

Rocky Mountain Fluid Mechanics Research Symposium 2018: Technical Program

Eaton Humanities Building
University of Colorado Boulder
August 13th-14th, 2018

Keynote Presentation

Dr. Greg Chini, (August 13th, 11:00 AM - 12:00 PM)

*A Tale of Two Quasi-Linear Dynamical Systems:
Modulated Waves and Shear-Driven Instabilities*

Presentation Schedule

Monday, August 13th, 2018

Session 1A: Experiments

9:30 AM - 10:30 AM (Room A)

9:30 AM Erin Connor (University of Colorado, Boulder, CO)

Experimental Quantification of Airborne Odor Plumes for the Development of Search Algorithms

9:45 AM Grant Dunbar (University of Colorado, Boulder, CO)

Design and Testing of a Multi-Hole Probe Geometry Insensitive to Manufacturing Variance

10:00 AM Daniel Sinner (University of Colorado, Boulder, CO)

Performance of an Unsteady, Low-Speed Wind Tunnel with an Upstream Lower System for Longitudinal Velocity Modulation

10:15 AM Lucas Droste (University of Colorado, Boulder, CO)

Continuous Pseudorandom Longitudinal Velocity Perturbations in an Unsteady Low-Speed Wind Tunnel

Session 1B: Engines

9:30 AM - 10:30 PM (Room B)

9:30 AM Diego Bernardi Bestel (Colorado State University, Fort Collins, CO)

Natural Gas and CFR Engine Modeling for Knock Prediction

9:45 AM McKay Stoker (Colorado State University, Fort Collins, CO)

CFD Model for an Automobile Refueling System

10:00 AM Radi Alsulami (Colorado State University, Fort Collins, CO)

Investigation on the Role of Fuel Droplet Vaporization and Atomization on Spray Flame Stability and Dynamics

10:15 AM Owen Brown (University of Colorado, Boulder, CO)

Computational Modeling of Propane Direct Injection for Advanced Compression Ignition Engines

Session 2A: CFD Methods**1:30 PM - 2:30 PM (Room A)**

- 1:30 PM Eric Peters (University of Colorado, Boulder, CO)
A Divergence-Conforming Hybridized Discontinuous Galerkin Method for the Incompressible Reynolds Averaged Navier-Stokes Equations
- 1:45 PM Eman Yahia (University of Colorado, Boulder, CO)
Central Moment Lattice Boltzmann Method for Computation of Flows on Stretched Lattice Grids
- 2:00 PM Adam Saad (University of Colorado, Denver, CO)
Non-Newtonian Fluid Flow Simulations using Cascaded Lattice Boltzmann Method
- 2:15 PM Scott Wieland (GATS Inc., Boulder, CO)
Mastering the Modality of the Rayleigh-Taylor Instability through Wavelet Based Adaptive Mesh Refinement

Session 2B: Porous Media**1:30 PM - 2:30 PM (Room B)**

- 1:30 PM Jincheng Lou (Colorado School of Mines, Golden, CO)
Numerical/Experimental Study of a Direct Contact Membrane Distillation System
- 1:45 PM Jacob Johnston (Colorado School of Mines, Golden, CO)
Application of Novel Immersed Boundary Method Techniques to Simulation of Flow Over a Cylinder in a Channel
- 2:00 PM Liam Pocher (Colorado School of Mines, Golden, CO)
Flow Regimes through Periodic Arrays of Cylinders (Part 1)
- 2:15 PM Zahra Khalifa (Colorado School of Mines, Golden, CO)
Flow Regimes Through Periodic Arrays of Cylinders (Part 2)

Session 3A: Fire**3:00 PM - 4:00 PM (Room A)**

- 3:00 PM Amanda Makowiecki (University of Colorado, Boulder, CO)
Dual Frequency Comb Spectroscopy for the Investigation of Ignition Behaviour of Wildland Fire Fuels
- 3:15 PM Jeff Glusman (University of Colorado, Boulder, CO)
A Chemical Kinetic Mechanism Reduction for Wildland Fire Direct Numerical Simulation and Experimental Validation
- 3:30 PM Caelan Lapointe (University of Colorado, Boulder, CO)
Fire Simulation Using Adaptive Mesh Refinement
- 3:45 PM Nicholas Wimer (University of Colorado, Boulder, CO)
Direct Numerical Simulations of Plumes and Pool Fires Using Adaptive Mesh Refinement

Session 3B: Geostrophysics**3:00 PM - 4:00 PM (Room B)**

- 3:00 PM Rachel Robey (Los Alamos National Laboratory, Los Alamos, NM)
An Assessment of a Mass Flux Closure for the Ocean Surface Boundary Layer
- 3:15 PM Talal Al Refae (University of Colorado, Boulder, CO)
The Effects of a Horizontal Magnetic Field on Rayleigh-Bénard Convection

3:30 PM Ming Yan (University of Colorado, Boulder, CO)
Thermal Conviction with a Strong Vertical Magnetic Field

3:45 PM Adam Binswanger (University of Colorado, Boulder, CO)
Experimental Investigation of Oblique Dispersive Shock Waves in Supercritical Shallow Water Flow

Tuesday, August 14th, 2018

Session 4A: Machine Learning 9:00 AM - 10:15 AM (Room A)

9:00 AM Michael Ying (National Center for Atmospheric Research, Boulder, CO)
Scale-dependent Localization for Ensemble Filtering of Quasi-Geostrophic Flows

9:15 AM Mokbel Karam (University of Utah, Salt Lake City, UT)
Applying Machine Learning to the Sedov-von Neumann-Taylor Blast Wave

9:30 AM Olga Doronina (University of Colorado, Boulder, CO)
On Markov Chain Monte Carlo Approximate Bayesian Computation Approach for Subgrid-Scale Model Development

9:45 AM Steven Issacs (University of Colorado, Boulder, CO)
Development of a Computational Modeling and Optimization Tool for Thin Flat Heat Pipes for Small Satellite Heat Dissipation

10:00 AM Michael Meehan (University of Colorado, Boulder, CO)
Characterization of Flapping in a Plane Turbulent Buoyant Jet Using Proper Orthogonal Decomposition

Session 4B: Biology 9:00 AM - 10:15 PM (Room B)

9:00 AM Alireza Sharifi (Colorado State University, Fort Collins, CO)
Impedance vs Peristaltic Pumping in Zebrafish 24-30 hpf Embryonic Heart

9:15 AM Banafsheh Zebhi (Colorado State University, Fort Collins, CO)
Computational Fluid Dynamic Simulation of Fetal Heart

9:30 AM Alison Wallbank (University of Colorado, Anschutz, CO)
Two-phase Flow Effects on Human Coagulation Factor X Activation in vitro

9:45 AM Joshua Pertile (University of Colorado, Denver, CO)
Parameters Governing Pressure Homogeneity in a 3D Printed Human Airway During Low Frequency Jet Ventilation

10:00 AM Joel Human (University of Colorado, Boulder, CO)
Wall-Bounded Vorticity in the Right Heart from 4DMRI Measurements

Session 5A: Turbulence 1:30 PM - 2:15 PM (Room A)

1:30 PM Samuel Whitman (University of Colorado, Boulder, CO)
Scaling and Collapse of Conditional Velocity Structure Functions in Turbulent Premixed Flames

1:45 PM Mitchell Krouss (University of Colorado, Boulder, CO)
The Influence of the Prandtl Number on the Inverse Cascade in Rapidly Rotating Convection

2:00 PM Elizabeth Strong (University of Colorado, Boulder, CO)
Designing a Noninvasive Laser-Based Vorticity Sensor

Session 5B: Exotic Fluid Flows

1:30 PM - 2:00 PM (Room B)

- 1:30 PM Ryan Darragh (University of Colorado, Boulder, CO)
Supersonic Turbulence Modulation in a Particle-Laden Jet
- 1:45 PM Dante Disharoon (Colorado School of Mines, Golden, CO)
Effects of Magnetic Torque on Microscale Spheres
- 2:15 PM Colin Towery (University of Colorado, Boulder, CO)
Spontaneous Detonation Initiation in Compressible Isotropic Turbulence

Session 6A: CFD Modeling

2:45 PM - 4:00 PM (Room A)

- 2:45 PM Meghan Kaminski (University of Virginia, Charlottesville, VA)
Gravo-Aeroelastic Additively Manufactured Design of a 1% Scale Wind Turbine Blade
- 3:00 PM Elizabeth Rasmussen (University of Washington, Seattle, WA)
Comparison of Multiple Equations of State in Numerical Simulation of Supercritical Carbon Dioxide Flow Around a Heated Cylinder
- 3:15 PM Riccardo Balin (University of Colorado, Boulder, CO)
Preliminary Steps to Scale-Resolving Simulations of Turbulent Boundary Layers with Flow Separation
- 3:30 PM Ryan Skinner (University of Colorado, Boulder, CO)
Modeling of Active Flow Control in an Aggressive Diffuser with Comparison to Experiment
- 3:45 PM Prakash Mohan (University of Texas, Austin, TX)
A Predictive Near-Wall Model for Large Eddy Simulations

Session 6B: Bubbles and Droplets

2:45 PM - 4:00 PM (Room B)

- 2:45 PM Jacob Gissinger (University of Colorado, Boulder, CO)
Drop Squeezing through Interparticle Constrictions with Insoluble Surfactant
- 3:00 PM Noemi Collado (University of Colorado, Boulder, CO)
Fast Agglomeration with Permeable Drops
- 3:15 PM Albert Maristany (University of Colorado, Boulder, CO)
Behavior of Droplets Through a Porous Membrane
- 3:30 PM Bashir Alnajjar (University of Colorado, Colorado Springs, CO)
A Spherical Model for an Encapsulated Microbubble Using Transient Network Theory
- 3:45 PM Fathia Arifi (University of Colorado, Colorado Springs, CO)
A Model for the Nonspherical Oscillation of Encapsulated Microbubbles Using Transient Network Theory

Keynote Presentation

Professor Greg Chini (11:00 AM - 12:00 PM)

Department of Mechanical Engineering, University of New Hampshire

A Tale of Two Quasi-Linear Dynamical Systems: Modulated Waves and Shear-Driven Instabilities

The quasi-linear (QL) approximation has facilitated the prediction and understanding of a broad variety of fluid dynamical phenomena, ranging from the quasi-biennial oscillation of the zonal winds in the equatorial stratosphere to the emergence of exact coherent states (ECS) in wall-bounded turbulent shear flows. The QL reduction involves a decomposition into mean and fluctuation components and retention of fluctuation/fluctuation nonlinearities only where they feed back on the mean dynamics. Although sometimes invoked as an *ad hoc* simplification, the QL approximation can be justified asymptotically for certain flows exhibiting temporal scale separation, as will be demonstrated here through two complementary examples. In the first example, a new type of acoustically-driven mean flow is identified and analyzed. Specifically, it is shown that when a high-frequency acoustic wave of small amplitude ϵ interacts with a stratified fluid, an unusually strong form of acoustic streaming can occur, with the time-mean flow arising at $O(\epsilon)$ rather than the more commonly realized $O(\epsilon^2)$ value. The resulting two-way coupling between the wave and streaming flow is self-consistently captured in a QL dynamical system. In the second illustration, a QL model of strongly stratified turbulent shear flows is derived. Spectrally non-local energy transfers, associated with small-scale non-hydrostatic instabilities induced by the relative horizontal motion of large-scale hydrostatic eddies, are economically represented. The model is used to compute ECS in strongly stratified Kolmogorov flow and to evaluate the mixing efficiency achieved by these nonlinear states. For both the wave- and shear-driven systems, new asymptotic analyses are developed that enable integration of the dynamics strictly on the slow time scale associated with the mean flow, yielding significant computational efficiencies while simultaneously promoting physical insight.

Speaker Biography:

Greg Chini is Professor of Mechanical Engineering and Co-Director of the Integrated Applied Mathematics Ph.D. Program at the University of New Hampshire. He earned his doctorate in Aerospace Engineering at Cornell University, with a focus on a fluid mechanics and applied mathematics, and has held visiting positions at Nottingham University, Caltech, the Institute for Pure and Applied Mathematics (IPAM) at UCLA, and the Kavli Institute for Theoretical Physics (KITP) at UCSB. In 2016, he was elected to the faculty of the Woods Hole Summer Program in Geophysical Fluid Dynamics. Prof. Chini's research centers on the application of nonlinear mathematics and high-fidelity numerical simulations to important environmental, energy, and resource challenges facing society. Specific research themes include self-organization and extreme transport in fluid turbulence, multiscale phenomena in geophysical fluid dynamics and geophysics, and mathematical modeling of energy and resource systems.

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Presentation Abstracts

Session 1A: Experiments

August 13th, 9:30 AM - 10:30 AM (Room A)

Experimental Quantification of Airborne Odor Plumes for the Development of Search Algorithms

Erin Connor, *Civil, Environmental, & Architectural Engineering, University of Colorado, Boulder*

Orit Peleg, *Computer Science, University of Colorado, Boulder*

John Crimaldi, *Civil, Environmental, & Architectural Engineering, University of Colorado, Boulder*

Using planar laser-induced fluorescence, we quantify the spatiotemporal structure of neutrally buoyant airborne scalar plumes ($Sc \approx 1.5$). We image the fluorescent tracer, acetone vapor, in a benchtop-scale low-speed wind tunnel as an ultraviolet laser excites fluorescence at a frequency of 15 Hz. The resulting concentration distributions have a detectability limit of 0.05% of the source concentration for a 16 cm by 30 cm field of view. We provide results for three different flow conditions in which the tracer is released isokinetically into the tunnel at 10 cm/s near a lower boundary, a second case at 10 cm/s released in the freestream of the tunnel, and 20 cm/s case also released in the freestream of the tunnel. Among the cases, we compare the spatial distributions of instantaneous concentration, mean concentration, root-mean-square fluctuations, and concentration intermittency. The work is motivated by an interest in olfactory navigation by animals and autonomous vehicles. Therefore, special attention is paid to evaluating the time-dependent information available to a searching agent. Further, we demonstrate the utility of real plume data in testing odor source localization algorithms such as infotaxis.

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Design and Testing of a Multi-Hole Probe Geometry Insensitive to Manufacturing Variance

Grant Dunbar, *Aerospace Engineering Sciences, University of Colorado, Boulder*

John Farnsworth, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Multi-hole probes are aerodynamic instruments that measure pressure at various points on their geometry. This array of pressures is used to estimate airspeed and flow angles through an established mathematical relationship. For existing multi-hole probes, this relationship is highly sensitive to the particular geometry of the probe. Due to manufacturing variances, each probe requires a unique calibration for its specific geometry, which is expensive and time consuming. Typical multi-hole probe configurations include hemispherical, conical, and pyramidal tip geometries. This project considers six probes spanning these common configurations and seeks to identify which geometry is least sensitive to manufacturing variance utilizing Reynolds-Averaged Navier-Stokes computational fluid dynamic simulations. These probes are tested for a range of simulated manufacturing variances, including non-uniform scaling, pressure port displacement, bumps and dips on the surface, and skewed geometries. The consistency of the pressure measurements from these probe geometries is compared for equivalent manufacturing variances. In future work, the least sensitive probe geometry will be manufactured through a stereolithographic additive manufacturing technique and evaluated experimentally.

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Performance of an Unsteady, Low-Speed Wind Tunnel with an Upstream Louver System for Longitudinal Velocity Modulation

Daniel Sinner, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Lucas Droste, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Daniel Bateman, *Aerospace Engineering Sciences, University of Colorado, Boulder*

John Farnsworth, *Aerospace Engineering Sciences, University of Colorado, Boulder*

The experimental simulation of unsteady flow can be obtained by moving a model relative to a flow or modifying the flow itself. In this study, the latter approach was used, utilizing the opening and closing of

flow-impeding louvers at the far upstream end of a low-speed, open-return wind tunnel. These louvers can rapidly tune the flow speed in the test section without altering the blower speed. Fixing the louvers in the fully closed position results in a 53% to 60% drop in flow speed from fully open, with the larger reductions at faster blower speeds. During dynamic louver operation, the test section flow speed does not instantly track with louver position. Additionally, the flow speed responds more quickly as the shutters are closed, dropping the speed, than when opened at the same rate. When commanding louver motion with equal opening and closing times, the flow speed can spend as much as 62% more time accelerating than decelerating. This effect is most pronounced for faster louver motions and lower blower speeds. Ultimately, this project aims to accurately predict the flow speed in the test section for any arbitrary louver position schedule.

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Continuous Pseudorandom Longitudinal Velocity Perturbations in an Unsteady Low-Speed Wind Tunnel

Lucas Droste, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Daniel Sinner, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Daniel Bateman, *Aerospace Engineering Sciences, University of Colorado, Boulder*

John Farnsworth, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Longitudinal velocity perturbations have been studied experimentally using active control methods over the last 75 years. To generate these perturbations in a wind tunnel, a system of counter-rotating louvers can be utilized to vary the blockage ratio and impose fluctuations in the test-section airspeed. Such a system has been implemented in the low-speed wind tunnel at the University of Colorado, Boulder which can be commanded to produce pseudorandom, longitudinal velocity perturbations. A pseudorandom louver motion was prescribed such that the test-section air speed would have a predicted energy decay rate proportional to the Kolmogorov energy cascade. Experiments were conducted to investigate the fluid system response to these pseudorandom louver motions. For an input signal with a prescribed energy decay rate proportional to the Kolmogorov energy cascade, the test-section airspeed decayed at the same rate but was attenuated above 7 Hz. Future work will investigate the coupling of these velocity perturbations with passive turbulence generation grids in the test-section.

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Session 1B: Engines August 13th, 9:30 AM - 10:30 AM (Room B)

Natural Gas and CFR Engine Modeling for Knock Prediction

Diego Bernardi Bestel, *Mechanical Engineering, Colorado State University*

Bret Windom, *Mechanical Engineering, Colorado State University*

Scott Bayliff, *Energy Institute, Colorado State University*

Alex Balu, *Mechanical Engineering, Colorado State University*

Knock is one of the major concerns when designing high thermal efficiency spark-ignited (SI) engines. Generally, tendency to knock is highly dependent on engine operating conditions and fuel anti-knock quality. Therefore, understanding the fuel-engine interactions is essential to achieving high efficiencies in SI engines, especially when designing on-road natural gas (NG) engines, which complicates the problem further due to the wide range of chemical reactivity in pipeline NG. For this reason, this work proposes to develop Converge CFD and GT-Power models of the Cooperative Fuel Research (CFR) engine to investigate fuel-engine interactions that lead to knock (e.g. various fuel reactivity, load conditions, Exhaust Gas Recirculation levels). Additionally, emissions tradeoffs and the relationship between End-Gas Autoignition (EGAI) heat release and knock intensity will also be studied. For this work, CFR engine experiments will be used to validate the computational models, which will ultimately be used to design an advanced engine control strategy for operation under controlled end-gas autoignition (C-EGAI).

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CFD Model for an Automobile Refueling System

McKay Stoker, *Mechanical Engineering, Colorado State University*

Mangesh Dake, *Mechanical Engineering, Colorado State University*

Luke Nibbelink, *Mechanical Engineering, Colorado State University*

Kyle Forrester, *Mechanical Engineering, Colorado State University*

Wanpeng Geng, *Mechanical Engineering, Colorado State University*

Marc Henderson, *Honda R&D Americas, Inc.*

Bret Windom, *Mechanical Engineering, Colorado State University*

Government regulations and customer satisfaction direct the performance of an automobile refueling system. Each new design must be prototyped and tested to ensure these requirements are satisfied. Often designs need multiple iterations, costing money and time in validation procedures. To conserve resources, it is desired to create a Computational Fluid Dynamics (CFD) tool to assist in design validation. Such a tool will be discussed here, simulating the entire refueling system. This includes boundary conditions of the pump nozzle, a line that returns vapors from the tank to the filler pipe, and an orifice that mimics the pressure drop across an activated carbon canister. Experiments are performed both to characterize boundary conditions for the CFD and to validate results from the model. Pressure data is gathered from both simulation and experiment. Comparison of tank pressure traces shows good correlation. Steady state pressures of each method trend the same and have similar magnitude at multiple fuel flow rates.

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Investigation on the Role of Fuel Droplet Vaporization and Atomization on Spray Flame Stability and Dynamics

Radi Alsulami, *Mechanical Engineering, Colorado State University*

Anish Jadhav, *Mechanical Engineering, Colorado State University*

Brye Windell, *Mechanical Engineering, Colorado State University*

Bret Windom, *Mechanical Engineering, Colorado State University*

Understanding the processes and the coupling of each step that takes place during the energy conversion of a liquid fuel has a great impact on enhancing the efficiency and limiting the emissions of the engine. Thus, the focus of this study is to investigate the importance of the atomization and vaporization processes, which control spray dynamics and reactant mixing in the majority of our transportation power systems, on flame

stability. Single component fuels, including n-heptane, n-dodecane, toluene, and 1,2,4-trimethylbenzene, carefully selected to cover a wide range of physical and chemical properties, as well as, two binary fuel mixtures were tested in a spray burner in which flame liftoff heights and blowout limits were measured. Using a derived correlation capable of predicting the gas phase global extinction behavior of simple hydrocarbon blends, the mixture compositions were formulated to match gas phase extinction performance but constructed such that the relative volatility of the reactive species (i.e. the n-alkane component) was switched. Despite having similar gas phase extinction limits, when utilized in the spray burner while maintaining a constant droplet size, the mixtures exhibited different stability behaviors marked by variation in flame liftoff height and blowout limits. The results demonstrate that atomization/vaporization dynamics can influence flame stability in liquid fueled applications. These results highlight the coupling between the physical and chemical processes that occur in liquid fueled engines and suggest the importance of accounting for both a fuel's physical and chemical properties in fuel surrogate formulation.

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Computational Modelling of Propane Direct Injection for Advanced Compression Ignition Engines

Owen Brown, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Matt Thornton, *Fuels Performance Group, National Renewable Energy Laboratory*

Brad Zigler, *Advanced Combustion and Fuels, National Renewable Energy Laboratory*

Simultaneously improving fuel efficiency while reducing emissions is driving development of novel internal combustion engine systems that incorporate recent advances in injector technologies with abundant domestic fuel sources. One current focus area is advancing engine combustion technology for liquified petroleum gas (LPG), commonly known as propane. Whereas current propane engines are generally spark ignition (SI) engines with low pressure port fuel injection, advanced combustion strategies will follow a shift to direct injection (DI) fueling. These combustion strategies may rely on technology adopted from diesel compression ignition (CI) fuel injectors at much higher pressures, potentially enabling LPG blends to be used in a highly efficient advanced CI strategy that may allow medium duty trucks to operate on LPG with low emissions. In this presentation, I will outline the steps involved in creating a computational fluid dynamics (CFD) model of propane injection through a diesel CI fuel injector and performing comparative studies against a diesel baseline. Parameters such as fuel properties (density, viscosity, surface tension) will be varied as well as injector design (number of nozzle holes, hole diameters) and fuel pressure. These CFD simulations will guide subsequent research engine studies of propane under advanced CI strategies.

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Session 2A: CFD Methods August 13th, 1:30 PM - 2:30 PM (Room A)

A Divergence-Conforming Hybridized Discontinuous Galerkin Method for the Incompressible Reynolds Averaged Navier-Stokes Equations

Eric Peters, *Aerospace Engineering Sciences, University of Colorado, Boulder*
John Evans, *Aerospace Engineering Sciences, University of Colorado, Boulder*

We introduce a hybridizable discontinuous Galerkin method for the incompressible Reynolds Averaged Navier-Stokes equations coupled with the Spalart-Allmaras one equation turbulence model for the scalar eddy viscosity. With a special choice of velocity and pressure spaces for both element and trace degrees of freedom, we arrive at a method which returns point-wise divergence-free velocity fields and properly balances momentum and energy at an element-level. We further examine the use of different polynomial degrees and meshes for the flow and turbulence variables to most efficiently represent the flow field (which is typically smooth) and the eddy viscosity (which is typically rough). As is standard with hybridized discontinuous Galerkin methods, static condensation can be employed to remove the element degrees of freedom and thus dramatically reduce the global number of degrees of freedom. Numerical results illustrate the effectiveness of the proposed methodology both in the case of no turbulence model as well as in the case of the Spalart-Allmaras turbulence model.

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Central Moment Lattice Boltzmann Method for Computation of Flows on Stretched Lattice Grids

Eman Yahia, *Mechanical Engineering, University of Colorado, Denver*
Kannan Premnath, *Mechanical Engineering, University of Colorado, Denver*

In order to significantly expand the scope of the lattice Boltzmann (LB) method to more practical applications, particularly in the simulation of complex fluid flows with multiscale flow physics (e.g., wall-bounded flows or mixing layer flows), the use of different grid resolutions in various coordinate directions is essential. This work aims at introducing a central moments-based lattice Boltzmann (LB) scheme using multiple relaxation times (CMRT) for anisotropic meshes. The proposed model is based on a simpler and more stable natural moment basis without using orthogonality and includes additional velocity gradient terms dependent on the grid aspect ratio directly on the post-collision second order central moments to fully restore the required isotropy of the transport coefficients of the normal and shear stresses. The transformation between the distribution functions and various central moments are accomplished via shift matrices. The consistency of CMRT-LB scheme with the Navier-Stokes equations is shown via a Chapman-Enskog expansion. Numerical study for a variety of complex benchmark flow problems demonstrate its accuracy and superior numerical stability at different values of the aspect ratios of the stretched grids, when compared to other existing LB models.

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Non-Newtonian Fluid Flow Simulations using Cascaded Lattice Boltzmann Method

Adam Saad, *Mechanical Engineering, University of Colorado, Denver*
Kannan Premnath, *Mechanical Engineering, University of Colorado, Denver*

Fluid motion with nonlinear rheological characteristics arise in various situations of interest, including those related to materials and food processing, chemical engineering applications, and geophysical flows. The complex rheology also includes other additional features such as memory and normal stress effects in the case of viscoelastic fluids. In this work, we present a cascaded lattice Boltzmann (LB) approach based on central moments and using multiple relaxation times to model non-Newtonian power-law models. A numerical validation is performed against a set of benchmark solutions for both shear thinning and shear thickening fluids, which demonstrate its accuracy, grid convergence and improvements in stability when compared to some other models. In addition, we present a LB method based on central moments for the simulation of viscoelastic flows represented using the upper convected Oldroyd-B model. In this approach, the viscoelastic

stresses are solved by means of a separate cascaded LB solver, which are then coupled to the LB scheme for the fluid motion via additional moment contributions in the collision step. The method is then validated against prior analytical and/or numerical solutions for different characteristic dimensionless parameters.

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Mastering the Modality of the Rayleigh-Taylor Instability through Wavelet Based Adaptive Mesh Refinement

Scott Wieland, *GATS Inc., Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Scott Reckinger, *Civil Engineering, Montana State University*

Daniel Livescu, *Los Alamos National Laboratory*

Rayleigh-Taylor instability (RTI) occurs when a heavier fluid is suspended above a lighter fluid in the presence of a gravity-like accelerative force. After a perturbation is introduced to the interface between the two fluids, the heavy fluid begins falling as the light fluid begins rising. This results in the initial small scale motions to grow to a much larger scale. Because of this inverse cascade, any extraneous disturbances can cause the late time modality of the instability growth to be significantly altered. A single mode study of the RTI has been carried out using wavelet based adaptive mesh refinement to ensure that these disturbances are minimized. Once this is completed, an investigation on the growth of the most unstable modes in compressible multi-modal RTI is then performed.

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Session 2B: Porous Media August 13th, 1:30 PM - 2:30 PM (Room B)

Numerical/Experimental Study of a Direct Contact Membrane Distillation System

Jincheng Lou, *Mechanical Engineering, Colorado School of Mines*

Johan Vanneste, *Civil and Environmental Engineering, Colorado School of Mines*

Tzahi Cath, *Mechanical Engineering, Colorado School of Mines*

Steven Decaluwe, *Mechanical Engineering, Colorado School of Mines*

Nils Tilton, *Mechanical Engineering, Colorado School of Mines*

Direct contact membrane distillation (DCMD) is a thermal process in which warm feed and cool distilled water flow on opposite sides of a hydrophobic membrane. The temperature difference causes water to evaporate from the feed, travel through the membrane, and condense in the distillate. To date, CFD studies of DCMD focus primarily on the challenge of temperature polarization. For high concentration brines, however, concentration polarization is another major challenge that reduces system efficiency and leads to mineral scaling. To study coupled temperature and concentration polarization phenomena in the DCMD treatment of high concentration brines, we develop an in-house CFD method to simulate 2-D/3-D, unsteady heat and mass transport within plate-and-frame DCMD systems. The coupled momentum, energy, and mass transport equations are solved using a finite-volume method with an efficient non-iterative unsteady scheme. Numerical results are also validated with comparison to dedicated experiments. For the 2-D simulations, we perform a parametric study of temperature and concentration polarization under a variety of operating conditions, including inlet velocity, temperature, and concentration. The numerical results are then used to investigate the spatial distribution of temperature, concentration, vapor flux and conductive heat loss along the membrane surface. We report that though permeate flux in DCMD is small compared to RO, concentration polarization is still significant. We also present 3D simulations demonstrating polarization occurring both in the downstream and lateral directions.

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Application of Novel Immersed Boundary Method Techniques to Simulation of Flow Over a Cylinder in a Channel

Jacob Johnston, *Mechanical Engineering, Colorado School of Mines*

Membrane separation processes, such as reverse osmosis and membrane distillation, have important applications in desalinating seawater and treating complex waste waters. Membrane systems filter water by flowing it between selectively-permeable membrane sheets. For efficiency, systems must pack as much membrane area as possible into limited system volumes. For this purpose, systems use “spacers,” which are woven mesh-like materials that separate tightly-packed membrane sheets. Spacers also play a central role in the undesirable accumulation and precipitation of salts on membrane surfaces. To better understand this process, we are developing a finite-volume CFD code that simulates spacers using immersed boundaries on Cartesian grids. Though the application of Dirichlet conditions with immersed boundaries is well understood, there is less published work on the application of Neumann conditions, which are required to simulate heat and mass transport in membrane systems. We consequently present a novel approach to applying second-order accurate Dirichlet and Neumann boundary conditions. We demonstrate the approach by simulating a channel flow with a heated cylinder. Time permitted, simulations of a feed spacer within a reverse osmosis system will also be presented.

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Flow Regimes through Periodic Arrays of Cylinders

Liam Pocher, *Mechanical Engineering, Colorado School of Mines*

Zahra Khalifa, *Mechanical Engineering, Colorado School of Mines*

Kody von Holdt, *Mechanical Engineering, Colorado School of Mines*

Ray Karam, *Mechanical Engineering, Colorado School of Mines*

Nils Tilton, *Mechanical Engineering, Colorado School of Mines*

Single-phase flow through porous media is well understood in the low-Reynolds number regime for which the pore-scale flow is governed by Stokes' equations and the macroscopic flow satisfies the Darcy equation. However, at higher Reynolds numbers, fundamental questions remain about the role of pore-scale inertial effects, particularly when the pore-scale flow transitions to unsteady flow due to hydrodynamic instability. Thus motivated, we perform a broad set of direct numerical simulations of incompressible single phase flow through periodic arrays of infinite cylinders using finite volume methods with immersed boundaries. We systematically vary the porosity (volume fraction of fluid) between $0.25 \leq \varepsilon \leq 0.95$, and the Reynolds number from the Stokes regime to the unsteady laminar regime with vortex shedding. We observe the interaction of viscous, inertial, and unsteady terms from the Navier-Stokes equation in the resultant flow. The interplay between these terms allow us to more fully classify the pore-scale flow.

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Flow Regimes Through Periodic Arrays of Cylinders

Zahra Khalifa, *Mechanical Engineering, Colorado School of Mines*

Liam Porcher, *Mechanical Engineering, Colorado School of Mines*

Kody von Holdt, *Mechanical Engineering, Colorado School of Mines*

Ray Karam, *Mechanical Engineering, Colorado School of Mines*

Nils Tilton, *Mechanical Engineering, Colorado School of Mines*

Single-phase flow through porous media is well understood in the low-Reynolds number regime for which the pore-scale flow is governed by Stokes' equations and the macroscopic flow satisfies the Darcy equation. At higher Reynolds numbers, however, fundamental questions remain about the role of pore-scale inertial effects, particularly when the pore-scale flow transitions to unsteady flow due to hydrodynamic instability. Thus motivated, we perform a broad set of direct numerical simulations of incompressible single phase flow through periodic arrays of cylinders using finite volume methods with immersed boundaries. We systematically vary the porosity (volume fraction of fluid) between $0.25 \leq \varepsilon \leq 0.95$, and the Reynolds number from the Stokes regime to the unsteady regime with vortex shedding. For a given porosity, we identify up to five regimes of macroscopic flow: (1) Darcy flow, (2) transitional flow, (3) Forchheimer flow, (4) steady post-Forchheimer flow, and (5) unsteady flow. For each regime, we identify corresponding macroscopic flow equations, and discuss how they vary with porosity.

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Session 3A: Fire August 13th, 3:00 PM - 4:00 PM (Room A)

Dual Frequency Comb Spectroscopy for the Investigation of Ignition Behaviour of Wildland Fire Fuels

Amanda Makowiecki, *Mechanical Engineering, University of Colorado, Boulder*
Julie Steinbrenner, *Mechanical Engineering, University of Colorado, Boulder*
Jeff Glusman, *Mechanical Engineering, University of Colorado, Boulder*
Nick Wimer, *Mechanical Engineering, University of Colorado, Boulder*
John Daily, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*
Gregory Rieker, *Mechanical Engineering, University of Colorado, Boulder*

As wildland fires become an increasing concern worldwide, there is a need to refine current computational models of wildfire spread. This in turn drives the need for experimental data with well-characterized boundary conditions to serve as validation data sets for computations. To meet this need, we have developed a diagnostic suite with carefully controlled and quantified initial and boundary conditions to provide benchmark data on the ignition and combustion of wildland fuel sources. Here, we present an investigation of hardwood and softwood wood species, to characterize the impact of wood composition on ignition and combustion behaviour. Due to the high precision required for model validation data, dual frequency comb spectroscopy (DCS) is used to measure in-situ gas temperatures and species concentrations above the wood samples. To further quantify the system, several other diagnostics are employed simultaneously with the DCS measurements. During testing, wood samples are subject to a constant radiative heat flux provided by a mass loss calorimeter. Surface temperature of the wood samples is measured with an infrared camera. Ignition time, charring rates and flame intensity are quantified using a visual camera. Mass loss history is measured by a load cell in the mass loss calorimeter.

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A Chemical Kinetic Mechanism Reduction for Wildland Fire Direct Numerical Simulation and Experimental Validation

Jeff Glusman, *Mechanical Engineering, University of Colorado, Boulder*
Amanda Makowiecki, *Mechanical Engineering, University of Colorado, Boulder*
Nick Wimer, *Mechanical Engineering, University of Colorado, Boulder*
Kyle Niemeyer, *Mechanical Engineering, Oregon State University*
Greg Rieker, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*
John Daily, *Mechanical Engineering, University of Colorado, Boulder*

A chemical kinetic mechanism for the gas-phase combustion of biomass is under development for use in a direct numerical simulation (DNS) of wildland fire. Due to the computational constraints of a DNS, a reduction in the number of reactions and species of the combustion mechanism is required. An existing pyrolysis mechanism will be used as the initial conditions for the combustion process. The detailed kinetic mechanism for the gas-phase combustion consists of 137 species and 4533 reactions developed by the Chemical Reaction Engineering and Chemical Kinetics (CRECK) group. The reduced kinetic model developed by directed relation graph with error propagation and sensitivity analysis (DRGEPSA) matches the laminar flame speeds and ignition delays predicted by the detailed model. A highly reduced and robust chemical mechanism was developed in combination with an existing pyrolysis model for use in a DNS of wildland fire. The pyrolysis model validation via experimentation is currently underway using Dual-Frequency Comb Diagnostics to obtain spectroscopy measurements and OpenFOAM, an open-source computational fluid dynamics (CFD) code to approximate entrainment.

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Fire Simulation using Adaptive Mesh Refinement

Caelan Lapointe, *Mechanical Engineering, University of Colorado, Boulder*
Nicholas Wimer, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

The spatial and temporal scales of large fires make simulations capturing both large and small scale dynamics intractable, motivating efforts to increase computational efficiency. Common methods to reduce computational expense include chemical mechanism reduction, employing approximations to increase minimum time steps, and intelligently refining regions of the computational domain in regions of interest. In this talk, we present a new solver for the open source code OpenFOAM that incorporates these techniques to reduce simulation cost. The solver developed for modeling turbulent diffusion flames, fireFoam, has been extended to allow run time mesh modification of steady or transient simulations using adaptive mesh refinement (AMR). We show that these changes greatly reduce the computational cost of simulations using AMR when compared to static (i.e. no mesh modification) simulations while maintaining the same level of accuracy. Preliminary tests of the solver are also showcased for cases including flame whirls and propagating flames.

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Direct Numerical Simulations of Plumes and Pool Fires Using Adaptive Mesh Refinement

Nicholas Wimer, *Mechanical Engineering, University of Colorado, Boulder*

Marc Day, *Center for Computational Science and Engineering, Lawrence Berkeley National Lab*

Amanda Makowiecki, *Mechanical Engineering, University of Colorado, Boulder*

Jeffrey Glusman, *Mechanical Engineering, University of Colorado, Boulder*

John Daily, *Mechanical Engineering, University of Colorado, Boulder*

Gregory Rieker, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Computational simulations of fire have the potential to provide new physical understanding of fire dynamics and evolution in both natural and built environments. However, such simulations are challenging due to the multi-physics, multi-scale nature of essentially all fires. In this talk, we present new results from a computational effort focused on understanding and characterizing wildland fire spread at small scales (roughly 1 m–1 mm) using direct numerical simulations (DNS). The cost of the simulations is reduced using adaptive mesh refinement (AMR), where resolution is provided only when and where it is needed to resolve physically-relevant fine-scale features. Simulation results are shown for both large-scale plumes and pool fires studied experimentally in the FLAME facility at Sandia National Lab. In the plume configuration, helium gas is released into ambient air from a 1 m inlet. In the pool fire configuration, methane is released into ambient air from the same 1 m inlet, before burning as a non-premixed diffusion flame. Comparisons are made between results from the simulations with and without AMR, and between the simulations and experiments. Focus is placed, in particular, on the computational savings enabled by the use of AMR, in addition to simulation accuracy.

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Session 3B: Geostrophysics August 13th, 3:00 PM - 4:00 PM (Room B)

[An Assessment of a Mass Flux Closure for the Ocean Surface Boundary Layer](#)

Rachel Robey, *Climate, Ocean, and Sea Ice Modeling, Los Alamos National Laboratory*

Luke Van Roekel, *Climate, Ocean, and Sea Ice Modeling, Los Alamos National Laboratory*

The turbulent ocean surface boundary layer (OSBL) mediates the transfer of heat, momentum, and tracers between the ocean and the atmosphere or sea ice above. Thus, it constitutes a critical component of the ocean climate. Within the boundary layer, small-scale turbulent eddies produce transport via vertical fluxes which cannot be directly resolved in Earth system models and must instead be parameterized. We explore the applicability of a mass flux closure to OSBL vertical turbulent transport in one-dimensional columns. Mass flux schemes represent a middle ground between the relative simplicity of the popular K-Profile Parameterization and the complexity of high-order Reynolds closures with a more robust estimation of the turbulence generation by processes not proportional to the mean vertical gradient. By assuming upward- and downward-moving plumes to have an associated probability distribution of state variables, higher-order turbulent moments may be represented in terms of lower order moments and the skewness. The results are compared against horizontally-averaged Large Eddy Simulations (LES) in cases spanning a number of mixing regimes. We find the mass flux closure to be generally consistent with LES with a notable robustness to vertical and temporal resolution variation.

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[The Effects of a Horizontal Magnetic Field on Rayleigh-Bènard Convection](#)

Talal Al Refae, *Physics, University of Colorado, Boulder*

Michael Calkins, *Physics, University of Colorado, Boulder*

Stefano Maffei, *Physics, University of Colorado, Boulder*

Ming Yan, *Physics, University of Colorado, Boulder*

We investigate the influence of a uniform horizontal magnetic field on Rayleigh-Bènard convection with the use of direct numerical simulation. In general, we note that imposing a horizontal magnetic field enhances heat transport relative to non-magnetic convection but only to a certain point. For a fixed Rayleigh number it is evident that as the magnitude of the magnetic field increases the Nusselt number approaches some ideal value, but only asymptotically. At relatively low Rayleigh numbers we observe stable convection rolls aligned along the direction of the magnetic field. For higher Rayleigh numbers, particularly with the onset of turbulence, we observe different flow structures that are dependent on the strength of the magnetic field. With weaker magnetic fields the flow quickly becomes three-dimensionally turbulent. For strong magnetic fields, the flow is predominantly two-dimensional with large-scale modulations in the direction of the magnetic field. These modulations tend to reduce the heat transfer, relative to non-magnetic convection.

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[Thermal Convection with a Strong Vertical Magnetic Field.](#)

Ming Yan, *Physics, University of Colorado, Boulder*

Michael Calkins, *Physics, University of Colorado, Boulder*

Stefano Maffei, *Physics, University of Colorado, Boulder*

Keith Julien, *Applied Mathematics, University of Colorado, Boulder*

Steven Tobias, *Applied Mathematics, University of Leeds*

Philippe Marti, *Earth Sciences, ETH Zurich*

The fluid outer core of the earth and many other planetary interiors possess large scale magnetic fields. These magnetic fields can change the dynamics of the flow significantly, thus in order to understand the mechanism of dynamo, it is important to look into the physics of magnetoconvection with strong magnetic fields. Here, we consider the extreme cases of small magnetic Prandtl number magnetoconvection with an imposed vertical magnetic field. We applied a quasi-static incompressible magneto-hydrodynamic model, and a set of direct numerical simulations is conducted in a Cartesian plane layer geometry. Three regimes

of flow are observed when we increasing the Rayleigh number Ra with fixed Chandrasekhar number Q , characterized by different flow structures and Nu - Ra scaling. In the first one, the boundary layer is not well formed and there is still a mean temperature gradient at mid-plane. In the second regime the interior of the flow becomes isothermal, and the Nu - Ra scaling agrees with marginal stability analysis, indicating that the convection is controlled by the boundary layer. At even higher Ra , the inertia takes the dominant balance over Lorenz force, resulting in a Nu - Ra scaling close to non-magnetic model. The distinguished changes of the dominant terms in the equations and the contribution of ohmic dissipation and viscous dissipation are analyzed. A reversed temperature profile occurs in the second regime, which associated with a stable plume structure, suggesting an efficient way of heat transfer. The result of this magnetoconvection research reveals the role magnetic field plays on natural dynamo.

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Experimental Investigation of Oblique Dispersive Shock Waves in Supercritical Shallow Water Flow

Adam Binswanger, *Applied Mathematics, University of Colorado, Boulder*

Patrick Sprenger, *Applied Mathematics, University of Colorado, Boulder*

Mark Hoefer, *Applied Mathematics, University of Colorado, Boulder*

A shallow water experiment is implemented in which a sluice gate controls a supercritical flow that is deflected by a slender wedge. Due to surface wave dispersion, the ensuing steady structure is a spatially extended, oscillatory pattern referred to as an oblique dispersive shock wave (DSW). Appropriate variation of water depth, flow speed, and deflection angle results in a bifurcation in the flow pattern. The Bond number B , measuring the effects of surface tension relative to gravity, characterizes the bifurcation. The quantity $B = 1/3$, corresponding to a fluid depth of approximately 5 mm, is the bifurcation point, where there is a transition between classical and non-classical DSW profiles. They are differentiated by monotonicity in their trailing solitary wave edges and the nonlinear wavetrain that ensues. Surface water wave profiles are measured via the Fourier transform profilometry technique. Ongoing work involves comparing the reconstructed surface profiles with theoretical predictions for the DSW structure via a previously developed approximate model.

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Session 4A: Machine Learning August 14th, 9:00 AM - 10:15 AM (Room A)

Scale-Dependent Localization for Ensemble Filtering of Quasi-Geostrophic Flows

Michael Ying, *Advanced Study Program, National Center for Atmospheric Research*

Covariance localization remedies sampling errors due to limited ensemble size in ensemble data assimilation. Previous studies suggest that the optimal localization radius depends on ensemble size, observation density and accuracy, as well as the correlation length scale determined by model dynamics. A comprehensive localization theory for multiscale dynamical systems with varying observation density remains an active area of research. Using a two-layer quasi-geostrophic (QG) model, this study systematically evaluates the sensitivity of the best Gaspari-Cohn (GC) localization radius to changes in model resolution, ensemble size and observing networks. Numerical experiment results demonstrate the scale dependency of the best localization radius for the QG flow. The best localization radius is rather insensitive to changes in model resolution, as long as the key dynamical processes are reasonably well represented by the low-resolution model with inflation methods that account for representation errors. Nonlocal observation-state correlations pose challenges for GC-based localization. The effect from varying observing network density is also demonstrated in this study.

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Applying Machine Learning to the Sedov-von Neumann-Taylor Blast Wave

Mokbel Karam, *Chemical Engineering, University of Utah*

Fady Najjar, *Lawrence Livermore National Lab*

Jiang Ming, *Center for Applied Scientific Computing, Lawrence Livermore National Lab*

James Sutherland, *Chemical Engineering, University of Utah*

Tony Saad, *Chemical Engineering, University of Utah*

A blast wave is the motion of fluid resulting from the deposition of energy in an infinitesimal volume. It can be approximated as a fluid front of compressed gas traveling at high speed followed by a region of low pressure. Blast waves occur in a variety of natural and man-made applications such as supernovae, volcanic eruptions, asteroid impacts, and energetic explosions. Around the 1940's, Leonid Ivanovitch Sedov, Jhon von-Neumann, and Geoffrey Ingram Taylor (SNT) developed an exact analytical solution for the propagation of a blast wave generated in a domain with uniform density. Given the initial energy and gas adiabatic index, the analytical solution predicts the values of the density, pressure, and velocity as a function of the distance from the origin at a certain point in time. The objective of our research is to develop a machine learning model able to predict the value of the initial energy and the time of the energy release given the values of the wave speed and maximum pressure at a certain distance from the origin. In this work, we investigated the predictive capacities of different machine learning models applied to the SNT problem, including linear and polynomial regressors, and Random Forest with Decision trees estimators. The high bias error for linear and polynomial regressors indicates a poor predictive power due to the low capacity of the models to capture the trends in the data. The Random Forest model succeeded in capturing the nonlinearity in the data and shows good predictive capabilities for values far from the boundaries of the training dataset. Also, we showed for the SNT problem that a non-uniform sampling in the adiabatic index space for the training dataset improves the accuracy of the model.

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On Markov Chain Monte Carlo Approximate Bayesian Computation Approach for Subgrid-Scale Model Development

Olga Doronina, *Mechanical Engineering, University of Colorado, Boulder*

Colin Towery, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

The predictive power of large eddy simulations (LES) depends on the accuracy of closure models used to represent subgrid-scale (SGS) fluxes. Traditionally, model parameters have been determined through either direct inversion of model equations given some reference data or using optimization techniques. However,

the former approach becomes complicated for models with many different parameters or when the model consists of partial differential equations, and the latter approach precludes the quantification of parameter uncertainty. In this talk, we use Approximate Bayesian computation (ABC) and Markov chain Monte Carlo (MCMC) methods to estimate parameter values, as well as their uncertainties, in SGS models. The MCMC-ABC approach avoids the need to directly compute a likelihood function during the parameter estimation, enabling a substantial speed-up as compared to full Bayesian analyses. The approach also naturally provides uncertainties in parameter estimates, avoiding the artificial certainty implied by optimization methods for parameter estimation. The MCMC-ABC approach is outlined, and both *a priori* and *a posteriori* test results for homogeneous isotropic turbulence are provided to demonstrate the accuracy and computational cost of the approach.

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Development of a Computational Modeling and Optimization Tool for Thin Flat Heat Pipes for Small Satellite Heat Dissipation

Steven Isaacs, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

With easier access to space and integration of power dense components, small-scale thermal management solutions are in demand for small satellite systems. With strict mass and volume requirements commanded by power dense small spacecraft, heat pipes with thin and flat architectures are excellent solutions for efficient heat transfer and dissipation. For traditional larger-scale heat pipes, performance is predominantly dictated by liquid wick parameters. As the scale of a heat pipe decreases the performance becomes increasingly more dependent on vapor core geometry and structural mechanics effects. In this study the motivation, development and application of a full computational heat pipe modeling and optimization tool is presented. First, simple analysis is used to define the small-scale design space in which vapor core and structural effects play significant roles. Next, the computational development of the liquid wick, vapor core and support structure is presented. Finally, the design tool is applied to a copper-water, flat heat pipe with a footprint of 8.4 cm×57.1 cm and a total thickness of 0.5 mm. The model is used to predict total thermal resistance, capillary limit evaporator heat load and case bending results. In addition, the tool is used to optimize the heat pipe design by minimizing total mass, volume and thermal resistance while maximizing heat dissipation.

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Characterization of Flapping in a Plane Turbulent Buoyant Jet Using Proper Orthogonal Decomposition

Michael Meehan, *Mechanical Engineering, University of Colorado, Boulder*

Jason Christopher, *Mechanical Engineering, University of Colorado, Boulder*

Caelan Lapointe, *Mechanical Engineering, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

The characteristics of the plane turbulent buoyant jet have been subject to a several experimental, numerical, and theoretical investigations with a growing emphasis on describing the global instability located near the jet exit. The instability is a result of the low density fluid accelerating upwards immediately upon injection into the higher density medium; the jet stream undergoes a ‘pinching and pulling’ process that results in a regular shedding of vortical structures, often referred to as puffing. Here, we perform direct numerical simulations of two-dimensional, high temperature buoyant jets with steady and sinusoidally forced inflow velocities to better understand the instability. We employ proper orthogonal decomposition (POD) to characterize the behavior of the vortices. The results of the POD show that the jet stream flaps, or intermittently oscillates normal to the direction of inflow, when the velocity of the inflow is steady and does not flap when sinusoidally forced. This result has practical implications for real combustion systems, such as industrial burners, in which the underlying fluid dynamics can influence the behavior of reacting flows. In addition, we demonstrate a potential technique to control this behavior.

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Session 4B: Biology August 14th, 9:00 AM - 10:15 AM (Room B)

Impedance vs Peristaltic Pumping in Zebrafish 24-30 hpf Embryonic Heart

Alireza Sharifi, *Mechanical Engineering, Colorado State University*

David Bark, *Mechanical Engineering, Colorado State University*

The first functional organ system to develop in vertebrate embryos is the cardiovascular system. In this stage heart consists of a primitive heart tube with no valve which pumps the blood through a simple vascular network. Pumping mechanism of the heart in this stage is still questionable. Valveless pumping in the heart tubes can be achieved by the use of impedance mismatch or by peristaltic motion. Impedance pumping is characterized by one stationary point of activation, inducing waves which then travel passively along the primitive heart tube. The passive waves create the blood flow. Peristalsis on the other hand is characterized by a series of adjacent contraction locations creating the appearance of a traveling wave along the wall. The mechanisms of valveless pumping have been observed in both physical experiments (Rinderknecht et al., *J. Micromechanics Microengineering*, 2005) and in numerical simulations (Manopoulos et al., *Phys. Fluids*, 2006). In particular, a new unpredictable phenomenon of valveless pumping was reported in previous work on the two-dimensional simulations of valveless pumping using the immersed boundary method: the direction and magnitude of a net flow are dependent on the parameters of the driving function, such as frequency or amplitude (Jung, et al., *SIAM J. Sci. Comput.*, 2001). In this study we investigate the both pumping mechanism and compare our results with experiments to find the accurate pumping mechanism as well as studying the blood flow behavior in 24 hours post fertilization zebrafish (hpf) zebrafish heart. Computational fluid dynamics (CFD) has been widely applied to simulate blood flow, to facilitate clinical decision-making, and to study the progression of cardiovascular diseases. In this study, we develop moving domain CFD model to model the progression of cardiac development. We study both peristaltic and impedance dynamic pumping mechanism to investigate which mechanism is closer to reality. We also studied the blood flow behavior as well as solid stress in these two configurations. We used Comsol multiphasic to simulate pumping mechanism in 24 hpf by using fluid-solid interaction (FSI) method. The structural mechanics computations use the assumption that the material is linear elastic, and they take geometric nonlinearities into account. The fluid flow is described by the incompressible Navier-Stokes equations. The equations are set up and solved inside the tube. The Navier-Stokes equations are solved on a freely moving deformed mesh, which constitutes the fluid domain. The deformation of this mesh relative to the initial shape of the domain is computed using Hyperelastic smoothing. On the solid-fluid boundary at the tube inner wall, the moving mesh follows the structural deformation. Geometrical and fluid/solid mechanical properties have been extracted from the previous studies (Yao et al., *J Biomech. Eng.*, 2012) (Zamir et al., *Ann Biomed Eng*, 2003). Blood flow simulation in both pumping mechanism has been studied and we also investigate the effect of different parameters (wave length, wave speed, applied force, fluid properties, elastic modulus of cardiac jelly and myocardium, Poisson's ratio of cardiac jelly and myocardium) on blood pumping in both configurations. We also studied the solid mechanic stress distribution in myocardium layer. Our results show both pumping mechanisms can deliver the desire amount of the blood.

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Computational Fluid Dynamic Simulation of Fetal Heart

Banafsheh Zebhi, *Mechanical Engineering, Colorado State University*

Hadi Wiputra, *Biomedical Engineering, National University of Singapore*

David Bark, *Mechanical Engineering, Colorado State University*

Yap Choon Hwai, *Biomedical Engineering, National University of Singapore*

Lisa Howley, *Fetal Care Center, Childrens Hospital Colorado*

Bettina Cuneo, *Fetal Care Center, Childrens Hospital Colorado*

Congenital Heart Defects (CHD) are the most common type of birth defects, affecting more than 1% of live births each year and 10% of aborted fetuses. Among these, Hypoplastic Left Heart Syndrome (HLHS) is one of the most complicated defects where the left side of the heart is underdeveloped. The commonly used surgical interventions to repair HLHS are highly complex and have limited success rates. Even when

surgical intervention is successful, it leaves patients with lifetime health issues. The long-term aim of our research is to 1) develop computational tools to simulate and evaluate outcomes of therapeutic interventions before the physical surgery occurs 2) provide novel prevention and treatment options for CHD. To approach these aims, we plan to leverage the response of cells to their mechanical environment. The mechanical forces caused by blood flow have long been considered to play a significant role in cardiac structure development. For instance, numerous animal studies have shown that reduced fluid flow in embryonic and fetal circulation creates underdeveloped cardiac structural formation. However, a direct link between the mechanical environment and congenital heart malformation in human fetuses has not yet been clearly shown. To fill this gap in knowledge, there is a critical need to quantify the relationship between normal blood flow with normal heart development, and the relationship between abnormal blood flow with underdeveloped heart structure so that we can develop new prevention and intervention approaches to improve patient outcomes. In this study, we optimize a physics-based computational simulation to quantify cardiovascular flow in healthy fetuses based on 4D Doppler ultrasound data. We collect 4D Doppler ultrasound data at ~ 22 and ~ 3 weeks gestation for healthy fetuses and fetuses diagnosed with HLHS. Then we reconstruct 3D geometries of right ventricle, and simulate cardiovascular flow field. The distribution of the blood flow parameters including wall shear stress, pressure, velocity, and vorticity are evaluated at various regions of the heart. We then evaluate how changes in blood flow parameters affect the morphological changes from early to late stages of development in normal and HLHS fetal hearts. WSS is known to be sensed by tissue cells, and distribution of pressure, velocity and vortex determines the mechanical environment. In general, the right ventricle in HLHS cases from 22 weeks to 35 weeks experiences higher wall shear stress. In both HLHS and normal 22 weeks as well as HLHS and normal 27/28 weeks, the highest wall shear stress can be seen at the back of the outlet during systole. At 22 weeks of gestation for both normal and HLHS, the highest WSS can be seen at the front and back of the inlet during diastole. While at 27/28 weeks of gestation for both normal and HLHS, the highest WSS can be seen at the apex of the right ventricle during diastole.

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Two-Phase Flow Effects on Human Coagulation Factor X Activation *in vitro*

Alison Wallbank, *Bioengineering, University of Colorado, Anschutz*

Karin Leiderman, *Applied Mathematics and Statistics, Colorado School of Mines*

Keith Neeves, *Chemical Engineering, Colorado School of Mines*

The effect of flow on coagulation substrate/enzyme reactions is well characterized, but the influence of red blood cells (RBCs) has yet to be elucidated. Experiments were conducted to understand how RBCs affect the conversion of zymogen factor X (fX) to enzyme factor Xa (fXa). Washed human RBCs were added to buffer containing fX to obtain four hematocrit (volume percent RBC) conditions: 0, 20, 30 and 40%. Tubular glass bioreactors were prepared with immobilized lipid bilayers containing tenase, which activates fX to fXa. Six shear rates ranging $50\text{-}2500\text{ s}^{-1}$ were tested for each condition. Generation of fXa was quantified by a chromogenic substrate assay. Experimental results show fXa production decreasing as functions of increasing hematocrit and increasing shear rate. Mathematical modeling was used to validate results. RBCs generate two-phase flow in vessels, necessitating a unique model to capture the fluid mechanics of substrate conversion. A PDE model of a variable sized reaction zone was used. We postulate that increased hematocrit hinders diffusion of fX to the wall of bioreactor, thereby diminishing the fXa present in collected effluent. Further, higher hematocrit yields faster velocity near the wall, causing fX to flow away from binding sites faster than diffusing to them.

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Parameters Governing Pressure Homogeneity in a 3D Printed Human Airway During Low Frequency Jet Ventilation

Joshua Pertile, *Bioengineering, University of Colorado, Denver*

Daniel Fink, *Otolaryngology, University of Colorado Hospital*

Bradford Smith, *Bioengineering, University of Colorado, Denver*

Low frequency jet ventilation is used during upper airway surgery to maintain airway access. Characterizing the parameters governing pressure distribution will improve safety and efficacy of the procedure. In order

to determine how jet position affects ventilation homogeneity the distal airway pressures were monitored in a physical model of the first five generations of the human airway tree while the jet needle position was adjusted with an automated system. As the jet needle depth into the trachea increased there was a decrease in distal airway pressure and ventilation homogeneity. In the proximal trachea, a homogenous flow pattern was able to form regardless of needle distance from the wall, leading to equal pressures across the lung model. When the ventilation needle was positioned in the distal trachea, central axis placement was necessary to achieve homogeneous ventilation due to the coanda effect along the wall of the trachea. A logarithmic relationship exists between the distal airway pressure and jet pressure. Conclusion During jet ventilation the ventilation needle should be centered and sufficiently far from the first bifurcation to allow for homogeneous flow in order to achieve ventilation homogeneity which is necessary for optimal gas exchange.

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Wall-Bounded Vorticity in the Right Heart from 4DMRI Measurements

Joel Human, *Mechanical Engineering, University of Colorado, Boulder*

Alejandro Perez, *Mechanical Engineering, University of Colorado, Boulder*

Reece Jones, *Mechanical Engineering, University of Colorado, Boulder*

Jamey Browning, *Engineering, Northeastern University*

Joyce Schroeder, *Cardiology, National Jewish Health*

Brett Fenster, *Radiology, University of Utah*

Jean Hertzberg, *Mechanical Engineering, University of Colorado, Boulder*

Time-resolved 3D cardiac magnetic resonance phase contrast flow imaging (4DMRI) was used to measure blood flow in the human heart in a small cohort of normal subjects and patients with pulmonary hypertension (PH). The ultimate goal of this work is to determine appropriate metrics to track the progress of diseases such as PH. Vorticity was derived from these measurements and decomposed into streamwise and helical components, with attention focused on the right ventricle RV and right atrium RA. The interaction of vorticity and structures such as valve leaflets, papillary muscles and chordae tendineae will be discussed.

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Session 5A: Turbulence August 14th, 1:30 PM - 2:15 PM (Room A)

Scaling and Collapse of Conditional Velocity Structure Functions in Turbulent Premixed Flames

Samuel Whitman, *Mechanical Engineering, University of Colorado, Boulder*

Colin Towery, *Mechanical Engineering, University of Colorado, Boulder*

Alexei Poludnenko, *Aerospace Engineering, Texas A&M University*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

A new scale-sensitive physical-space conditional analysis is outlined and used to examine the scaling and collapse of velocity structure functions in turbulent premixed flames. The conditioning is based on local instantaneous temperatures in the premixed flame, and structure function scaling and collapse are examined using Kolmogorov-type dimensional arguments and scaling relations. Longitudinal structure functions are computed using the local flame normal as reference direction. The analysis shows that as the turbulence intensity increases, and for locations near the unburnt reactants, conditional structure functions approach the inertial range scaling predicted by Kolmogorov. Furthermore, as the turbulence intensity increases, structure functions throughout the flame approach a collapse to a single profile when scaled with conditionally-calculated variables, with a more complete collapse observed for smaller scales within the analytic (or dissipative) range. These results suggest that, at sufficiently high intensities, Kolmogorov-type scaling laws and dimensional arguments may retain some validity in premixed flames, provided that scaling variables are computed on a conditional basis for different temperatures.

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The Influence of the Prandtl number on the Inverse Cascade in Rapidly Rotating Convection

Mitchell Krouss, *Physics, University of Colorado, Boulder*

Michael Calkins, *Physics, University of Colorado, Boulder*

Stefano Maffei, *Physics, University of Colorado, Boulder*

We are focused on understanding the dynamics of rapidly rotating convection as it pertains to planetary interiors. Large-scale vortices (LSVs), generated by an inverse cascade of kinetic energy, have been observed in rotating convective turbulence with Prandtl numbers (Pr) of unity or less. When present, LSVs grow to fill the entire computational domain. Here, we extend this previous work to Prandtl numbers greater than unity. For $Pr = 1.5$ we have observed the formation of LSVs for values of the convective Reynolds number (Re) greater than 6.74. At $Pr = 2$, we do not see the LSV until much higher Reynolds numbers, indicating that the vigor of the convection alone is not a sufficient criteria for establishing the presence of an inverse cascade, or more specifically, formation of a LSV. Increasing the Prandtl number tends to quench the formation of LSVs by saturating the inverse cascade at equivalent Rayleigh numbers.

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Designing a Noninvasive Laser-Based Vorticity Sensor

Elizabeth Strong, *Mechanical Engineering, University of Colorado, Boulder*

Alex Anderson, *Chemical and Biological Engineering, University of Colorado, Boulder*

Juliet Gopinath, *Electrical, Computer and Energy Engineering, University of Colorado, Boulder*

Greg Rieker, *Mechanical Engineering, University of Colorado, Boulder*

Vorticity is a quantity of fundamental importance in the realm of fluid dynamics, especially given that the increase in vorticity associated with vortex stretching is the primary mechanism for energy transfer between length scales in turbulent 3D flows. Measures of vorticity at and near the smallest so-called Kolmogorov length scales are necessary to evaluate transfers of energy; however, such measurements are challenging to make. Noninvasive, state-of-the-art techniques for determining vorticity involve using such techniques as PIV or LDA to first determine and then differentiate velocity fields; yet these strategies are computationally intensive and can have limited spatial resolution. Here, we discuss our work developing a noninvasive

laser-based vorticity sensor which infers components of the vorticity vector based on rotational Doppler frequency shifts of light scattered from tracer particles in the flow. Such frequency shifts result when light endowed with orbital angular momentum (OAM) scatters from tracer particles moving the flow. We present preliminary results from optics experiments in which we evaluate the potential of our sensor by testing it on moving tracer particles simulated with a digital micromirror device.

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Session 5B: Exotic Fluid Flows August 14th, 1:30 PM - 2:15 PM (Room B)

Supersonic Turbulence Modulation in a Particle-Laden Jet

Ryan Darragh, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Bryan Schmidt, *Mechanical and Aerospace Engineering, The Ohio State University*

Jeffrey Sutton, *Mechanical and Aerospace Engineering, The Ohio State University*

Particle-laden turbulent flows are found in a wide range of flow systems. In many cases, particles in these flows modulate the turbulence by either enhancing or diminishing the turbulence intensity, and by affecting the properties and coherence of turbulent structures. Particle size, loading, mass, clustering, and Reynolds number all play complicated roles in determining how the turbulence is modulated, and the addition of shock waves in supersonic particle-laden flows further complicates how these parameters interact with the turbulence. Currently, turbulence modulation in such supersonic particle-laden flows remains incompletely understood and has not yet been studied to the same degree as the subsonic case. Turbulence in a numerically simulated supersonic jet will be validated by experiments and provide a comparison case for future particle-laden simulations.

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Characterization and Control of Gap Width Between Self-Propelling Superparamagnetic Colloids and Glass

Dante Disharoon, *Chemical and Biological Engineering, Colorado School of Mines*

Keith Neeves, *Chemical and Biological Engineering, Colorado School of Mines*

David Marr, *Chemical and Biological Engineering, Colorado School of Mines*

We observe a novel hydrodynamic lift force on 8.3 μm spheres that are induced to rotate by a magnetic torque. Sphere rotation rate, translational velocity and the gap between sphere and surface are measured using total internal reflection microscopy. Before manipulation via the magnetic field, the spheres settle to 15 nm from the prism's glass surface. When rotating they experience a lift force and rise to between 20 nm and 80 nm from the surface depending on the rotational frequency of the sphere. The hydrodynamic lift force is significant (order 10^{-13} N) even at Reynolds numbers in the gap on the order of 10^{-3} . Higher rotation rates result in a greater lift force as evidenced by a larger gap width. The translational velocity increases linearly with sphere rotation rate from $9.2 \pm 4.2 \mu\text{m/s}$ at a particle rotation rate of 4 Hz to $51.4 \pm 21.3 \mu\text{m/s}$ at a rotation rate of 30 Hz. We demonstrate that the interaction between the spheres and the glass prism can be tuned using a direct current magnetic load force. A load equal to a sixth the gravitational force applied in the same direction of gravity decreases the gap width during translation by 22%, whereas the same load applied opposite the direction of gravity increases the gap by 28%.

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Spontaneous Detonation Initiation in Compressible Isotropic Turbulence

Colin Towery, *Mechanical Engineering, University of Colorado, Boulder*

Alexei Poludnenko, *Aerospace Engineering, Texas A&M University*

Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Theory and computations have shown that local hot spots in highly compressible turbulent reactive mixtures can lead to spontaneous detonation initiation. However, present theory and models are restricted to single hot spots that i) are well-separated from other local maxima in temperature; ii) are formed on timescales comparable to, or shorter than, the chemical induction and acoustic crossing times of the hot spot; and iii) evolve freely in a gas with zero initial velocity fluctuations. In this talk, by contrast, we examine detonation initiation in non-monotonic temperature fields with local maxima that are tightly spaced and evolve over a range of timescales, from an outer scale comparable to the mean induction time to a much shorter inner diffusive timescale. We perform a series of direct numerical simulations of homogeneous isotropic turbulence in reactive gas mixtures that sweep over a range turbulent Mach numbers and test both a thermally-regulated

single-step Arrhenius reaction mechanism and a chain-branching-regulated detailed hydrogen-air mechanism. Although we find some evidence of spontaneous detonation initiation due to compressible turbulence, distributions of temperature-gradient magnitudes and wave propagation speeds are inconsistent with previous theory.

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Session 6A: CFD Modeling August 14th, 2:45 PM - 4:00 PM (Room A)

Gravo-Aeroelastic Additively Manufactured Design of a 1% Scale Wind Turbine Blade

Meghan Kaminski, *Mechanical Engineering, University of Virginia*
Eric Loth, *Mechanical and Aerospace Engineering, University of Virginia*
Chao Qin, *Mechanical and Aerospace Engineering, University of Virginia*
Todd Griffith, *Mechanical Engineering, University of Texas at Dallas*

A gravo-aeroelastic scaling (GAS) method is developed to capture the full-scale non-dimensional dynamics and deflections on a sub-scale model to inexpensively and rapidly test new designs. The GAS method scales the complete blade loads (including aerodynamic and gravitational) and the blade dynamics of the full-scale model. As compared to conventional scaling, the GAS method scales gravitational loading and blade dynamics to more accurately represent the full-scale model. Through scaling, three non-dimensional key scaling values are given priority in order to retain proper dynamics: flapping frequency, tip deflection, and tip-speed-ratio. These values lead to GAS parameters for the sub-scale model. In the presented work, the GAS method is applied to the 13.2 MW 100-meter SNL100-03 wind turbine blade creating a 1/100th scale model resulting in a 1-meter model. To the authors' knowledge, this is the first model of such a significant scale due to the difficulties in developing a model of this size. A series of scale models were designed and tested using additive manufacturing. To achieve scaling, bio-inspired structural design and carbon fiber reinforcements are applied. The final version has errors for total mass as 3%, tip deflection as 15.6%, and flapping frequency as 8.1%.

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Comparison of Multiple Equations of State in Numerical Simulation of Supercritical Carbon Dioxide Flow Around a Heated Cylinder

Elizabeth Rasmussen, *Mechanical Engineering, University of Washington, Seattle*
Shashank Yellapantula, *High Performance Algorithms and Complex Fluids, National Renewable Energy Laboratory*
Michael Martin, *High Performance Algorithms and Complex Fluids Group, National Renewable Energy Laboratory*

Supercritical carbon dioxide appears in a range of engineering applications, including novel material synthesis, turbomachinery for advanced energy systems, and carbon sequestration. Simulations are key to understanding and successfully designing these systems. However, lack of physical understanding in behavior of supercritical fluids near the critical point, and the challenges of simulating under these conditions, can lead to inaccurate results. In this talk, we examine how results vary when different equations of state are employed. The system is two-dimensional flow of supercritical carbon dioxide over a cylinder at Reynolds number ranging from 0.1 to 10. We apply the ideal gas law, Soave-Redlich-Kwong, and Peng-Robinson equations of state to the system and report on the varying results. For each of these models, cases with temperatures of 310 K-320 K, an operating pressure of 8 MPa, and cylinder temperatures of 310 K-360 K are presented. We compare flow and heat transfer characteristics between non-ideal and ideal models.

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Preliminary Steps to Scale-Resolving Simulations of Turbulent Boundary Layers with Flow Separation

Riccardo Balin, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Eric Peters, *Aerospace Engineering Sciences, University of Colorado, Boulder*
John Evans, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Kenneth Jansen, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Due to the large computational cost associated with DNS and LES, most engineering flows are currently modeled with RANS. However, RANS models perform poorly when dealing with boundary layers affected

by strong adverse pressure gradients and flow separation, plaguing the prediction and design of systems exhibiting such characteristics. Therefore, it is of great value to better understand the physics involved in separation of a turbulent boundary layer, and to gather data for such flows with the hope of improving the prediction of closure models of different fidelity. To accomplish this task, a series of scale-resolving simulations of a separating turbulent boundary layer over a Gaussian bump will be carried out. The smooth, two-dimensional bump causes a rapid succession of strong favorable-to-adverse pressure gradients, resulting in a separation bubble on the downstream side. At the start of the bump, the Reynolds number based on the momentum thickness is 3,200, and the boundary layer thickness is of the order of the bump height. The preliminary work performed to set up the simulations is discussed.

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Modeling of Active Flow Control in an Aggressive Diffuser with Comparison to Experiment

Ryan Skinner, *Aerospace Engineering, University of Colorado, Boulder*

Jeremy Gartner, *Aerospace Engineering, Rensselaer Polytechnic Institute*

Michael Amitay, *Aerospace Engineering, Rensselaer Polytechnic Institute*

Kenneth Jansen, *Aerospace Engineering, University of Colorado, Boulder*

This computational work explores active flow control for separation mitigation in an asymmetric, aggressive diffuser of rectangular cross-section at inlet Mach ~ 0.4 and $Re \sim 1.3M$. Unsteady tangential blowing is used to control separation on the single ramped face. Different methods of modeling the unsteady jet are evaluated, and the corresponding Spalart-Allmaras DDES and RANS simulations are compared to experimental PIV and pressure data.

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A Predictive Near-Wall Model for Large Eddy Simulations

Prakash Mohan, *Institute for Computational Engineering and Sciences, The University of Texas at Austin*

Robert Moser, *Institute for Computational Engineering and Sciences, The University of Texas at Austin*

Large eddy simulations directly represent larger scale turbulent motions and model the effects of small scale motions. However in the near-wall region the large, dynamically important eddies are on the order of viscous scales, which makes resolving them very expensive. It is therefore desirable to formulate an approach where the near-wall region is modeled, leading to the so-called wall-modeled LES. Spectral analysis of DNS data indicates that thin-layer asymptotics is a promising approach to model the interactions between the near-wall layer and the outer flow. For this approach an asymptotic analysis of the filtered Navier-Stokes equations is pursued in the limit in which the horizontal filter scale is large compared to the thickness of the wall layer. It is shown in this limit that the filtered velocities in the near-wall layer are determined to zeroth order by filtered velocities at the boundary of the wall layer. Further, the asymptotics suggest that there is a scaled universal velocity profile f in the near-wall region. This profile, f is evaluated through analysis of DNS data from channel flow at $Re = 5200$. The resulting f is used to formulate a predictive near-wall model.

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Session 6B: Bubbles and Droplets August 14th, 2:45 PM - 4:00 PM (Room B)

Drop Squeezing through Interparticle Constrictions with Insoluble Surfactant

Jacob Gissinger, *Chemical and Biological Engineering, University of Colorado, Boulder*
Alexander Zinchenko, *Chemical and Biological Engineering, University of Colorado, Boulder*
Robert Davis, *Chemical and Biological Engineering, University of Colorado, Boulder*

Despite the prevalence of surfactants in confined biological and subsurface settings, their influence on drop dynamics under tight squeezing conditions remains largely uncharacterized. Using a fully three-dimensional boundary-integral algorithm, the interfacial behavior of surfactant-laden drops squeezing through tight constrictions in uniform far-field flow is modeled under an extensive range of fluid and surfactant properties. A characteristic aspect of this confined and contaminated multiphase system is the rapid development of steep surfactant-concentration gradients during the onset of drop squeezing, due to the interplay between drop hydrodynamics and Marangoni stresses. The presence of surfactant, even at low degrees of contamination, is found to significantly decrease the critical capillary number for droplet trapping, due to the accumulation of surfactant at the downwind pole of the drop and its subsequent elongation. Surfactant transport is enhanced by low drop-to-medium viscosity ratios, at which extremely sharp concentration gradients form during various stages of the squeezing process. Increasing the degree of contamination decreases drop squeezing times, up to a maximum value above which the addition of surfactant negligibly affects squeezing dynamics.

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Fast Agglomeration with Permeable Drops

Noemi Collado, *Chemical and Biological Engineering, University of Colorado, Boulder*
Robert Davis, *Chemical and Biological Engineering, University of Colorado, Boulder*
Alexander Zinchenko, *Chemical and Biological Engineering, University of Colorado, Boulder*
Sydney Baysinger, *Chemical and Biological Engineering, University of Colorado, Boulder*

The purpose of this project is to study a new process for the recovery of fine particles from an aqueous suspension: fast agglomeration with permeable drops. This method, proposed by Prof. Galvin at the University of Newcastle, uses a binder that contains salted-water drops surrounded by thin surfactant-stabilized oil layers to capture the particles through hydrophobic interactions. This salted water creates an osmotic flow of water into the drop, which carries even the smallest particles to the oil-water interface. A model is under development to achieve a better understanding of this process. In the first phase of this project, the model describes permeable drops but without an osmotic driving force. A trajectory analysis was performed to calculate particle capture rates by permeable drops in compressional (or extensional) flow. In the case of impermeable spheres, lubrication resistance prevents collisions, so the collision efficiency (collision rate including hydrodynamic interactions divided by the one in absence of them) is zero. It was found that the presence of permeability (K) leads to non-zero values of E_{pd} , even for small values of K . The effect of on the mobility functions along and normal to the line-of-centers was also studied. It is shown that causes a greater effect when the particle and the drop are in near contact, as lubrication resistance is reduced due to permeation into the drop. However, the effect of is weak for cases in which the particle and the drop are widely separated.

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Behavior of Droplets Through a Porous Membrane

Albert Maristany, *Chemical and Biological Engineering, University of Colorado, Boulder*
Cassandra Giammo, *Chemical and Biological Engineering, University of Colorado, Boulder*
Alexander Zinchenko, *Chemical and Biological Engineering, University of Colorado, Boulder*
Rocio Vazquez, *Chemical and Biological Engineering, University of Colorado, Boulder*
Robert Davis, *Chemical and Biological Engineering, University of Colorado, Boulder*

In this work, we study the behavior of a deformable droplet in a Stokes flow across a porous membrane geometry. First, flow equations are solved for the fluid flow field without the droplet, and then the flow

including the droplet inside is calculated using a ‘moving frame’ and performing boundary-integral simulations. To find relevant results for the theoretical research on membranes, we are interested in finding the trapping and breakage conditions of the droplets, which are useful for characterization of the membrane for emulsion filtration. 3D-simulations show that droplets with high capillary numbers (ratio of viscous stresses to interfacial tension) are more difficult to trap and more likely to break across the pore-geometry, because they easily deform. In contrast, larger drops are more easily trapped and also more easily break than do smaller drops. Video results of our simulations for both breakage and trapping are displayed.

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A Spherical Model for an Encapsulated Microbubble using Transient Network Theory

Bashir Alnajar, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*

Michael Calvisi, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*

Encapsulated microbubbles (EMBs) are widely used to enhance contrast in ultrasound sonography and are finding increasing use in biomedical therapies such as drug/gene delivery and tissue ablation. EMBs consist of a gas core surrounded by a stabilizing shell made of protein, polymer, or lipid. We propose a novel model for a spherical EMB that utilizes a statistically-based continuum theory for the encapsulating material using transient networks. The use of transient network theory provides a general framework that allows a variety of viscoelastic shell materials to be simulated, including a purely elastic solid or a viscous fluid. The model permits macroscopic continuum quantities – such as stress, elastic energy, and entropy – to be calculated based on the network configuration. Using measured properties for a phospholipid bilayer, the model accurately reproduces the experimentally-measured radial response of an ultrasonically-driven, spherical, lipid-coated microbubble, and provides a better fit than that given by common spherical EMB models by Marmottant et al., Chatterjee and Sarkar, and Hoff. The model can be readily extended to finite nonspherical EMB deformations, which are important in many biomedical applications.

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A Model for the Nonspherical Oscillation of Encapsulated Microbubbles using Transient Network Theory

Fathia Arifi, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*

Bashir Alnajar, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*

Michael Calvisi, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*

An axisymmetric analytical model has been developed for small nonspherical oscillations of a microbubble encapsulated by a viscoelastic membrane and subjected to ultrasound. We use transient network theory by Franck et al. (2017) to obtain an appropriate constitutive law for the viscoelastic bubble encapsulation. We incorporate in-plane stress into the membrane, but transverse shear tension, which results from the bending moment, is neglected due to the assumption of a thin shell. By following Prosperetti (1977) and Liu et al. (2012), we derive a nonlinear evolution equation for the radial motion from the governing equations that describe the perturbed radial flow of an incompressible, viscous fluid. The radial motion is represented by a Rayleigh-Plesset type equation with additional terms to account for the influence of the membrane. From a dynamic balance at the bubble surface, evolution equations for the shape modes are obtained by using Legendre polynomials to describe the shape perturbations in the radial and tangential directions. In future work, optimal control theory will be applied to this model to determine the acoustic forcing that optimizes the nonspherical shape oscillation of encapsulated microbubbles for a given application, e.g., sonography or drug delivery.

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