Rocky Mountain Fluid Mechanics Research Symposium 2021: Technical Program

August 10th, 2021

Keynote Presentation

Dr. Sara McAllister, (01:00 PM - 02:00 PM)

Wildland fire: how did we get here and research needed to move forward

Presentation Schedule

Session 1A: Advanced Numerical Methods
09:30 AM – 11:00 AM (Breakout Room 1)

09:30 AM Steven Kiyabu (National Renewable Energy Laboratory)
Modeling Combustion Reaction ODEs with Neural Networks

09:45 AM Parvathi Kooloth (National Renewable Energy Laboratory)
Data-driven Adaptive Mesh Refinement in PeleC

10:00 AM Caelan Lapointe (University of Colorado Boulder)
Towards Efficient Simulations of Fire Spread in the Wildland-Urban Interface

10:15 AM Julian Quick (University of Colorado Boulder)
Multifidelity Multiobjective Optimization for Wake Steering Strategies

10:30 AM Chayut Teeraratkul (University of Colorado Boulder)
Two way coupled fluid-particle coupled interaction using immersed finite element method

10:45 AM Eunji Yoo (National Renewable Energy Laboratory)
One-Dimensional Flow of Cryogenic Helium Below 4K

Session 1B: Engineering Applications
09:30 AM – 11:00 AM (Breakout Room 2)

09:30 AM Sean Bohling (University of Colorado Boulder)
Experimentally Demonstrating a Structed Light and Machine Learning based Flow Velocimeter

09:45 AM Dasha Gloutak (University of Colorado Boulder)
Impact of Surging Streamwise Flow on Laminar Separation Bubble Dynamics for a Finite-Span Wing

10:00 AM Matt Kronwall (Colorado State University)
Erosion Rates of Graphite Nozzles in Hybrid Rocket Motors

10:15 AM Luke McLaughlin (University of Wyoming)
The Influence of Airflow on Aerosol Production from Commercial Fire Pits

10:30 AM Aaron True (University of Colorado Boulder)
Distortion of passive scalar structure during suction-based sampling of airborne odor plumes

10:45 AM Brye Windell (Colorado State University)
Development of Advanced Combustion Strategies for Direct Injection Heavy Duty LPG Engines to Achieve Near-Diesel Engine Efficiency

Session 2A: Multiphase Flows
11:15 AM – 12:15 PM (Breakout Room 1)

11:15 AM Davis Conklin (University of Colorado Boulder)
Modeling self-limited surface reactions on particles in a fluidized bed ALD reactor

11:30 AM Andrew J. Gibson (University of Colorado Colorado Springs)
Application of Koopman LQR to the control of nonlinear bubble dynamics

11:45 AM William Schupbach (University of Colorado Denver)
Central Moment Lattice Boltzmann Schemes with Fokker-Planck Guided Collision for Simulation of Multiphase Flows with Surfactant Effects

12:00 PM Ashish Srivastava (University of Colorado Boulder)
Numerical Simulation of Viscous Microdroplets Flowing Through Straight Microchannels

Session 2B: Modeling
11:15 AM – 12:15 PM (Breakout Room 2)

11:15 AM Filipe Henrique (University of Colorado Boulder)
Double Layer Charging Inside a Nanopore of Arbitrary Debye Length

11:30 AM Nathan Jarvey (University of Colorado Boulder)
Impact of Faradaic Reaction of the Structure of Electrical Double Layer: A Perturbation Expansion Model

11:45 AM Grant Norman (University of Colorado Boulder)
Mesh Element Topologies in Large Eddy Simulation

12:00 PM Gauri Wadhwa (University of Colorado Boulder)
Flow-mediated Infection Transmission in a Dynamic Social Environment in Indoor Occupied Spaces

Session 3A: Atmospheric and Oceanic Flows
02:15 PM – 03:00 PM (Breakout Room 1)

02:15 PM Emily de Jong (National Renewable Energy Laboratory)
Understanding Low Level Jets in the US Atlantic Offshore

02:30 PM Skyler Kern (University of Colorado Boulder)
Progress towards automatic parameter estimation in BFM17 using observing system simulation experiments

02:45 PM Jaylon McGhee (University of Colorado Boulder)
The Impact of Atmospheric Stability and Wake Turbulence on the Wind Turbine Blade Aerodynamics

Session 3B: Turbulence
02:15 PM – 03:00 PM (Breakout Room 2)

02:15 PM Michael Meehan (University of Colorado Boulder)
Vorticity dynamics in buoyant helium plumes

02:30 PM Samantha Sheppard (University of Colorado Boulder)
Generalizing the Concept of the Surface Layer

02:45 PM Samuel Whitman (University of Colorado Boulder)
Thermal Effects in the Turbulent Wake of a Strongly Heated Bluff Body

Keynote Presentation

Dr. Sara McAllister (1:00 PM - 2:00 PM)
RMRS Missoula Fire Sciences Laboratory, USDA Forest Service, 5775 W US Highway 10, Missoula, MT 59808, USA
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Wildland fire: how did we get here and research needed to move forward

Chances are that if you live in the Rocky Mountains, you will be impacted by wildland fires, either through the smoke or directly from fire itself. These impacts have seemingly only increased as wildfires now routinely make headlines, burning more structures and area every year. This talk will begin by introducing the causes of the current "wildfire problem" in the U.S.: the growth of the Wildland-Urban Interface (WUI), climate change, and the more than one hundred years of fire exclusion from the landscape. Our history of wildland fire relates to both the cause and the cure for the current "wildfire problem," especially in the Rocky Mountains. The path forward requires accepting that wildland fires will, and should, happen, but it needs to be the right kind of fire under the right conditions. Unfortunately, fundamental understanding of the processes controlling wildland fire behavior is lacking and this limits our ability to safely train our firefighters, predict fire behavior, and understand how to change it. An overview of the current work at the Missoula Fire Sciences Lab to address this lack of understanding will be given, highlighting the important role of fluid dynamics in wildfire behavior. However, much more work needs to be done before we have confidence in our prediction capabilities and be able to reduce the impact of wildland fire on our communities. The talk will conclude with a discussion of these outstanding research needs.

Speaker Biography:
Sara McAllister earned her Ph.D. in Mechanical Engineering in 2008 from the University of California, Berkeley. Her Ph.D. dissertation, sponsored by NASA, focused on material flammability in spacecraft. Since 2009, she has been a Research Mechanical Engineer with the U.S. Forest Service at the Missoula Fire Sciences Laboratory in Missoula, Montana. As part of the National Fire Decision Support Center, Sara's research focuses on the fundamental governing mechanisms of wildland fire spread. Specifically, her research includes understanding the critical conditions for solid fuel ignition, flammability of live forest fuels, ignition due to convective heating, and fuel bed property effects on burning rate. She has authored a textbook on combustion fundamentals and over 80 peer-reviewed publications and conference papers. In her spare time, Sara enjoys cycling, running, and racing in triathlons.

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Presentation Abstracts

Experimentally Demonstrating a Structed Light and Machine Learning based Flow Velocimeter

Sean Bohling, Mechanical Engineering, University of Colorado Boulder
Elizabeth Strong, Mechanical Engineering, University of Colorado Boulder
Alex Anderson, Electrical Engineering, University of Colorado Boulder
Nazanin Hoghooghi, Mechanical Engineering, University of Colorado Boulder
Juliet Gopinath, Electrical Engineering, University of Colorado Boulder
Greg Rieker, Mechanical Engineering, University of Colorado Boulder

Light scattered from particles moving in a flow can be analyzed to determine the velocity of the flow. Laser Doppler Velocimetry (LDV) uses this basic concept. In LDV, structured light illuminates the region of interest within a fluid, and the scattered light signal is encoded with information relating to the linear velocity components of the flow. Yet, because LDV relies on the limiting assumption that particles travel along linear pathlines, this technique may misrepresent the velocity of particles traveling along curved pathlines. Previously, we have developed a concept and signal processing means for generalizing LDV to measure more velocity-related quantities. Here, we test this framework in a fluidic device by measuring flow rates at locations where conventional velocimetry techniques would fail due to the curved pathlines. These tests run in parallel with simulations of the fluid-particle interaction which support the experimental analysis. Here, we will discuss our experiments and simulations. In particular, we detail the rapid prototyping techniques we employ to fabricate these devices, the simulations we conduct to support the signal processing, and our preliminary results.

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Modeling self-limited surface reactions on particles in a fluidized bed ALD reactor

Davis Conklin, Chemical and Biological Engineering, University of Colorado Boulder
Julia Hartig, Chemical and Biological Engineering, University of Colorado Boulder
Alan Weimer, Chemical and Biological Engineering, University of Colorado Boulder

New manufacturing technologies are needed to support production of high-performance battery components and promote vehicle electrification. Particle atomic layer deposition (ALD) is a coating technique which utilizes sequential, self-limiting surface reactions to produce highly controllable coatings which can significantly improve the cycling stability of lithium-ion battery cathodes. This approach is challenging to commercialize due to a lack of predictive reactor-scale models for the ALD coating process. Here we develop a CFD-DEM model which simulates surface-limited ALD reactions and particle motion in a fluidized bed reactor to de-risk scale up of particle ALD for advanced battery component manufacturing.

A multiphase fluid simulation tool MFIX is used to model a lab-scale fluidized bed reactor during one ALD half-cycle. The minimum fluidization velocity obtained from simulation is compared to the expected result based on correlations of experimental data. Kinetic rate laws for the ALD surface reaction are implemented with user-defined functions and the time profiles of reaction product and precursor breakthrough are compared to results from a laboratory ALD reactor. This research promotes commercialization of particle ALD as a new coating method for advanced batteries.

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Understanding Low Level Jets in the US Atlantic Offshore

Emily de Jong, Mechanical Engineering, National Renewable Energy Laboratory
Eliot Quon, National Renewable Energy Laboratory
Shashank Yellapantula, National Renewable Energy Laboratory

Low level jets (LLJs) in the atmosphere exhibit a local windspeed maximum in the boundary layer, with positive shear beneath the jet and negative shear above the jet. Wind turbines tend to experience increased loads with varying wake recovery characteristics in the presence of an LLJ, therefore understanding the mechanism

and impact of LLJs is crucial to wind energy development. The US Mid-Atlantic offshore region is a huge potential wind energy resource, yet LLJs in this area are poorly understood. In particular, the coastal offshore environment does not exhibit the same diurnal cycle that leads to strong LLJs in the well-characterized Great Plains region. In this study, we use the Weather Research and Forecasting model (WRF) plus lidar buoy data to identify case studies for LLJ events in 2020 in the New York Bight. A reduced order model is presented to explain the onset of these events based on the competing effects of baroclinicity and eddy diffusivity. Finally, using the macro-scale WRF, we drive a micro-scale large eddy simulation (LES) to generate a more detailed characterization of the Marine Boundary Layer during an LLJ. Gaining a better understanding of LLJs and their impacts on offshore wind in the mid-Atlantic is crucial for a transition toward renewable energy.

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Application of Koopman LQR to the control of nonlinear bubble dynamics

Andrew J. Gibson, Aerospace Engineering, University of Colorado Colorado Springs
Xin (Cindy) Yee, Aerospace Engineering, University of Colorado Colorado Springs
Michael L. Calvisi, Aerospace Engineering, University of Colorado Colorado Springs

Koopman operator theory has gained interest in the past decade as a framework for analyzing nonlinear dynamics by embedding in an infinite-dimensional function space. This enables the use of linear control and estimation methods for strongly nonlinear systems. Recently, the linear quadratic regulator (LQR) problem for nonlinear dynamics was formulated in Koopman eigenfunction coordinates and its feasibility demonstrated; however, applications were limited to controlling the Hamiltonian for conservative systems. Here, we extend this framework to use multiple complex eigenfunctions and illustrate its enhanced power by driving several classical nonlinear oscillators to follow arbitrary, prescribed trajectories. We then control nonlinear bubble dynamics, as described by the well-known Rayleigh-Plesset equation, with two novel objectives: 1) stabilization of the bubble at a nonequilibrium radius, and 2) simple harmonic oscillation at amplitudes large enough to incite nonlinearities. Control is implemented through a single-frequency transducer whose amplitude is modulated by the Koopman LQR controller. This work is a step towards controlling nonspherical shape modes of encapsulated microbubbles, which has applications in biomedicine for ultrasound imaging and intravenous drug delivery.

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Impact of Surging Streamwise Flow on Laminar Separation Bubble Dynamics for a Finite-Span Wing

Dasha Gloutak, Aerospace Engineering, University of Colorado Boulder
John Farnsworth, Aerospace Engineering, University of Colorado Boulder

The impact of unsteady streamwise flows on a finite, semi-span, NACA 0015 wing is examined for mean chord-based Reynolds Numbers of 100,000 and 150,000. The unsteady lift response is primarily dominated by the coupling of the surging streamwise flow with the laminar separation bubble dynamics at low to moderate angles of attack, and with the vortex shedding characteristics at angles of attack post-stall. For low reduced frequencies at low angles of attack, the laminar separation bubble elongates at the minimum velocity, thereby increasing the suction pressure on the suction surface and enhancing lift. For low reduced frequencies at post-stall angles of attack, shedding of low pressure coherent structures from the leading edge convect more slowly and coalesce, creating lift plateaus during the lower velocity portion of the cycle, but does not have an impact on the phase averaged lift.

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Double Layer Charging Inside a Nanopore of Arbitrary Debye Length

Filipe Henrique, Chemical and Biological Engineering, University of Colorado Boulder
Ankur Gupta, Chemical and Biological Engineering, University of Colorado Boulder

Electrical-double-layer (EDL) charging in porous media plays a pivotal role in modern energy storage devices such as supercapacitors and hybrid capacitors. Typical models on EDL charging address either the thin-double-layer- or the overlapping-double-layer limit. However, pore radii in typical electrodes range from

less than a nanometer to tens of nanometers, and thus the models that hold for arbitrary Debye lengths are critical to accurately guiding electrode design. Here, we develop a perturbation expansion model based on Poisson-Nernst-Planck equations to capture the effect of an arbitrary ratio of pore size to Debye length. Two key features arise from the model: i) charging timescale depends on the pore size, ii) electric potential undergoes a jump discontinuity at the mouth of the pore. We also derive an expression of effective capacitance, calculated from the steady-state charge density in the pore, and find that our analysis is able to explain the experimental results of nanopore capacitance reported in the literature.

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Impact of Faradaic Reaction of the Structure of Electrical Double Layer: A Perturbation Expansion Model

Nathan Jarvey, Chemical and Biological Engineering, University of Colorado Boulder
Ankur Gupta, Chemical and Biological Engineering, University of Colorado Boulder

Electrical double layers (EDLs) and faradaic reactions are commonly observed in electrochemical systems such as batteries, fuel cells and hybrid capacitors. However, the impact of faradaic reactions on the structure of EDLs is typically neglected, making it harder to accurately predict the concentration, charge, and current profiles. Here, we propose a perturbation expansion model in the thin EDL limit that accounts for a constant Faradaic flux at the Stern layer/diffuse layer boundary. We conclude that while Boltzmann distribution is valid for the thin double layer limit, the structure of the electrical double layer is fundamentally altered by the introduction of a faradaic reaction. This change in structure allows us to connect the micro-scale transport problem near the electrical double layer with the macro-scale bulk transport problem and allows us to qualitatively predict the limiting current for these systems.

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Progress towards automatic parameter estimation in BFM17 using observing system simulation experiments

Skyler Kern, Mechanical Engineering, University of Colorado Boulder
Mary Mcguinn, Mechanical Engineering, University of Colorado Boulder
Peter Hamlington, Mechanical Engineering, University of Colorado Boulder
Katherine Smith, Los Alamos National Laboratory

DAKOTA is an open source numerical toolbox which provides a flexible framework for performing optimizations with arbitrary, user defined models. In this work, the optimization capabilities of DAKOTA are being leveraged to perform parameter estimation studies of the simplified Biogeochemical Flux Model with 17 state variables, BFM17. This is accomplished by performing optimizations of the parameter values with an objective of minimizing the error between the model output and a reference data set. An observing system simulation experiment (OSSE) is used to test the robustness of the optimization algorithm and its implementation by using a synthetic set of data from a nominal run of the model as the reference data. The parameter estimation is then performed from a perturbed set of parameter values. In this presentation the coupling of BFM17 to DAKOTA and results from OSSEs of BFM17 using 5 model parameters will be discussed.

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Modeling Combustion Reaction ODEs with Neural Networks

Steven Kiyabu, Mechanical Engineering, National Renewable Energy Laboratory
Nicholas Wimer, National Renewable Energy Laboratory

The chemistry of combustion reactions is complex as it involves many species and reactions. In practice, such a system is often modeled computationally using an empirically derived chemical mechanism. Given the large range of reaction rates, the system is then time evolved using a stiff ODE solver. However, even when reduced chemical mechanisms are employed, the system can become computationally expensive for two-dimensional or three-dimensional systems. Such systems can also face problems with instability. As such, it is desirable to find a cheaper, stable alternative to solving the reaction system. Neural networks offer the potential to learn these reaction ODEs and time evolve a combustion reaction in a more cost-efficient manner *than stiff ODE solvers. In this study, a variety of neural networks are trained on zero-dimensional Cantera simulations of methane combustion with varying initial conditions. Several predictive approaches as well as several neural network architectures (artificial neural network with dropout, ResNet, and Neural ODE) are compared in their ability to predict combustion trajectories. Promising models are then identified.*

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Data-driven Adaptive Mesh Refinement in PeleC

Parvathi Kooloth, Applied Mathematics, National Renewable Energy Laboratory
Bruce Perry, National Renewable Energy Laboratory

Many of the current AMR (Adaptive Mesh Refinement) frameworks use heuristic criteria that rely on user intuition to identify regions of the computational grid that require refinement. We explore the possibility of replacing the ad-hoc tagging of grid cells for refinement with a neural net that can discern regions of high spatial discretization error using instantaneous flow field data. We compare the efficacy of various neural net architectures including fully connected networks and convolutional neural nets (CNN) by conducting a priori tests on a turbulent high pressure CO_2 jet. Results from a posteriori tests carried out by integrating the neural net in PeleC, a reacting fully compressible Navier-Stokes solver that is built on the AMReX library, are also presented.

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Erosion Rates of Graphite Nozzles in Hybrid Rocket Motors

Matt Kronwall, Mechanical Engineering, Colorado State University
Bret Windom, Mechanical Engineering, Colorado State University
Anthony Marchese, Mechanical Engineering, Colorado State University

Preliminary work is pursuant to the measurement and evaluation of nozzle erosion rates, specifically relating combustion chamber pressure and fuel chemistry to carbon nozzle erosion in hybrid rocket motors. Oxidizing species, such as, OH, CO2 and H2 O, have been shown to be the largest contributors to nozzle erosion in carbon-based materials, wherein surface carbon reacts with the oxidizing species present in the exhaust products, forming CO. Although earlier studies have assumed a linear relationship between erosion rates and pressure, our research indicates that this linear assumption may not hold at combustion chamber pressures below 3.4 MPa. Initial numerical modeling shows a non-linear decrease in boundary layer thicknesses with increasing pressures up to 3.4 MPa, with increasing linearity seen above 3.4 MPa. As such, the modeled results suggest a non-linear relationship between nozzle erosion and pressure at lower chamber pressures caused by non-linear diffusion of the oxidizing species to the surface of the nozzle. To test the effect of low chamber pressure and hydrocarbon fuels on erosion rates, a HTPB-N2O hybrid rocket motor was designed, built, and tested. Significant erosion has been measured from a 30 second burn at a combustion chamber pressure of 1.5 MPa.

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Towards Efficient Simulations of Fire Spread in the Wildland-Urban Interface

Caelan Lapointe, Mechanical Engineering, University of Colorado Boulder
Peter Hamlington, Mechanical Engineering, University of Colorado Boulder

Fires in the wildland urban interface (WUI) are challenging to study computationally, in part, due to topographical variations as well as large scale separation between smaller, local geometric features (e.g., buildings or houses) and larger flow-scale features (e.g., the atmospheric boundary layer and computational domains on the size of hundreds of meters or kilometers). Adaptive mesh refinement (AMR) can be used to bridge this gap and increase resolution only where its needed; for large fire spread problems characteristic of the WUI this may be just a fraction of the computational domain. In this talk, we present a new OpenFOAM solver for multi-region, AMR-based fire spread simulations in the WUI. The new solver, called multiRegionFireDyMFoam, leverages unstructured mesh and arbitrary mesh interface (AMI) capabilities of OpenFOAM to incorporate AMR in gas and solid regions. Test cases representative of fire spread in the WUI are discussed to showcase new capability.

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The Impact of Atmospheric Stability and Wake Turbulence on the Wind Turbine Blade Aerodynamics

Jaylon McGhee, Aerospace Engineering, University of Colorado Boulder
Ganesh Vijayakumar, National Renewable Energy Laboratory
John Farnsworth, Aerospace Engineering, University of Colorado Boulder

Significant challenges remain in understanding wind turbine performance within the turbulent atmospheric boundary layer (ABL) and the wakes of upstream turbines. To help address these points, large-eddy simulations of the convective ABL under a range of stability states and inflow velocities are computed with two IEA-15 megawatt turbines separated by seven rotor diameters in a 5 km by 5 km by 1 km domain using the AMR-Wind solver from NREL. A comparison is made between the length- and time-scales encountered by the turbine in the global reference frame and the relative or local scales encountered by the rotating blade as a function of the ABL state and the rotor span. Since the ABL turbulence contains length scales much larger than the blade chord length; it has often been treated as a quasi-steady change in the local blade angle of attack and relative velocity. However, recent research from Vita et al. (2020) suggests that turbulence effects are non-negligible on blade aerodynamic performance even at integral length scales up to 3 times the local chord length. This study aims to elucidate these differences as a function of the ABL state, to better isolate the quasi-steady, unsteady, and turbulent flow conditions imposed on a wind turbine blade.

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The Influence of Airflow on Aerosol Production from Commercial Fire Pits

Luke McLaughlin, Mechanical Engineering, University of Wyoming
Erica Belmont, Mechanical Engineering, University of Wyoming
Shawn Urbanski, Fuels and Combustion Science, U.S.F.S. Missoula Fire Sciences Laboratory

Different commercial fire pits utilize unique airflow patterns through their fire pits, influencing the amount of oxygen available during burning. Air flow influences fire behavior and plays a significant role in the rate of formation and properties of aerosols formed during biomass burning. Closely related to air flow is combustion chemistry which occurs in an oxidative environment and influences the type, size, and volatility of aerosols formed from biomass burning. This work investigated the number, size, and volatility of aerosol emissions from two different commercial fire pits with different modern air flow designs to better understand how air flow influences aerosol emissions from commercial fire pits. Increased airflow was associated with a larger modified combustion efficiency in this work. Results obtained during a steady burn showed that the stove suggesting to have increased airflow produced a lower particle number formation rate, similar particle mass formation rate, larger particle sizes, and less volatile particles compared to the stove with less air flow. The results suggest that oxygen availability during fire pit burning influences the physical and chemical properties of the aerosols produced, and fire pit air flow can be altered through fire pit design.

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Vorticity dynamics in buoyant helium plumes

Michael Meehan, Mechanical Engineering, University of Colorado Boulder
Peter Hamlington, Mechanical Engineering, University of Colorado Boulder

Axisymmetric buoyant plumes are often characterized by the large-scale vortical structures that form upon the upward injection of a lightly fluid into the heavier ambient. These structures can be found in a variety of naturally occurring phenomena, such as hydrothermal vents and volcanic eruptions, and have a leading-order effect in reacting plumes found in heat treatment processes and pool fires. In order to improve optimization and prediction capabilities, we need to improve our understanding of the flow characteristics. In this work, we conduct highly-resolved numerical simulations using adaptive mesh refinement of helium plumes and analyze the plumes using the Reynolds-averaged enstrophy transport equation. We find that in laminar plumes, despite preserving symmetry instantaneously, each transport term contributes appreciably; this is particularly notable for vortex stretching which must be zero in pure two-dimensional flows. As the Richardson and Reynolds number are increased, the flow becomes more chaotic, and heavier ambient fluid penetrates farther into the core of the plumes; this is associated with a sharp increase in vortex stretching. Lastly, scaling relationships between transport terms for different Reynolds and Richardson numbers are identified and explained.

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Mesh Element Topologies in Large Eddy Simulation

Grant Norman, Aerospace Engineering, University of Colorado Boulder
Aviral Prakash, Aerospace Engineering, University of Colorado Boulder
Kenneth Jansen, Aerospace Engineering, University of Colorado Boulder
John Evans, Aerospace Engineering, University of Colorado Boulder

Even with the acceleration of computational hardware, Direct Numerical Simulation is too expensive for countless applications of interest, particularly for problems involving turbulence. For the subset of these cases involving unsteady features or flow separation, we may turn to Large Eddy Simulation (LES), fully resolving the larger scales of motion, while hoping to model how energy cascades to the smaller scales. These interactions from larger resolved scales to smaller unresolved scales are theoretically captured by the subgrid scale (SGS) tensor. However, without resolving all the scales of motion, we are left with a problem of closure and can only approximate this object.

For practical applications, we want a closure model that works well on complex geometries, where the domain of interest is often represented by an unstructured grid composed of various types of anisotropic mesh elements. For a few closure models, we use the test case of forced Homogeneous Isotropic Turbulence (HIT) to examine the differences caused by meshing with hexahedral, tetrahedral, and prismatic elements, at various levels of mesh anisotropy. The results compare energy spectra between the different meshes, DNS data, and Kolmogorov's 1941 theory.

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Multifidelity Multiobjective Optimization for Wake Steering Strategies

Julian Quick, Mechanical Engineering, University of Colorado Boulder
Ryan King, National Renewable Energy Laboratory
Peter Hamlington, Mechanical Engineering, University of Colorado Boulder

Wake steering is a wind power plant control strategy where upstream turbines are intentionally yawed away from the incoming wind, thereby steering wakes away from downstream turbines. The potential increase in power and reduction of fatigue loading achieved through this control strategy is the subject of continuing investigation. In this study, we present a multiobjective multifidelity optimization approach for exploring these trade-offs. Numerical simulations with different resolutions are used to model the system at multiple computational fidelities. Single-fidelity and multifidelity Bayesian optimization studies are performed, maximizing an acquisition function in each iteration, after some initial sampling of the system. Each optimization uses the expected hypervolume improvement acquisition function. In the multifidelity case, the acquisition function is weighted by the total cost of a proposed model evaluation. Our multifidelity approach identifies a Pareto front of optimal control strategies that balance competing power and loading objectives. Preliminary results suggest the multifidelity approach is twice as fast as the single-fidelity approach, and we expect this advantage to grow as we consider more expensive simulations.

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Central Moment Lattice Boltzmann Schemes with Fokker-Planck Guided Collision for Simulation of Multiphase Flows with Surfactant Effects

William Schupbach, Mechanical Engineering, University of Colorado Denver
Kannan Premnath, Mechanical Engineering, University of Colorado Denver

We present central moment lattice Boltzmann (LB) schemes, whose collision steps are represented by a novel Fokker-Planck (FP) kinetic model, for computations of multiphase hydrodynamics, interface tracking and surfactant evolution. Our approach involves matching the changes in different discrete central moments under collision to those of the continuous central moments as given by the drift-diffusion based FP model of the Boltzmann equation. This effectively results in relaxations to equilibria, the Markovian central moment attractors, which depend on the lower order moments. Based on this, a LB scheme for the pressure and velocity fields in multiphase flows at high density ratios is constructed. The interface motions are captured using the Allen-Cahn equation computed by another FP-guided LB scheme. The surfactant concentration is evolved by a model that accounts its preferential adsorption on interfaces, which is solved by a third LB scheme using FP collision. The Langmuir isotherm then parameterizes the effect of surfactant concentration

on surface tension and its tangential gradients. Various simulations involving the effect of surfactant concentrations on multiphase systems are presented and the advantages of using the FP model are demonstrated.

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Generalizing the Concept of the Surface Layer

Samantha Sheppard, Aerospace Engineering, University of Colorado Boulder
James Brasseur, Aerospace Engineering, University of Colorado Boulder
John Farnsworth, Aerospace Engineering, University of Colorado Boulder
John Christos Vassilicos, Laboratoire de Mecanique des Fluides de Lille

The classical description of a surface layer is a wall-adjacent region within a high Reynolds number turbulent boundary layer in which turbulence fluctuations are directly modified by surface impermeability and where turbulence integral scales scale with z, the distance from the surface. This description includes both modulation by surface blockage and production by mean shear. To generalize the concept of a surface layer, we consider these effects separately. Canonical boundary layer PIV data from LMFL is compared to SPIV measurements of grid turbulence blown over an impermeable flat plate to characterize the direct influence of surface impermeability on turbulence structure. We identify a region for the grid turbulence case where integral length scales of fluctuating vertical velocity grow with z and where there exists a deficit in turbulent kinetic energy. The latter is not observed in the canonical turbulent boundary layer data but is consistent with theory developed by Hunt Graham (1978) and experiments of Thomas Hancock (1976). By isolating surface blockage effects on grid turbulence, we aim to isolate key surface layer elements associated with the creation of attached turbulence eddies in the absence of turbulence production.

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Numerical Simulation of Viscous Microdroplets Flowing Through Straight Microchannels

Ashish Srivastava, Chemical and Biological Engineering, University of Colorado Boulder
Gesse Roure, 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

Understanding the behavior of drops in microchannels is of utmost importance for the design of microfluidic systems, such as microreactors and lab-on-chip systems. Understanding droplet deformation and motion inside microchannels can help to guide new developments in these areas. One of the main methods to simulate drop motion is the Boundary Integral Method, in which only the boundary is discretized, rather than the entire fluid domain. However, for very large channels, these simulations are computationally demanding. To overcome this issue, we introduce a moving frame around the droplet, within which our equations are solved. In this work, we simulate a deformable droplet flowing in a straight, infinitely-long microchannel with a rectangular cross section. Our simulations show that droplets with higher capillary numbers, Ca, have higher steady state velocities and higher deformation. In contrast, increasing the viscosity ratio, λ, leads to lower steady state velocities, and also more deformable droplets. At higher values of Ca and λ, we observe the formation of instabilities, characterized by the formation of a tail structure in the back portion of the droplet, which may hinder the drop to reach steady state and can eventually lead to drop breakup.

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Two way coupled fluid-particle coupled interaction using immersed finite element method

Chayut Teeraratkul, Mechanical Engineering, University of Colorado Boulder
Debanjan Mukherjee, Mechanical Engineering, University of Colorado Boulder

Fluid-particle interaction problems are prevalent in many engineering, biomedical, and environmental applications. Despite several existing approaches, handling simultaneous coupling for multi-particle systems remain a challenge. In this work, an implementation of two way coupled fluid-particle interaction simulation is presented. The fluid-particle coupling is resolved using immersed finite element method in which

the particle structure is represented by a Lagrangian mesh moving on top of a Eulerian fluid mesh. This allows for the fluid mesh to be generated independently from the solid structure and thus greatly simplifies the meshing process for multi-particle systems. The no-slip condition and the interaction force at the fluid-solid interface is enforced using a mesh-to-mesh interpolation via basis function transformation techniques. Support size on which the fluid-structure interaction force is applied is the size of elements touching the particle domain and therefore optimal in an element-wise sense. Simplified particle collisions are used to demonstrate the implementation. Results from two canonical problems: (a) rigid sphere dropping in a channel; and (b) two particle drafting-kissing-tumbling phenomena are presented to illustrate and validate the implementation.

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Distortion of passive scalar structure during suction-based sampling of airborne odor plumes

Aaron True, CEAE, University of Colorado Boulder
Dionys Beck, CEAE, University of Colorado Boulder
John Crimaldi, CEAE, University of Colorado Boulder

Many odor plume and olfaction studies use photoionization detectors (PID) to quantify spatiotemporal odor distribution. PIDs use suction to draw ambient air through a sampling needle, producing a temporal odor concentration record. Little is known about how suction distorts the spatial structure of odor filaments, or how this may alter the sensor-level signal. We numerically model the geometry and dynamics of a widely-used PID to investigate effects of relative suction rate (ratio of average needle velocity to ambient flow speed) and passive scalar geometry (filament width) on sensor-level concentration records, relative to that measured by a nonintrusive probe. Our results show that suction can modify the arrival time, peak concentration, and pulse shape, relative to the undistorted filament structure. We derive a nondimensional parameter based on a sink flow model that robustly predicts distortion levels and delineates distortion regimes at order 1. This parameter intuitively represents the ratio of the size of the suction-induced distortion region of the PID (function of relative suction rate and needle geometry) to filament size. The analytical expression derived allows us to assess distortion potential for typical PID operational regimes and to inform mitigation strategies.

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Flow-mediated Infection Transmission in a Dynamic Social Environment in Indoor Occupied Spaces

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Covid-19 and its high risk of spread indoors has generated significant interest in studying infection transmission in dynamic social environments within occupied indoor spaces. This is essential for formulating preventative measures and solutions related to HVAC systems and movement strategies to combat infection spread. Fluid flow is known to play a key role in the spread of infection indoors. However, using full-scale CFD or experiments for an indoor dynamic social environment, involving multiple human occupants, is prohibitively expensive. Hence, stochastic infection dynamics models are commonly employed, which do not account for the indoor air flow. Here, we develop a flow-dependent infection spread model coupled with the social force model, to study infection transmission in a social environment comprising 60 people in an indoor layout. Results reveal that the extent of infection transmission is significantly affected by the inclusion of air flow pattern data in the transmission analysis. Through this study, we establish the utility and efficacy of flow-integrated probabilistic models based on social dynamics to study infection transmission.

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Thermal Effects in the Turbulent Wake of a Strongly Heated Bluff Body

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We investigate the impact of heat transfer from a triangular prism bluff body on the development of turbulent wake dynamics, using adaptive mesh refinement (AMR) to locally resolve physics of interest, producing the highest Reynolds number simulations of any bluff body study of comparable resolution to date. We perform simulations for non-heated and strongly heated bluff bodies and examine the resulting variations in the flow structure and dynamics, specifically analyzing the near-field effects of varying fluid density, viscosity, diffusivity and local Reynolds number caused by the heating. We find a resolution-dependent effect of heat transfer on mean flow statistics, including recirculation zone length. Strong gradients along the boundary and shear layers, which affect the dynamical importance of specific terms in the vorticity transport equations, are analyzed in this context as a potential explanation. Comparisons are made to bluff body stabilized flame cases from the available literature, which share several important features with the current simulations. All results highlight the importance of capturing strong gradients in simulations of bluff body flows, enabled here by the use of AMR.

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Development of Advanced Combustion Strategies for Direct Injection Heavy Duty LPG Engines to Achieve Near-Diesel Engine Efficiency

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Internal combustion engines are a huge part of the transportation sector as well as heavy-duty applications. Liquified petroleum gas (LPG) is a promising leap to help mitigate these issues as well as being economically friendly for heavy-duty applications. Before LPG is widely accepted, an LPG engine must be comparable in efficiency to similar diesel engine platforms. The fundamental limitations of LPG will be experimentally tested in a constant volume high pressure spray chamber using multiple imaging techniques, such as Schlieren, Mie, and planar laser induced fluorescence (PLIF) to verify computer models. Direct injection engines are known to achieve higher efficiencies than other conventional methods. Using direct injection and imaging techniques, certain parameters will be used to measure and define the characteristics of a spray, simulating a direct injection event in an engine. Parameters such as penetration length, speed, and angle will help characterize how LPG reacts at near engine like conditions as well as display vaporization and mixing processes. With the successful completion of this study a better understanding of LPG and a finely tuned LPG model, will help research progress forward understanding LPG heavy-duty applications while reaching diesel like efficiencies.

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One-Dimensional Flow of Cryogenic Helium Below 4K

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Efficient cooling of quantum technologies requires the use of low-temperature liquid helium. Because qubits must be maintained at temperatures ranging from 15K to 4K, a complex equations of state (EoSs) is needed to characterize fluid properties. The effect of these properties on the fluid behavior is not yet understood. To investigate this, we implemented a comprehensive solver package of the EoS introduced by McCarty and Arp in 1990 and various properties for wide temperature and pressure range. This package also provides the computation for a temperature or pressure point from enthalpy and entropy changes. We then couple the EoS solution with conservation equations for one-dimensional compressible flow with heat addition. Although the Mach number for liquid helium is low, the density change is large enough to be required a compressible formulation. We present the impact of the amount of heat on the energy system, including the stability, solution time, and physical accuracy. We plan to compare the solutions obtained from other computational fluid dynamics (CFD) solvers for realistic energy systems simulation.

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