

Session K Abstracts

Numerical simulations and data generation for learning closure models

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Closure models are critical in accurately capturing unresolved or subgrid-scale processes in complex physical systems, such as fluid dynamics, climate modeling, and material deformation. Recently, there has been a rise of interest in using high-fidelity simulated data or experimental data to learn closure models using techniques such as operator learning and differential programming. However, there is a lack of standardized and well-documented testing problems and datasets, which makes it challenging to systematically compare the strengths and limitations of different learning methods across various mechanistic systems. We address this issue by designing simple and representative test problems, generating datasets, and evaluating the performance of learning methods. Emphasis was put on reproducibility and accessibility--the designed test problems, code, and datasets will be shared with the broader research community to foster collaboration and further advancements in the field.

Numerical analysis of low-Mach time-integration schemes for 3D variable density flows

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Mentors: Guillaume Blanquart and Aaron Nelson

The low-Mach limit gives rise to numerical challenges in turbulent flows where density changes over time and space. We study the performance of an iterative time-integration scheme for such flows using direct numerical simulations of a stationary homogeneous buoyant turbulent flow in a triply periodic domain. The parameters tested include the Courant–Friedrichs–Lewy (CFL) number, scalar transport scheme, scalar rescaling to enforce conservation, number of subiterations, and grid resolution. Results show that the effects of rescaling and transport scheme depended on the CFL and subiteration settings, where rescaling improved density conservation at low CFL but could greatly increase equation-of-state error, and the semi-Lagrangian scheme tended to yield slightly lower residuals than the Eulerian scheme but was less stable in some high-CFL cases. Additionally, while both had similar convergence rates for low CFL, the semi-Lagrangian scheme had a much faster convergence rate than the Eulerian scheme at high CFL, with rescaling amplifying the effects. These findings provide guidance for selecting parameters that balance accuracy, stability, and computational cost in low-Mach turbulence simulations. Future work will extend this study to shear-generated variable-density turbulence.

Extending frequency-based spatiotemporal reduction techniques to periodic systems

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Mentors: Tim E. Colonius and Caroline Cardinale

Model reduction techniques have traditionally focused on spatial representations, but recent advancements have explored the use of spatiotemporal bases to improve the accuracy of reduced-order models. The proper orthogonal decomposition (POD) method, which computes modes of the state matrix in the spatial domain, has been the standard approach. However, it can suffer from reduced accuracy when only a limited number of modes are retained. In contrast, spectral proper orthogonal decomposition (SPOD) offers a more efficient framework by incorporating Fourier-transformed POD modes of each trajectory in the state space, improving the representation of the system's dynamics. This approach involves solving the governing partial differential equation (PDE) algebraically for the linear term, while the nonlinear term is approximated using the discrete empirical interpolation method (DEIM). The reduction process consists of two key phases: an offline stage to approximate the necessary operators, and an online stage that performs the projection. When compared to traditional POD-based methods, SPOD demonstrates superior accuracy with respect to

the number of retained modes and computational time. However, a limitation of SPOD is its assumption of periodicity, which may cause spectral leakage when applied to nonperiodic systems. To assess the technique's performance and limitations, we extend the SPOD framework to the Kuramoto-Sivashinsky equation, a well-known chaotic system that exhibits both periodic and nonperiodic behavior across different bifurcations.

Inverse scattering solution for kidney stone detection

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Mentors: Tim E. Colonius and Chris Zhang

This project develops a computational framework for the non-invasive detection of kidney stones using inverse acoustic wave scattering. A Gaussian pulse is propagated through body fluids, and the pressure field of the scattered wave is recorded by probes positioned around the domain. By formulating the problem as an inverse optimization task, we infer the stone's size and location from the measured pressure data. The methodology integrates forward modeling with inverse problem-solving techniques, examining the effectiveness of local methods such as the Gauss-Newton and Levenberg-Marquardt algorithms, full waveform inversion, global methods such as the particle swarm optimization, and hybrid global-local approaches, ensuring robust convergence with limited prior knowledge. Extensions to two-dimensional and potentially three-dimensional reconstructions further enhance accuracy, enabling a viable framework for kidney stone imaging, optimizing accuracy and computational cost.

Improving the modeling of cement carbonation and carbon uptake

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Mentors: Melany L. Hunt and Ricardo A. Hernandez

The production process of concrete is a substantial contributor to carbon emissions; however, due to a set of carbonation reactions, cement also acts as a carbon sink by absorbing atmospheric CO₂. The current estimate of the mass of CO₂ that can be absorbed by cement is 40-50% of the CO₂ emitted in manufacturing cement. However, the model used in this estimate is an approximation with assumptions that are inconsistent with the real world. Our research develops a refined model incorporating more realistic porosity and atmospheric CO₂ concentrations.

By employing a finite element method (FEM) using COMSOL Multiphysics we simulate the CO₂ diffusion throughout a block cement and incorporate the carbonation reactions that are missing in the approximate model. This improved FEM model provides a more accurate assessment of the amount of carbon absorbed through time and matches experimental data more accurately than the approximate model. Ultimately, this research will support the development of sustainable concrete production and utilization strategies to mitigate climate change.

Scalable second-life battery management system for stationary energy storage

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Mentor: Runar Unnthorsson

The rapid growth of electric vehicles has generated an abundance of end-of-life lithium-ion cells, presenting an opportunity for cost-effective stationary energy storage if reliable second-life management systems can be developed. This project develops and validates a scalable battery management system (BMS) for repurposed electric-vehicle cells in stationary energy storage applications. Starting with a 4-cell proof-of-concept, we have refined both hardware and firmware to support 30 V and 50 V assemblies, including improved current and temperature sensing, enhanced thermal management, and reliable relay control. We have adapted existing control software for automated cycling and balancing validation, and designed compact enclosures that integrate factory thermistors and BMS electronics. These 30 V and 50 V modules are designed to be deployed in parallel banks, allowing capacity to be scaled to multi-kilowatt-hour levels for grid-tied or off-grid applications.

Ongoing work encompasses comprehensive capacity and cyclability testing under IEC 61960-3 protocols, the development of passive balancing strategies for idle periods, and field deployment at off-grid sites. Together, these efforts aim to demonstrate a cost-effective, reliable second-life energy storage solution that advances sustainable, circular-economy practices.

Exploring the role of flax fiber on the structural and mechanical behavior of 3D-printed *Chlorella vulgaris* biocomposites

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Mentors: Chiara Daraio and Israel Kellersztein

The long-term persistence of petroleum-based plastics in natural ecosystems creates serious environmental concerns, and even many biodegradable alternatives, such as biopolymers or wood, require ideal conditions to break down effectively. Biomass-based composites provide a renewable and biodegradable option that adapts to diverse applications. However, improving their structural reliability and mechanical performance remains an area of active research. In this SURF project, we used flax fibers, extracted from agricultural waste, to investigate their reinforcement effect on *Chlorella vulgaris* microalgae and hydroxyethyl cellulose (HEC) biocomposites. We process our materials via extrusion 3D printing at room temperature and without the use of any petrochemical components, resulting in lightweight materials with tailored properties and geometries. High fiber loadings affect the printability of the structures due to nozzle clogging and irregular extrusion. Dimensional analysis shows reduced shrinkage in the x-y plane, attributed to fiber alignment because of flow during printing. Structural analysis through scanning electron microscopy (SEM) demonstrated that the *Chlorella* cells remained intact after 3D printing processing, showing the microalgae cell resilience to high shear stress. Quasi-static three-point bending shows an improved flexural modulus of 1211 MPa, which is 25 % higher than the reference material (967 MPa), while maintaining comparable bending strength. We identify pull-out phenomena at fracture surfaces as the main mechanism of energy absorption.

These results identify flax fibers as a promising reinforcement of microalgae-based materials, providing a sustainable alternative to wood and plastics, for diverse engineering applications such as packaging, construction, or furniture.

New experimental platform for investigating soliton and wave dynamics in 1D and 2D Polycatenated Architected Materials (PAMs)

Kensuke Shimojo

Mentors: Chiara Daraio and Xiaoxiao Xiong

Polycatenated Architected Materials (PAMs) are a new class of metamaterials composed of interlocked ring-like elements, which offer unique, tunable nonlinear dynamics and energy-dissipative behavior under mechanical loading. Compared to conventional architected or granular materials, PAMs exhibit highly customizable resistance to specific deformation modes, due to the high internal degrees of freedom in their interlocked and per-unit topology. This enables their potential use in advanced shock absorption applications, such as impact-resistant helmets or vehicle protection systems, where tailored mechanical responses are desirable. Because most existing experiments only investigate static properties of PAMs, investigations into the dynamics of PAMs are necessary to fill the knowledge gap for such applications. To this end, we developed an experimental platform to investigate force and soliton propagation in 1D and 2D PAM systems. Using this platform, we obtained high-quality, analyzable data from experiments investigating 1D chains, junctions of chains, and 2D chainmail meshes. These experiments allowed us to compare experimental signatures of nonlinear wave propagation with theory. The setup's modular design allows for various different configurations of PAMs and actuation modes, such as transverse or rotational actuation and the integration of various sensors into the PAM units, yielding great potential for future experimentation.

Computational and experimental study of irregular architected metamaterials

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Mentors: Chiara Daraio and Chelsea Fox

Irregular networks are found in a variety of biological materials, resulting in a diversity of structurally dependent mechanical properties. An algorithm based on a lattice of truncated octahedra has been developed to generate irregular pseudo-random structures. These structures are examined both computationally and experimentally, and in both quasi-static and dynamic compression.

Sensor-integrated head design for robust perception in humanoid robots

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Mentors: Aaron D. Ames, Adrian Boedtker Ghansah, and Sergio A. Esteban

The AMBER Lab at Caltech conducts research on locomotion, control, and human-robot interaction, aiming to build robots that can safely operate in human environments. Recently, the lab has been working with the Unitree Humanoid G1, a humanoid designed for research in robotics and human-robot interaction. Ensuring safety in humanoid operation requires robust perception, as the robot must reliably sense and respond to its environment. This project focuses on enhancing perception of the G1 robot through the development of a new head design that integrates multiple visual sensors. The redesigned head integrates four RGB-D cameras, providing a comprehensive field of view for safer navigation and interaction. Early results show smooth integration of the cameras with ongoing progress in visualization. Future work will refine the head's mechanical design to further improve perception, robustness, and safety.