}, Zn^{2+}, Cr^{3+}, Ni^{2+}, Co^{2+} and Cd^{2+} were reduced by over 90% at a pH of 3-4. Consequently, wool fabric dyed with

the polyhydroxyl-nitroso dye exhibits potential as a material for removing heavy metallic ions from industrial wastewater.

Keywords: multifunctional dyes, metal absorbent material, polyhydroxyl-nitroso dye, wool fabric.

Synergizing Machine Learning, Molecular Docking, and Dynamics Simulations to Uncover Potent HDAC2 Inhibitors

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Abstract

Histone deacetylase 2 (HDAC2) inhibitors are promising therapeutic agents, particularly in cancer treatment. However, discovering novel inhibitors with high specificity and binding affinity is challenging. Recent advancements in machine learning (ML) and cheminformatics offer new avenues for drug discovery by integrating QSAR models with molecular docking and molecular dynamics simulations.

Keywords: HDAC2 inhibitor; QSAR based ML; docking, molecular dynamic simulations

Ab-initio based Kinetic Modeling of Dissociation Reactions Sodiated Monosaccharides under Collision-induced Dissociation Mass Spectrometry Conditions

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Abstract: Recently, the so-called logically derived sequence tandem mass spectrometry (LODES/MSn) using collision-induced dissociation (CID) developed by C.-K. Ni and co-workers has been successfully applied for the structural identification of cation-tagged sugars from biological samples. The obtained structural information includes the identity of the monosaccharide building blocks, their linkage positions, and anomeric configurations. Further, it can also differentiate between branched and linear oligosaccharides. To apply this method, it is essential to know how different cation-tagged sugar monomers decompose under CID conditions. Thus, a computational approach has been employed to perform mechanistic studies for various monosaccharides.

The mechanism for the dehydration and cross-ring dissociation processes, i.e., the reactions associated with the major ion fragments observed in the CID mass spectra, have been examined based on ab-initio reaction barriers. In addition, the rate constants for these competing dissociation reactions have been calculated by different approaches. These results have been employed to set up a kinetic model at MP2/6-311+G(d,p) level of theory to estimate the dissociation products' relative concentration and rationalize the experimental mass spectrometry results. The computational results are in line with experimental observations and support the assignment of the mass spectrum of different anomers of monosaccharides.

Keywords: dissociation reactions, kinetic modeling, mass spectrometry, monosaccharides, MP2

Collective excitations in 4-BLG: Inhomogeneity effects

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Abstract

We investigate the plasmon properties of a 4-BLG structure on an inhomogeneous background dielectric within the random-phase approximation. We obtain plasmonic excitations in layered structures can be found from the zeroes of the frequency-dependent dielectric function $\varepsilon\ q,\omega_p - i\gamma\ = 0$ (ω_p denotes the frequency of collective excitations at a given wave vector q while γ denotes the decay rate of plasma oscillations) and then calculate respective broadening functions. Computations demonstrate that there are four solutions to the zero-point equation of the dynamical dielectric function, corresponding to four phases of collective excitations in the system. Three of them, acoustical modes, are lower than that in BLG at the same parameters while the optical mode has a higher frequency at a given wave vector. Secondly, we present that both the inhomogeneity of background dielectric and the inter-layer separation strongly decrease the plasmonic frequency and respective broadening functions. Moreover, the inhomogeneity of the environment strengthens the effects of separation on plasmon properties. Lastly, the increase in doping density in BLG layers decreases strongly both plasmon frequency and its broadening functions. We observe that due to the pronounced contributions to plasmon properties of 4-BLG systems of the inhomogeneity, this factor should not be neglected in calculations

Keywords: Bilayer graphene; Inhomogeneity effects; Multilayer graphene; Plasmon properties.

Creep and Long-term Strength of High-entropy Alloys

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Abstract: High-entropy alloys (HEAs) are actively being investigated for next-generation structural materials. Gaining a comprehensive understanding of their creep behavior is necessary. These aspects of mechanical properties are especially important because creep resistance determines the use of the alloys in high-temperature applications. Because the materials with superior properties are continuously searched, high-entropy alloys (HEAs), formed by the metallurgy of five or more metallic elements with equal or nearly equal quantities, emerge as a class of revolutionary materials. One decade of dedicated research has revealed that many HEAs possess unparalleled properties in comparison with traditional alloys, for instance, great thermal and microstructural stability, high hardness, high strength at a wide range of temperatures, and excellent resistance to wear, corrosion, fatigue, fracture, and high-temperature softening. Given these merits, applications of HEAs in various fields, particularly in the structural engineering (e.g., used for gas-turbine engines), is being actively explored. Among many performance indices, a thorough understanding of creep behavior of HEAs is crucial and indispensable to their complex engineering applications.

In the work to describe the creep and long-term strength of HEAs a damage conception is used. A system of interconnected kinetic equations for the creep rate and damage parameter is formulated. A compressible medium is considered and the mass conservation law is taking into account. The damage parameter is specifying in the form of the ratio of the current density of the material to the initial one. Exact and approximate analytical solutions of these equations are obtained. The theoretical creep and long-term strength curves are plotted and compared with the experimental results for CrMnFeCoNi alloy. It is shown, that the experimental results are in good agreement with

the theoretical ones. Thus, the proposed system of interrelated kinetic equations allows us to describe the creep and long-term strength behavior of HEAs.

Keywords: Creep, damage parameter, high-entropy alloys, long-term strength.

First-principle Calculations of Structural and Electronic Properties of Xenes (X=Si, Ge and Sn) Surfaces with CO or NO2 Adsorption

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Abstract: In this work, the adsorption of toxic gas molecules (CO or NO_2) on Xenes (X = Si, Ge, Sn) has been studied by density functional theory (DFT). The optimized adsorption site of the adsorbates (CO, NO_2) on Xenes (X = Si, Ge, Sn), the corresponding adsorption energies, band gap, band structure and density of states of Silicene, Germanene and Stanene are discussed. We observed that, Xenes (X = Si, Ge, Sn) weakly physically adsorb CO, from which we show that Xenes (X = Si, Ge, Sn) are not suitable for gas sensing application of CO. On the other hand, NO_2 can be adsorbed on Xenes (X = Si, Ge, Sn) with the moderate adsorption energy (respectively is 0.813 eV, 0.716 eV and 0.776 eV). In addtion, the band gap of Xenes (X = Si, Ge, Sn) is expanded after adsorption of NO_2 in varying degrees, which indicates that Xenes (X = Si, Ge, Sn) may be a promising candidate as the sensor of NO_2. Finally, we assume that Xenes (X = Si, Ge, Sn) has not potential in developing catalysts for CO or NO_2 due to these gas molecules are not strongly chemisorbed on Xenes (X = Si, Ge, Sn) (adsorption energies < 1.00 eV). Our research results not only help to understand the properties of Xenes (X = Si, Ge, Sn) but also suggest research directions for the application of its potentials as catalysts and gas sensors as well as applications in the electronics field.

Keywords: adsorption, adsorption energies, band structure, density of states and density functional theory

Design and simulation of a novel magnetorheological brake with T-shaped multilayer rotor

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Abstract: This paper presents the design and simulation of a novel magnetorheological (MR) brake with a T-shaped multilayer rotor. The objective is to enhance the braking performance and operational stability of MR brakes for a wide range of industrial applications. The proposed design incorporates a T-shaped rotor configuration consisting of multiple layers of magnetorheological fluid (MRF) and ferromagnetic materials. The multilayer rotor structure enables the generation of a stronger magnetic field and provides enhanced braking torque. The design process involves the optimization of the T-shape multilayer rotor geometry, considering factors such as the number of layers, thicknesses, and materials used. Finite element analysis (FEA) simulations are conducted to evaluate the magnetic field distribution and torque generation of the brake. The simulation results guide the design iteration process and aid in achieving an optimal rotor configuration. Comparisons between the simulated results of the proposed design and previously developed MR brake configurations are conducted. The objective is to assess the performance improvements achieved by the T-shaped multilayer rotor. The simulation outcomes provide valuable insights into the advantages of the proposed design, including enhanced braking performance and increased torque generation.

Keywords: Magnetorheological fluid (MRF), MR barke, T-shaped rotor, multilayer MRF, optimization.

A study on velocity profile of magnetorheological Fluid in an annular duct based on finite element analysis

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Abstract: This paper investigates the velocity profile of magnetorheological (MR) fluid within an annular duct using finite element analysis. MR fluids are intelligent materials that exhibit reversible and tunable changes in rheological properties when subjected to a magnetic field. Understanding the flow behavior of MR fluids is crucial for modeling and optimizing their applications in various engineering systems. The study employs a finite element analysis approach to simulate the flow of MR fluid in an annular duct using the Bingham and Herschel plastic rheological model. The velocity profile of the MR fluid in the annular duct is derived from the finite element solution. The effects of key parameters, including annular duct geometry, fluid properties, and magnetic field intensity, on the velocity profile are investigated. The results demonstrate the influence of these parameters on the flow behavior of MR fluids, highlighting the potential for controlling and manipulating fluid flow by adjusting the magnetic field strength. The knowledge gained from this investigation contributes to the development of advanced engineering applications, such as dampers, clutches, and adaptive devices, where precise control of fluid flow is essential.

Keywords: Magnetorheological fluid (MRF), annular duct, velocity profile, finite element analysis, Bingham plastic rheological model, Herschel plastic rheological model

Free vibration analysis of magneto electro-elastic plates reinforced with carbon nanotubes: a moving Kriging meshfree approach

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Abstract: This paper investigates the free vibration characteristics of carbon nanotube-reinforced magneto-electro-elastic (CNTMEE) plates using a moving Kriging meshfree method (MKM). The investigation explores the influence of various carbon nanotube (CNT) distribution patterns (uniform, O, V, and X) within the MEE plate thickness. By employing Hamilton's principle and C^0-higher order shear deformation theory with seven variables, the governing equations for free vibration analysis are derived. The moving Kriging approach is then implemented to approximate the displacement field, electric potential, and magnetic potential. A comprehensive analysis is conducted to examine the impact of several factors on the vibrational frequency of the CNTMEE plate. These factors include: external magnetic and electric loads, CNT distribution patterns, CNT volume fraction, and plate geometry. Numerical results are compared to published findings in the literatures.

Keywords: Moving Kriging meshfree method, free vibration, electro-magneto-elastic plate, carbon nanotube reinforcement.

Implementing Sobol's Global Sensitivity Analysis to SFRC's Flexural Strength Predictive Equation

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Abstract: The integration of steel fibers into plain concrete enhances concrete performance. The addition of steel fibers improves a significant property of concrete, which is its flexural strength. Flexural strength, crucial for Steel Fiber Reinforced Concrete (SFRC), significantly improves with steel fiber inclusion, bolstering resistance to cracking and bending loads, ensuring durability. Current research investigates the impact of fibers and other concrete compositions on SFRC's flexural strength properties and the lack of predictive models. This study focuses on four key areas: selection of tests databases, validating data distribution, analyzing parameter correlations, and developing accurate predictive models for SFRC flexural properties. Utilizing Sobol's method for global sensitivity analysis, 211 experimental recordings from 18 researchers form a comprehensive database. Bayesian Model Averaging identifies significant structural components affecting overall strength, refining prediction, and regression models. The study used Sobol's method for assessing the sensitivity of various input parameters to SFRC flexural strength, including water, cement, aggregates, etc., and fiber characteristics.

Keywords: Sobol' Method, Global Sensitivity Analysis, Flexural Strength, SFRC, Linear Regression, Bayesian Model Averaging

A Study on Structure Stiffness of 3D Printed Continuous Carbon Fibers Frames

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Abstract: In this paper, the effect of carbon continuous fibers (CCF) on the stiffness of 3D printed frames is investigated. Fused deposition modelling (FDM) technology is employed to build three typical frames with 15% of CCF and 85% Polyamide 12 combined 10% short carbon fibers (PA12-CF) for compress testing. The 3D models of the frames including grid 45 CCF, triangle CCF and grid 90 lattices are designed based on slicing parameters and simulated in Abaqus before conducting experiment. An MTS–45 system (USA) is used for compress testing to measure the stiffnesses and peak loads of the models. The contribution of CCF to enhancing the stiffness of the printed models are pointed out. Finally, the comparison between simulation and experiment results are also discussed. It shows that the two results quite fit together. This investigation is worth in the extension of CCF printing application.

Keywords: Behavior of 3D Printed Structures, Carbon Fibers, 3D Printing Lattices, Polyamide 12, Fused Deposition Modelling.

Absorption coeficient in a GaAs/InAs/GaAs cylindrical semicinductor quantum well with a three level ladder configuration

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Abstract: From the density matrix equation, the paper has presented the interaction between the electromagnetic field and electron in the cylindrical semiconductor quantum well with a three level ladder configuration. We study the change of absorption coefficient in InAs is embedded in a GaAs barrier material and frequency of probe laser and coupling laser. From the research results, we determine the values of Ω_p , Ω_c, Δ_p, Δ_c for the appearance of the electromagnetically induced transparency effect.

Keywords: semiconductor quantum well, absorption coefficient, electromagnetically induced transparency**.**

Nonlinear optical absorption in hyperbolic quantum wells

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Abstract: In this work, the nonlinear optical absorption properties have been theoretically investigated via two-photon processes in a hyperbolic quantum well (HQW). We obtain the analytical expression for the magneto-optical absorption coefficient (MOAC) by using the perturbation theory to consider the transition probability for the absorption of photons. The obtained results affirm that the shape of confined potential is strong affected to the MOAC, the width at half maximum (HWHM) of the MOAC in both linear and nonlinear absorption cases, as well as magnetic field and temperature. So, by changing specific parameters in HQW model, we can be controlled the magneto-optical properties of the materials. These results are also compared with the shape of with different confinement potentials.

Keywords: hyperbolic quantum wells; magneto-optical absorption; two-photon processes electron – phonon scattering.

Polytopal composite finite elements for pseudo-lowerbound limit analysis of two dimensional structures

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Abstract: We present a polytopal composite finite element (PCE) used in conjunction with second-order cone programming (SOCP) to evaluate the pseudo-lowerbound limit analysis of two dimensional structures. Limit analysis can be utilized to directly compute the ultimate load of structures without the need for costly elastic-plastic analysis. The fundamental idea behind PCE is to create a polynomial projection of compatible strain fields using the least-squares approximation. We construct two projection operators of the volumetric and deviatoric stresses that lead to the stability of the pressure solution in nearly incompressible situations. The approach works well with arbitrary polygonal elements, as well as typical triangular and quadrilateral ones, which are considered special situations. We limit the treatment to the analysis of von Mises-type materials in this paper, but it can easily be extended to other materials. Numerical tests are done, which demonstrate that the suggested method has good accuracy and a low evaluation load, allowing us to solve large-scale limit analysis problems.

Keywords: Polygonal FEM, limit analysis, polytree mesh, SOCP.

Study on optimizing the amount of RFCC in high performance concrete (HPC)

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Abstract: In this paper, we delve into the optimization of mixed technique for high-performance concrete (HPC) using residue fluid catalytic cracking (RFCC) for component. Additionally, we explore the integration of AI-inspired big data analytics and use machine learning to predict the optimum amount of RFCC in HPC.The primary aim remains finding an optimal balance among workability, compressive strength, flexural strength, slipting strength in concrete mixture design. Utilizing the simplex centroid design approach, grounded on packing density, we optimize the composition of cement, RFCC, and sand paste, alongside the ideal ratio between paste, fine aggregate, and coarse aggregate, tailored to a specified strength grade. Our findings indicate that the correlations among workability and paste volume fraction serve as valuable indicators for determining the optimal total cementitious material content. Furthermore, characteristics and compressive strength of concrete, incorporating ternary cementitious components, aid in identifying the most effective replacement of excess cementitious materials. By employing the simplex centroid design approach, we demonstrate the feasibility of optimizing concrete mixture designs concerning compression strength, spread flow, flexural, and splitting characteristics, particularly pertinent to their application in RFCC within the realm of HPC.

Keywords: Machine learning, Simplex centroid design method, Residue Fluid Catalytic Cracking (RFCC), High-Performance Concrete (HPC), compressive strength, flexural and splitting characteristics.

Free vibration analysis of functionally graded triply periodic minimal surface nanoplates using meshfree method

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Abstract: This study presents the size-dependent effects on the free vibration characteristics of functionally graded (FG) triply periodic minimal surface (TPMS) nanoplates. Employing the higher order shear deformation theory (HSDT) alongside the moving Kriging meshfree method, and integrating nonlocal Eringen's elasticity theory, we explore two types of porous nanostructures: Primitive and Gyroid patterns. Four distinct volume distribution scenarios are analyzed for each pattern. Mechanical properties, such as elastic modulus, shear modulus, and Poisson's ratio, are determined through a fitting curve model based on a two-phase piece-wise function. Numerical results are meticulously compared to original reference data obtained from existing literature.

Keywords: Triply periodic minimal surface; Cellular materials; Higher order shear deformation theory; Moving Kriging meshfree method.

Unsteady thermoelastic-diffusion vibrations of a Bernoulli-Euler beam on an elastic foundation

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Abstract: The paper deals with the problem of unsteady vibrations of the Bernoulli-Euler beam, taking into account relaxation of temperature and diffusion processes. The original mathematical model includes a system of equations of unsteady bending vibrations of the beam taking into account heat and mass transfer, which is obtained from the general model of thermoelastic diffusion for continuum using variational D'Alembert principle.

On the example of a simple supported three-component beam made of an alloy of zinc, copper, and aluminum, which is under the influence of mechanical load distributed along the length, the interaction of mechanical, temperature and diffusion fields is investigated. The influence of relaxation effects on the kinetics of heat and mass transfer is analyzed. The solution is presented in analytical form and in the form of graphs of the dependence of the desired fields of movement, temperature increments, and increments of concentration of medium components on time and coordinates

Keywords: Thermoelastic diffusion, Laplace transform, Fourier series, Green's functions, Bernoulli-Euler beam, unsteady problems

A locking-free plate element based on asymptotically first order shear deformation theory

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Abstract: We present an approach to prevent the volumetric and shear locking of the plate element by simple scaling technique. The asymptotically accurate theory based on first order shear deformation approach is employed to characterize the weak and strong form of the plate element. We combine it with Isogeometric Analysis (IGA) to facilitate model construction and improve the accuracy of the analysis by hpk-refinement technique. Bezier decomposition is used in implementation to improve the scalability and computational throughput of the numerical code.

Keywords: Plate finite element, Asymptotically first order theory, shear and volumetric locking.

Nonlinear vibration and dynamic buckling responses of stiffened functionally graded graphene-reinforced cylindrical, parabolic and sinusoid panels using the higher-order shear deformation theory

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Abstract: The nonlinear vibration and dynamic responses of functionally graded graphene-reinforced composite (FG-GRC) laminated cylindrical, parabolic, and sinusoid panels stiffened by FG-GRC stiffeners in the uniformly distributed temperature variation are presented in this paper. An improved smeared stiffener technique is used to model the added stiffnesses of stiffeners to the total stiffnesses of panels. The higher-order shear deformation shell theory (HSDT) with the geometrical nonlinearities of von Kármán is applied to establish the governing formulations. The stress function form is estimated using the approximated technique for complex curvature panels. Lagrange function and Euler-Lagrange equations are applied, and the Rayleigh dissipation function is taken into account to obtain the nonlinear equation of motion. Numerical examples are investigated using the Runge-Kutta method to obtain the dynamic responses of panels, and the critical dynamic buckling loads of panels are considered using the Budiansky-Roth criterion. Some significant remarks on the nonlinear vibration and dynamic buckling responses of three types of stiffened panels can be recognized from the numerical examples.

Keywords: Functionally graded graphene-reinforced composite; Vibration and dynamic buckling; Higher-order shear deformation shell theory; Thermal environment; Complex curvature panels.

A new analytical approach for nonlinear thermo-mechanical postbuckling of FG-GPLRC circular plates and shallow spherical caps stiffened by spiderweb stiffeners

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Abstract: This study considered the problem of nonlinear postbuckling of circular plates and shallow spherical caps reinforced by meridian, parallel stiffeners, and spiderweb stiffeners based on the Donnell shell theory (DST) and von Kármán geometric nonlinearities. The caps/plates and stiffeners were made of functionally graded graphene platelet-reinforced composite (FG-GPLRC). These stiffened structures were subjected to uniformly distributed external pressure or/and uniformly distributed thermal loads. By expanding Lekhnitskii's smeared stiffener technique and employing the Ritz method of energy, the formulas to determine the postbuckling curves of the external pressure–deflection and thermal load-deflection relations of stiffened plates/spherical caps were derived. The various influences of FG-GPLRC stiffeners, material distributions of plate/cap and stiffeners, and geometrical, material, and foundation parameters were investigated.

Keywords: Nonlinear postbuckling; Donnell shell theory; FG-GPLRC; Spiderweb stiffener; Ritz energy method.

Dynamic Regimes for Compressing of Thin Plastic Layers

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Abstract: More recently, in 2023, one hundred years have passed since the publication in ZAMM of the pioneering work by L.Prandtl, dedicated to the quasi-static compression and spreading of a thin flat perfect rigid plastic layer between approaching absolutely rigid rough plates. A decade later, H.Geiringer and W.Prager constructed a velocity field in this problem corresponding to an incompressible plane flow. The analytical history of the Prandtl problem which includes many generalizations and ramifications begins with these two papers.

This work is devoted to the generalization of the Prandtl problem in the case when it is necessary to take into account the inertial effects arising from the spreading of a thin layer. In addition, the velocity of convergence of rigid plates may depend on time being one of the control parameters in the system. The dynamic formulation of the problem includes three characteristic dimensionless parameters. One of them, a small geometric parameter equal to the ratio of the thickness of the layer to its length, clearly depends on time, and over time the order of its smallness increases with respect to another two dimensionless parameters — a number equal to the inverse Euler number and dimensionless acceleration of rigid plates convergence. These values are also assumed to be much smaller than one. In relation to ratio of these parameters, i.e. at different time intervals, using the asymptotic integration procedure, solutions are constructed in the form of integer power expansions. The validity of the search for a solution in this form is substantiated. The possibility of smooth crosslinking in time of asymptotic expansions is shown. Various dynamic regimes of compressing are investigated, namely, when the plates approach uniformly, as well as according to power or exponential laws.

Keywords: asymptotic analysis, compressing, dynamics, perfect plasticity, thin plane layer.

Two-photon optical absorption in a quantum dot with the Yukawa potential

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Abstract: We investigate the optical absorption characteristics of a quantum dot featuring a Yukawa potential, with a specific focus on the two-photon absorption (TPA) phenomenon. GaAs/AlGaAs material serves as our illustrative example. Our findings reveal that the intraband transition exhibits a narrower energy transition compared to the interband transition. Consequently, TPA spectra associated with intraband transitions are confined within a smaller energy range and display higher peak values compared to those of interband transitions. Moreover, the relationship between the absorption peak position and the transition order, denoted as 'n', varies between intra- and inter-band transitions. Our exploration holds promise for facilitating the design of innovative photonic devices, ultra-fast optical switches, and highly efficient solar cells by optimizing the properties of quantum dot materials.

Keywords: Two-photon absorption, quantum dot, Yukawa potential.

Essential properties of emergent monolayered semiconductors

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Abstract: Using the highly accurate hybrid functional, we have developed a complete first-principles theoretical framework to fully identify the critical formation mechanism and clarify the physical and chemical picture of the Si-doped 1D graphene nanoribbons within armchair and zigzag edges, in which the critical formation mechanism of the critical quasi π and σ hybridizations was firstly introduced. Specifically, the quasi π and quasi σ bands show a weak separation that evidences the weak quasi sp^2 hybridization, which is an origination of the good structural stability of the doped 1D semiconductors. Our theoretical results can not only provide a complete understanding of the chemically doped 1D semiconductors for future semiconducting applications but also bring a promising platform for the following experimental verification. Furthermore, this developed theoretical framework based on highly accurate first-principles calculations can be effectively generalized to many other chemically doped systems.

Keywords: Density functional theory, graphene nanoribbons, substitution, electronic band structure, spin density

The generation of entangled state in a nonlinear coupling coupler pumped in modes is driven by broadband laser

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Abstract: We explore a configuration consisting of two nonlinearly interconnected oscillators. These oscillators are stimulated by two external classical fields, which are divided into deterministic components and white noise. Through the application of the nonlinear quantum scissors mechanism, we establish that the system's development can be restricted to a finite set of Fock states, resulting in the creation of maximally entangled states. Noteworthy is the noticeable change observed in the maximally entangled states when contrasted with situations where the noise parameter of the laser field is not present. The credibility of our results is affirmed by comparing them with previous studies.

Keywords: Maximally entangled state, Nonlinear coupler, Parameter related to the chaotic part, Stochastic process, White noise.

A novel decoupled RBDO approach for structural optimization with probabilistic constraints

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Abstract: Reliability-based design optimization (RBDO) is termed for structural optimization with probabilistic constraints. The problem aims at the cost-effective design of structural integrity, addressing simultaneously inherent indeterministic uncertainties. This ensures that the structure performs reliably under practical design specifications. Processing the RBDO problem often poses challenges involving the accurate estimation of failure probabilities transgressing limit-state functions. This paper proposes the novel and efficient decoupled RBDO, called subset simulation – comprehensive learning particle swarm optimization (SS-CLPSO), method to iteratively converge the optimal design solution. The decoupled approach separates reliability analysis from the design improvement in the RBDO process. It transforms uncertain variables into deterministic ones through connected constraints and thus allows for an exploration of the most suitable design within the specified design space. More explicitly, the initial stage performs the CLPSO under deterministic parameters using the most probable points (MPPs), constructing the principle for limit-state functions. As the reliability assessment progresses, CLPSO adjusts its optimization performance evolving limit-state functions, and SS predicts the spectrum of limit-state functions under uncertain parameters. The probabilistic analysis prediction significantly reduces the need for computationally expensive Monte-Carlo simulations (MCSs), enabling the precise failure probability approximation. The SS-CLPSO effectively maps failure probabilities using generated samples, aligning with predefined thresholds. The application of the decoupled SS-CLPSO approach is illustrated through the reliability-based designs of steel structures in the presence of probabilistic uncertainties. A primitive design example can describe the robustness and accuracy of

the proposed method, which importantly provides good potential for handling extended complex engineering design problems.

Keywords: Comprehensive learning, Particle swarm optimization, Probabilistic analysis, Reliability-based design optimization, Subset simulation.

NSGA-II, SPEA2+SDE and AMOSA: A comparative study

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Abstract: Design Optimization is research area which was carried out a lot on the world, with many applications in the specifications of mechanical engineering, aerospace engineering, civil engineering. The global optimization methods are more effective than local optimization methods. In this article, the authors will deal with multiobjective global optimization methods, such as: NSGA-II, SPEA2+SDE, AMOSA. The authors will do novel research about comparing the efficiencies of these multiobjective optimization methods. It is investigated that AMOSA is the most effective multiobjective optimization method, AMOSA can converge faster and smoother towards the final optimal solutions. SPEA2+SDE will rank secondly. It has been found that SPEA2+SDE outperforms NSGA-II. SPEA2+SDE is better than NSGA-II when size of population and number of iterations are small, the increasement in population size does not make an increasement in performance. SPEA2+SDE is also faster in finding the best Pareto front.

Keywords: Design Optimization, Multiobjective Optimization Methods, AMOSA, SPEA2+SDE, NSGA-II.

Atomistic simulation of high strain rate deformation and shock compression of metal crystals

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Abstract: We perform molecular dynamic simulations of shock-wave loading for copper and molybdenium crystals of micrometer length in a wide range of temperatures and impact velocities. Crystal models with different initial distribution dislocations are considered: perfect crystals with no dislocations, crystals with dislocations in a selected region along the shock wave direction, and uniform distribution of dislocations across the crystal with different densities. The role of solutes in the case of Cu crystals is also studied. The time series of stress, particle velocities and temperature along the shock wave direction are obtained from the simulations. The features of the shock wave structure, such as the elastic precursor decay, the Hugoniot elastic limit and the rise time of the plastic wave, are investigated.

We show that In Mo crystals with preexisting dislocations, the HEL decays monotonically, and the decay rate and the stress values weakly depends between [110] and [111] orientations. The HEL decreases slightly with increasing temperature for [110] crystal and taking close values for [111] crystal at the shock wave propagates of about 1 micron. In perfect Mo crystals, the HEL decreases with temperature for all crystal considered.

The results show that in Cu solid solution crystals with dislocations, the HEL decays slower with an increase in the misfit parameter of the solute, resulting in higher HEL values at a certain shock propagation distance. The Cu-Al solid solutions with the largest misfit parameter exhibit the largest deceleration of HEL decay. When the concentration of Al atoms increases to 20 at.%, the HEL almost does not change with shock propagation distance and a plateau shape of the elastic precursor is observed, as in the case of perfect crystals.

The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University and MVS-10P clusters at the Joint Supercomputer Center of the Russian Academy of Sciences (JSCC RAS). The reported study is supported by the Russian Science Foundation (RSF), research project №22-71-00088.

Limit state analysis of structures under cyclic loads using bubble-enriched smoothed finite element method

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Abstract: This study presents an efficient approach that combines the bubble-enriched edge-based smoothed finite element method (bES-FEM) with conic programming to accurately compute the load- carrying capacity of structures under both monotonic and variable repeated loads. Enhancing the cubic bubble function within the ES-FEM framework results in a notable improvement in solution accuracy while successfully addressing the common issue of volumetric locking phenomena in plane strain problems. Kinematic and equilibrium constraints are satisfied on average within the smoothing domains associated with the edges, resulting in a minimized problem size. The optimization problem is formulated as second-order cone programming (SOCP), enabling efficient solutions using high-performance interior-point solvers. The proposed method accurately determines the upper-bound and pseudo-lower-bound shakedown and collapse loading factors with optimal computational cost. A series of numerical examples are presented to validate the performance and effectiveness of the approach.

Model-free data-driven simulation of elasto-plastic materials

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Abstract: Data-driven computational mechanics offers an alternative to traditional constitutive models by performing simulations directly from strain-stress data. This approach minimizes the distance between the model's stress-strain response and a pre-defined dataset subject to equilibrium and compatibility constraints. While successful for elasticity, incorporating history-dependent materials remains a challenge.

This paper overviews the data-driven framework for elasto-plasticity with isotropic hardening, which is augmented by two essential elements:

1. **Tangent Space Information:** Directions in the tangent space of points within stress-strain space are included, capturing the material's local response.

1. **Data Subsets and Transition Rules:** The data is divided into subsets corresponding to different material behaviors. Transition rules map the selection between these subsets based on the material state.

In addition, the methodology utilizes Haigh-Westergaard coordinates, which provide information about the material's yield surface. A combined tension-torsion test captures this information, while a single tensile test determines the tangent space data. By minimizing the distance over the Haigh-Westergaard space, augmented with tangent space directions under compatibility and equilibrium conditions, the framework offers a robust solution to inelastic problems with isotropic hardening. Taking into account material symmetries allows generating sufficient experimental data with limited effort.

Modeling of Unsteady Vibrations of a Bernoulli-Euler Beam on an Winkler Foundation with Considering Heat and Mass Transfer

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Abstract: The immense practical applications in science and technology have led to a constant interest in understanding the mechanics of interconnected fields of different physical origins. Nowadays, models have been developed using established equations from continuum mechanics, heat and mass transfer, electrodynamics, and thermodynamics to capture the interactions between mechanical, temperature, diffusion, electromagnetic, chemical, and other fields.

The research introduces a concept for analyzing non-stationary thermal injection fusion vibrations in an orthotropic Bernoulli-Euler beam subjected to a distributed transverse load. The beam is supported by an elastic base modeled as a Winkler base. The problem is mathematically formulated as a closed system of Bernoulli-Euler beam bending equations incorporating heat and mass transfer. This formulation is derived from the generalized d'Alembert principle based on the thermoelastic diffusion model for continuous media. Additionally, the model considers the final speed of heat and diffusion propagation, accounting for relaxation effects. The problem is further defined by homogeneous boundary conditions representing hinge support and zero initial conditions indicating the absence of internal disturbances at the beginning of the analysis.

The problem is approached by utilizing Green's functions and presenting the solution as convolutions of influence functions with functions that describe non-stationary perturbations distributed along the beam's length. Green's functions are obtained through the Laplace transformation over time and expansion into Fourier series with respect to the longitudinal coordinate. Consequently, the original set of equations governing the thermohazardoffusion vibrations of the beam is transformed into a system of linear algebraic equations involving the

Fourier coefficients of the desired functions in the Laplace transform domain. The inversion of the Laplace transform is accomplished through deductions and operational calculation tables.

Keywords: Thermoelastic diffusion, Laplace transform, Green's function, Bernoulli-Euler beam.

Influential Features Analysis and AI-Driven Accuracy Enhancement: A Study Case For DDoS Detection

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Abstract: Cybersecurity is known today as one of the greatest challenges of the modern era. Among the various types of cyber-attacks that threaten our security, the Distributed Denial of Service (DDoS) attack is among some of the most common, effective, and well-recognized attack strategies. Since this form of attack is meant to disrupt the availability factor covertly, it can be detrimental to the targeted machines and difficult to be discovered. Because of that, there have been a number of approaches, as well as solutions that have been devised in order to detect it as accurately and efficiently as possible. Impressively, data mining methods have been employed to identify patterns of DDoS attacks from the computer network traffic. Nevertheless, the recent works' results have not yet mentioned which factors of the computer network traffic play the most vital role in indicating the potential for true positive attacks. Additionally, with the Machine Learning approach, there are still ample opportunities to enhance the attack prediction accuracy of the detection model. As such, in this paper, we attempt to explore factors that would influence the classification result, and leverage a variety of Machine Learning algorithms, i.e. Random Forest, Naive Bayes, Logistic Regression, and Multilayer Perceptron, for the purpose of improving the accuracy of data classification. The experiments were deployed using CICIDS2017 dataset and compared with the other related works on the same dataset. The experimental outcomes of our methodologies and analyses demonstrate some potential and effectiveness enhancement compared to previous works. Moreover, we analyzed and concluded the insight of how side factors affect the attack identification result. The collected information from our analysis identifies dominant factors, and opens a new view for their hidden correlationship directly affecting the attack labeling.

Keywords: Distributed Denial of Service (DdoS), Random Forest (RF), Naive Bayes (NB),

Logistic Regression (LR), Multilayer Perceptron (MLP).

A Machine Learning Approach fo a Statistical Homogenization Method fo Elastic Two-Phase Materials Topic: Data-driven Computational Mechanics and Machine Learning

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Abstract: Statistical homogenization methods are widely used to predict the response of a heterogeneous material to loading. The key idea is to find the average behavior of the material, i.e. looking at a homogenized version of it and determining its mechanical properties.

To apply the methods, a key challenge is the choice of a suitable probability function which describes the spatial correlation within the material.

Limitations in experimental and theoretical tools often lead to difficulties in finding a good approximation of the statistical descriptor.

We propose an approach that employs machine learning techniques to address the difficulty of finding the correct correlation function for a class of 2D two- phase-microstructures. A neural network is used to extract the probability functions from the microstructure image.

Extracting the size distribution of gold nanoparticles from a UV-visible spectrum: an artificial neural network model

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Abstract: A nondestructive detection of the size distribution of nanoparticles (NPs) is desired in various applications. The conventional method utilizes the dynamic light scattering from which the sizes of NPs are drawn by using the Stokes-Einstein relation. We propose a novel method to draw the size distribution of NPs from the UV-visible spectrum. Our method utilizes an artificial neural network (ANN) model trained against an extensive dataset generated by Mie theory. The promising performance of the present ANN model is demonstrated.

Keywords: gold nanoparticle, artificial neural network, Mie theory, extinction spectrum, size distribution

Analysis of the vibration behavior of continua with physics-informed neural networks

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Abstract: Investigating oscillations becomes a challenging task for complex structures and high frequencies as needed in acoustic design or earthquake risk assessment. Besides modal analysis for the linear regime, time-stepping algorithms after domain discretization by the finite element method (FEM) as well as for multi body simulations (MBS) are a standard approach. They exhibit a trade-off between numerical stability and accuracy which is signaled by a steady loss of the calculated system energy over the simulated time.

Neural Networks (NNs) are universal function approximators which proved to be effective in high-dimensional spaces. For the solution of physical problems, PINNs are a promising and powerful architecture. Their training objective is not based on given data tuples, but on the residual of partial differential equations (PDE). The architecture is set up so that the NN predicts the field variables which solve the PDE. Then, its weights and biases are optimized so that the residual of the prediction and the deviation from the given boundary conditions are minimized.

The approach presented here is designed to include different data sources and techniques to improve and accelerate the solution, such as data-driven pre-training (e.g. from measurement data), transfer learning based on results from comparable calculation tasks, estimates for eigenfrequencies and/ or amplitudes (e.g. from modal analysis of a simplified model or another NN based estimator) and equations or inequations that apply to the physical task.

Possible scenarios for this approach are i) acceleration of the simulation of nonlinear oscillations based on existing, related data, ii) acceleration of optimization tasks, iii) calculation of the sound transmission loss (STL) and acoustic properties of structures and iv) hybrid experimental and numerical investigations.

Case studies on simple oscillating structures in 1D and 2D show that the approach is promising and capable to capture the oscillatory behavior of structures with sufficient accuracy for a range of applications.

Keywords: Vibrations, Nonlinear oscillations, Physics-Informed Neural Networks, Machine Learning, Data-driven methods

Comparative Study of xLSTM with Conventional Deep Learning Models on Bitcoin Price Trends

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Abstract: Recent advancements in sequence modeling have led to significant improvements in predicting complex time-series data. This article introduces the Extended Long Short-Term Memory (xLSTM) model, which encompasses single-layer LSTM (sLSTM) and multi-layer LSTM (mLSTM) architectures, designed to enhance prediction accuracy and computational efficiency. We conduct a comprehensive comparison of xLSTM with traditional Recurrent Neural Networks (RNNs), Long Short-Term Memory Networks (LSTMs), Gated Recurrent Units (GRUs), and Transformers, employing the dataset of Bitcoin prices published by Binance. Our evaluation criteria focus on predictive accuracy, learning time, and model robustness in handling the highly volatile nature of cryptocurrency markets. The results indicate that xLSTM models, particularly the mLSTM configuration, provide superior performance in capturing the temporal dynamics and volatility of Bitcoin prices compared to other models. This study not only confirms the efficacy of xLSTM in financial time-series forecasting but also demonstrates its potential applicability in broader economic and predictive analytics domains.

Keywords: xLSTM, RNNs, LSTMs, GRUs, Transformers

Analysis of large datasets measured on non-linear oscillators for application in data-driven machine learning

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Abstract: In recent years, the application of data-driven machine learning models (ML models) in combination with large collections of data has become very popular in different areas. Also, in the field of nonlinear dynamics, various initiatives are underway to improve or even replace classical modelling with machine learning techniques. Classical non-linear dynamics modelling is usually understood as the description of the system using differential equations which are derived from the dominant physical phenomena. Meanwhile, data- driven ML models are generally trained with large amounts of data without the knowledge of underlying physics. Regardless of the type of model, the aim remains to approximate the dynamics of the system under specific boundary or initial conditions as accurately as possible.

A common practice for evaluating the quality of data-driven models is currently to compare them with simulation data from classical models. In nonlinear dynamics, special forms of the duffing oscillator are often used for this purpose. However, investigations in which a ML model is trained and tested directly on actual measurement data of a real system are rare.

For this reason, a dataset generated precisely for this purpose, which will be freely accessible, will be introduced and analyzed in this talk. The data set consists of numerous measured time series representing the response of a nonlinear oscillator. In classical modelling, this system can be approximated as a Duffing oscillator with one or two degrees of freedom. Furthermore, different ML approaches for modelling from different areas are compared with regard to their ability to describe the real system in comparison to the classic approach.

Keywords: Experimental Data, Vibrations, Nonlinear oscillations, Machine Learning, Data-driven methods

Multiscale modeling of calcified polymer hydrogels

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Abstract

Hydrogels, a significant group of highly hydrated polymers, represent the best choice for the potential application to bone fracture regeneration, which goes back to their bioactivity, affinity for biologically active proteins and compatibility with the bone tissue. However, this kind of materials also shows a serious disadvantage, namely, it loses its mechanical strength through swelling. This makes its straightforward usage difficult and motivates the development of different enhancement procedures. One of the most modern techniques for this purpose is calcification or, in a more general sense, mineralization. This method is inspired by the natural process of the bone growth where the enzyme alkaline phosphatase causes mineralization of the bone by cleavage of the phosphate from organic molecules. An analogous process induces homogeneous mineralization of a hydrogel and increases its mechanical strength. Recently, optical and electron microscopy has revealed that calcification yields different types of microstructure dependent on the type of the underlying polymer, and thus has clearly indicated that computational modeling can significantly contribute to the targeted investigation of effective behavior and material parameters. The current contribution uses the multiscale finite element method to simulate the effective material behavior of calcified hydrogels. Within this framework, representative volume elements (RVEs) are generated to depict the biphasic material microstructure consisting of the organic hydrogel and anorganic calcium phosphate [1]. Most commonly, the anorganic phase appears in the form of spherical inclusions or honeycomb grids where the characteristic size of a typical unit might vary. The approach proposed treats the calcified regions as linear elastic material and assumes the Ogden model for the hydrogel. Diffusivity is another important aspect in this context [2]. Its study requires a profound knowledge on the processes on the nanoscale. This time, the effective behavior is investigated by using the asymptotic homogenization approach.

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Keywords: Multiscale analysis, Multiscale FEM, Hydrogels, Diffusion

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