Rocky Mountain Fluid Mechanics Research Symposium 2019: Technical Program

Sustainability, Energy and Environment Complex (SEEC)
University of Colorado, Boulder
July 29th, 2019

Keynote Presentation

Dr. Jacqueline O'Connor, (1:00 PM - 2:00 PM)
The Role of Fluid Mechanic Instability in Gas Turbine Combustor Operability

Presentation Schedule

Session 1A: Wings
8:45 AM - 10:15 AM (Room A)

8:45 AM Joseph Pointer (University of Colorado, Boulder, CO)
Fine-Wire Sensor Calibration System for Low Velocity Flows at Stratospheric Conditions

9:00 AM Dasha Gloutak(University of Colorado, Boulder, CO)
Influence of Surging Flow Frequency on Lift Coefficient for Finite Wings

9:15 AM Hunter Ringenberg (University of Colorado, Boulder, CO)
Sparse Identification of Non-linear Dynamics for an Unsteady Pitching Wing Section

9:30 AM Emmanuele Costantino (University of Colorado, Boulder, CO)
Influence of Aspect Ratio on Lift Coefficient for Finite Wings in Surging Flow

9:45 AM Julian Quick (University of Colorado, Boulder, CO)
Capturing a Blade Tip Vortex

10:00 AM Riccardo Balin (University of Colorado, Boulder, CO)
Scale Resolving Simulations of Separated Flow over a Bump

Session 1B: Model Development
8:45 AM - 10:15 AM (Room B)

8:45 AM Jeffrey Glusman (University of Colorado, Boulder, CO)
Initial Verification of a Reduced Combustion Model of Douglas Fir

9:00 AM Noemi Collado (University of Colorado, Boulder, CO)
Fast Agglomeration with Permeable Drops

9:15 AM Alireza Sharifi (Colorado State University, Fort Collins, CO)
Mechanics and Efficiency of Zebrafish 30HPF Heart

9:30 AM Skyler Kern (University of Colorado, Boulder, CO)
Towards a Reduced Biogeochemical Flux Model for Large Eddy Simulations of the Upper Ocean

9:45 AM Nicholas Yearout (Colorado School of Mines, Golden, CO)
Membrane Distillation Experiments with 3D Printed Spacers

Session 2A: Combustion
10:30 AM - 11:45 AM (Room A)

10:30 AM David Yun (University of Colorado, Boulder, CO)
Updating High Temperature Methane Absorption Models Using Dual Comb Spectroscopy Data

10:45 AM Jesse Schulthess (Colorado State University, Fort Collins, CO)
Transient, High Pressure Oil-gas Dilution Study

11:00 AM Samuel Whitman (University of Colorado, Boulder, CO)
Simulation of Bluff-Body-Stabilized Flames Using PeleC, a Combustion Code for Exascale Computing

11:15 AM Stephen Lucas (Colorado State University, Fort Collins, CO)
Combustion and Droplet Behavior of JP-8 Surrogates in a Two-Phase Reacting Flow

11:30 AM Lydia Meyer (Colorado School of Mines, Golden, CO)
Azeotrope Formation During the Evaporation Process of Fuel Blends

Session 2B: Making CFD Work
10:30 AM - 11:45 AM (Room B)

10:30 AM John Patterson (University of Colorado, Boulder, CO)
Inflow Boundary Conditions for Scale Resolving Simulations

10:45 AM Michael Meehan (University of Colorado, Boulder, CO)
Synthetic Turbulence Generation Method to Simulate Turbulence Generating Plates

11:00 AM Miguel Valles Castro (Colorado State University, Fort Collins, CO)
Computational Fluid Dynamics of a Heavy Hydrocarbon Direct Injected Unmanned Aerial Vehicle

11:15 AM Julia Ream (Florida State University, Tallahassee, FL)
Numerical Simulations of the Supercritical Carbon Dioxide Round Turbulent Jet

11:30 AM Mokbel Karam (University of Utah, Salt Lake City, UT)
On a Class of High-Order, Low-Cost Time Integrators for the Navier-Stokes Equations

Session 3A: Machine Learning
2:15 PM - 3:30 PM (Room A)

2:15 PM Olga Doronina (University of Colorado, Boulder, CO)
On Approximate Bayesian Computation Approach for Turbulence Model Development

2:30 PM Carlos Michelen-Strofer (National Renewable Energy Laboratory, Golden, CO)
New Fluid Flow Data Assimilation Formulations Using Perceptual Loss Networks

2:45 PM Andrew Glaws (National Renewable Energy Laboratory, Golden, CO)
Deep Learning for In-Situ Data Compression of Large CFD Simulations

3:00 PM Karen Stengel (National Renewable Energy Laboratory, Golden, CO)
Physics-Informed Super-Resolution of Climatological Wind Data

3:15 PM Matt Sorrells (University of Colorado, Anschutz, CO)
A Microfluidic Model of Bleeding to Probe the Fluid Mechanics and Biochemistry of Bleeding Disorders

Session 3B: Engineering Applications 2:15 PM - 3:30 PM (Room B)

2:15 PM Caelan Lapointe (University of Colorado, Boulder, CO)
Efficient Simulation of Complex Fire Phenomena

2:30 PM Jeffery Allen (National Renewable Energy Laboratory, Golden, CO)
Accounting for Complex Terrain to Optimize Wind Farm Layouts Using WindSE

2:45 PM Benjamin Appleby (Colorado School of Mines, Golden, CO)
Rheological Analysis of Conditioned Soil Material for Soft Ground Tunneling

3:00 PM Colin Towery (University of Colorado, Boulder, CO)
Detonation Initiation by Compressible Turbulence Thermodynamic Fluctuations

3:15 PM Courtney Mattson (University of Colorado, Anschutz, CO)
Fluid Dynamic Forces Affect the Spatial Distribution of Cellular Injury During the Progression of Ventilator-Induced Lung Injury

Session 4A: Heat Transport 3:45 PM - 5:00 PM (Room A)

3:45 PM Mark Dudley (Colorado School of Mines, Golden, CO)
Numerical Study of Membrane Heating in a Vacuum Membrane Distillation System

4:00 PM Steven Issacs (University of Colorado, Boulder, CO)
Development and Application of a Thin Flat Heat Pipe Design Optimization Tool for Small Satellite Systems

4:15 PM Eman Yahia (University of Colorado, Denver, CO)
Simulation of High Rayleigh Number Natural Convection Flows using a Central Moment Lattice Boltzmann Method on a Rectangular Grid

4:30 PM Jacob Johnston (Colorado School of Mines, Golden, CO)
Direct Numerical Simulation of Unsteady Mixing in Direct Contact Membrane Distillation Systems with Membrane Spacers

4:45 PM Choah Shin (University of Oregon, Eugene, OR)
Simulation of Low-Temperature Helium Flow in a Heated Microchannel

Session 4B: Advanced Fluids 3:45 PM - 5:00 PM (Room B)

3:45 PM Sean Coughenour (University of Colorado, Colorado Springs, CO)
Modes of Droplet Breakup in Confined Shearing Flow

4:00 PM Ryan Darragh (University of Colorado, Boulder, CO)
Particle Pair Dispersion in a High-Speed Premixed Flame

4:15 PM Sam Simons-Wellin (University of Colorado, Boulder, CO)
An Efficient Proper Orthogonal Decomposition Algorithm for Adaptively Refined Meshes

4:30 PM Alison Wallbank (University of Colorado, Denver, CO)
Fluid Mechanical Forces in a Sepsis Mediated Model of Ventilator-Induced Lung Injury

4:45 PM Forest Mannan (Colorado School of Mines, Golden, CO)
Modeling the Synchronization of Flagella on the Exterior of a Sphere

Keynote Presentation

Professor Jacqueline O'Connor (1:00 PM - 2:00 PM)

Department of Mechanical Engineering, The Pennsylvania State University

The Role of Fluid Mechanic Instability in Gas Turbine Combustor Operability

Gas turbine engines are a highly efficient source of power for a variety of applications, including electricity generation, aircraft propulsion, and industry. These engines are not only efficient, but can also meet strict emissions regulations. However, these improvements in emissions and efficiency dont come without significant technical challenges, the greatest of which is combustion instability. Combustion instability is a potentially disastrous feedback cycle between combustor acoustics and flame heat release rate fluctuations in the combustor. These processes couple through fluid mechanic pathways in the complex combustor flow field, making suppression of instabilities a very difficult task. In this talk, we will discuss the fundamentals of combustion instability and see the critical role that fluid mechanic instability plays in the instability feedback loop. In particular, we focus on the behavior of two common flows in gas turbine combustors: bluff-body flows and swirling jets. Both flows are used to stabilize flames as a result of their large recirculation zones, but they display a range of hydrodynamic instability modes that can interact with the resonant acoustics in combustion chamber. Coupled experimental, theoretical, and modeling studies will be used to illustrate the importance of these fluid dynamic structures in the coupling process. Implications for future gas turbine design will be discussed.

Speaker Biography:
Dr. Jacqueline O'Connor is an Associate Professor of Mechanical Engineering and the director of the Reacting Flow Dynamics Laboratory at the Pennsylvania State University. Her research focuses on unsteady combustion phenomena in power and propulsion technologies, including power generation gas turbines, aircraft engines, and diesel engines, using high-speed laser diagnostics. Previously, she was a post-doctoral researcher at Sandia National Laboratories in Livermore, California in the Engine Combustion Department. She received a BS from MIT in Aeronautics in 2006, and a MS and Ph.D. in Aerospace Engineering from Georgia Tech in 2009 and 2012. She is the recipient of the 2016 Irvin Glassman Young Investigator Award from the Eastern States Section of the Combustion Institute and the 2018 Dilip R. Ballal Early Career award from the ASME International Gas Turbine Institute.

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Presentation Abstracts

Accounting for Complex Terrain to Optimize Wind Farm Layouts Using WindSE

Jeffery Allen, *National Renewable Energy Laboratory*
Ryan King, *National Renewable Energy Laboratory*
Garrett Barter, *National Renewable Energy Laboratory*

Wind farm simulations in complex terrain are especially challenging due to terrain-induced effects such as flow separation and curvature. These effects make it difficult to achieve accurate results with traditional engineering flow models based on linear superposition. To address these challenges, we have added a complex terrain modeling capability to NRELs open source computational fluid dynamics (CFD) software WindSE. WindSE is a Reynolds-averaged Navier Stokes (RANS) solver built in Python with the capability to solve flows in 2D and 3D, steady state or time varying, and it can also compute gradients of objective functions using automatic differentiation. In this talk, we discuss modifications to WindSE that enable complex terrain studies, and report on results from test cases involving a Gaussian hill and terrain from a utility scale wind farm. Our results show significant vertical and spanwise velocities are induced by the terrain, resulting in deviations from normal inflow angles and as substantial wake deflections. Capturing these effects will critical to effective layout optimization and wake steering strategies.

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Rheological Analysis of Conditioned Soil Material for Soft Ground Tunneling

Benjamin Appleby, *Chemical and Biological Engineering, Colorado School of Mines*
Joseph Samaniuk, *Colorado School of Mines*
Michael Mooney, *Civil and Environmental Engineering, Colorado School of Mines*

The purpose of this project is to study the use of foam in Earth Pressure Balance Tunnel Boring Machines (EPB TBM), an industry standard equipment for creating large-scale tunnels in soft ground, to improve tunneling speed and efficiency. Soft ground consists of sands and clays with varying water content, composition, and mixtures. Depending on soil conditions, foam is tailor-made and injected into the soil by the cutter-head during boring. The foam does two jobs, reduces the torque load on the cutter-head and modifies the consistency of the soil to minimize clogging and improve extraction rate as it is removed by a rotating screw conveyor. However, it is not well understood how the foam does this. Bulk rheology is used to better understand this three-phase mixture by probing yield stress and the viscosity over a range of relevant shear rates. The methodology is to understand individually the constituents of sand and clay with variation in water content and pressure. Followed by the introduction of foam at ratios of foam to soil and foam quality. Then in the future, a large-scale rheometer will characterize the soil-foam material under representative EPB TBM conditions, giving both insight into the connection between small and large-scale bulk rheology and expand upon difficult to measure soils that cannot be characterized in traditional rheometers.

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Scale Resolving Simulations of Separated Flow over a Bump

Riccardo Balin, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Kenneth Jansen, *Aerospace Engineering Sciences, University of Colorado, Boulder*

A turbulent boundary layer over a Gaussian bump is computed with a series of scale resolving simulations of the incompressible Navier-Stokes equations. The two-dimensional bump causes a rapid succession of favorable-to-adverse pressure gradients that can lead to smooth separation on the downstream side, both of which are characteristic of the flow over the flap of an aircraft wing in high-lift configurations. At the inflow, the momentum thickness Reynolds number is approximately 1,000, and the boundary layer thickness is 1/8 of the bump height. Comparisons of the results from a wall-modeled large eddy simulation (WMLES) and a direct numerical simulation (DNS) show the deficiencies of the WMLES to accurately capture the effects of the pressure gradients on the boundary layer turbulence.

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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*

The purpose of this project is to model 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 salt-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 when there is an imposed extensional flow due to stirring. In our previous work, the model only described permeable drops but without an osmotic driving force. A new model has been developed in order to calculate trajectories of a solid particle relative to a permeable drop that expands with time due to osmotic flow. The description includes a new dimensionless parameter N, which corresponds to the ratio of the osmotic flow velocity to the imposed velocity. The effect of N has been studied; it is seen that higher values of N lead to faster collision rates, as drop growth enhances particle collection.

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Influence of Aspect Ratio on Lift Coefficient for Finite Wings in Surging Flow

Emanuele Costantino, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Dasha Gloutak, *Aerospace Engineering Sciences, University of Colorado, Boulder*
John Farnsworth, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Increasing aspect ratio (AR) of a semi-span NACA0015 wing in an unsteady freestream modified the instantaneous coefficient of lift. At a mean Reynolds number of 150,000, the wind tunnel gusting flow followed an approximate sinusoidal profile at a frequency of 1 Hz. Data for full-span AR of 4, 6, and 8 were tested at angles of attack between 0 and 20 degrees, in increments of 5 degrees. While both steady state and unsteady, attached flow, lift coefficients demonstrated a positive correlation with AR and lift coefficient, the unsteady lift coefficient at stall was inversely proportional to AR. For fully separated flows, lift coefficient collapsed for AR of 6 and 8. This indicated the significance of wing tip vortex strength in relation to the detached flow region of stalled wing.

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Modes of Droplet Breakup in Confined Shearing Flow

Sean Coughenour, *University of Colorado, Colorado Springs*
Sean Coughenour, *Mechanical and Aerospace Engineering, University of Colorado, Colorado Springs*
Hui Wan, *Mechanical and Aerospace Engineering , University of Colorado, Colorado Springs*

The deformation of an isolated droplet confined in a fluid channel was analyzed using Gerris, a computational fluid dynamics solver using Volume of Fluids method. The deformation behavior was analyzed for both simple shear flow and oscillatory shear flow. Within each case, the effects of various Reynolds number, Weber number, viscosity ratio, density ratio, degree of confinement, and oscillation frequency were studied. The resulting deformation was categorized by whether the droplet experienced breakup or not. In the cases of droplet breakup, it was further categorized into one of three modes: midpoint pinching, edge breakup, and homogeneous breakup. Current results were obtained using two-dimensional simulations. Three-dimensional simulations will be conducted in future study.

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Particle Pair Dispersion in a High-Speed Premixed Flame

Ryan Darragh, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Colin Towery, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Particle pair dispersion has long been of interest and studied in non-reacting flows, primarily homogeneous

isotropic turbulence. Theory developed in these non-reacting flows describes how quickly fluid particles separate in time and has produced Richardsons well-known 4/3rds law which has since been described using the classical turbulence theory of Kolmogorov. An analysis of particle pairs is conducted in a high Karlovitz number premixed flame using an unconfined domain direct numerical simulation. The results suggest that Richardsons theory, and thus Kolmogorovs theory still applies at this large Karlovitz number.

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On Approximate Bayesian Computation Approach for Turbulence Model Development

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

Approximate Bayesian computation (ABC) is used in this study to estimate unknown model parameter values, as well as uncertainties, in a nonequilibrium anisotropy closure for Reynolds averaged Navier-Stokes (RANS) simulations. The ABC approach does not require the direct computation of a likelihood function, thereby enabling substantially faster estimation of unknown parameters as compared to full Bayesian analyses. The approach also naturally provides uncertainties in parameter estimates, avoiding the artificial certainty implied by optimization methods for determining unknown parameters. Details of the ABC approach are described, including the use of a Markov chain Monte Carlo technique to accelerate the parameter estimation. Nonequilibrium turbulence model parameters are estimated based on turbulence kinetic energy reference data for sheared homogeneous turbulence. The ABC method is shown to yield parameter values for the nonequilibrium anisotropy closure that provide a good agreement between model results and the reference data.

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Deep Learning for In-Situ Data Compression of Large CFD Simulations

Andrew Glaws, *National Renewable Energy Laboratory*
Ryan King, *National Renewable Energy Laboratory*
Mike Sprague, *National Renewable Energy Laboratory*

The ExaWind project seeks to develop blade-resolved LES simulations of wind turbines for next-generation exascale computing architectures. Such simulations expect to generate data with at least O(10^9) degrees of freedom and O(10^5) time steps. Due to this large amount of data, significant computational resources must be dedicated to data storage, visualization, and analysis. In many cases, performing these tasks on the full dataset is intractable, prompting the need for in-situ data compression. The singular value decomposition (SVD) is the standard matrix compression approach; however, the linear nature of the low-rank approximation limits its ability to reconstruct highly nonlinear flow data. In this work, we explore deep learning methods for in-situ data compression and reduced order modeling. In particular, we develop a deep convolution autoencoder network that learns nonlinear relationships in the data that map 3D turbulent flow fields to a low-dimensional latent space, yielding better performance than single-pass SVD-based approaches. We compare these two data compression techniques in lossy restart studies where a flow simulation is checkpointed and restarted. Such a scenario is typical of the computationally intensive LES simulations resulting from the ExaWind project.

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Influence of Surging Flow Frequency on Lift Coefficient for Finite Wings

Dasha Gloutak, *Aerospace Engineering Sciences, University of Colorado, Boulder*
Emanuele Costantino, *Aerospace Engineering Sciences, University of Colorado, Boulder*
John Farnsworth, *Aerospace Engineering Sciences, University of Colorado, Boulder*

Surging flows at different frequencies influenced the behavior of instantaneous lift coefficient for semi-span, NACA 0015 wings. At a mean Reynolds Number of 100,000, the wind tunnel gusting flow followed an approximate sinusoidal profile at frequencies of 0.1, 0.5 and 1.0 Hz. Lift coefficients were calculated from hot wire anemometer velocity measurements and aerodynamic forces obtained from the load cell, installed

on the wing root. For attached flows, the data revealed a quasi-steady lift response to the 0.1 Hz gust, and an unsteady lift response with local peaks for 0.5 and 1.0 Hz gusts. At stall, the lift coefficient for 0.1 and 0.5 Hz gusts plateaued periodically, indicating periods of reattachment in a largely separated flow. The timing and amplitude of these maxima demonstrated a lift dependence on both frequency and gusting phase.

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Initial Verification of a Reduced Combustion Model of Douglas Fir

Jeffrey Glusman, *Mechanical Engineering, University of Colorado, Boulder*
Kyle Niemeyer, *School of Mechanical, Industrial, and Manufacturing Engineering, Oregon State University*
Amanda Makowiecki, *Mechanical Engineering, University of Colorado, Boulder*
Nicholas Wimer, *Mechanical Engineering, University of Colorado, Boulder*
Caelan Lapointe, *Mechanical Engineering, University of Colorado, Boulder*
Gregory Rieker, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*
John Daily, *Mechanical Engineering, University of Colorado, Boulder*

New skeletal chemical kinetic models have been created by reducing a detailed model for the combustion of Douglas Fir pyrolysis products. These skeletal models are intended to reduce the cost of high-fidelity wildland fire simulations, while incurring minimal changes in accuracy. The detailed model contains 137 species and 4,533 reactions and is reduced via the directed relation graph with error propagation and sensitivity analysis methods, followed by further reaction elimination. Three skeletal models were produced with each at varying levels of accuracy: a 71 species, 1,179 reaction model with 1% error, a 54 species, 637 reaction model with 24% error, and a 54 species, 204 reaction model with 80% error when compared to the detailed model. Using the skeletal models, the peak temperature, volumetric heat release rate, premixed laminar flame speed, and diffusion flame extinction temperatures are compared with the detailed model, revealing an average maximum error of these metrics to be less than 1% for the larger model, 10% for the intermediate model, and 24% for the smaller model. Therefore, all three skeletal models are sufficiently accurate and efficient for use in high-resolution wildfire simulations, where other model errors and uncertainties are likely to dominate.

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Development and Application of a Thin Flat Heat Pipe Design Optimization Tool for Small Satellite Systems

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

With easier access to space and the increasing integration of power-dense components, small-scale thermal management solutions are in-demand for small satellite systems. Due to the strict mass and volume requirements commanded by such power-dense small spacecraft, heat pipes with thin and flat architectures provide a nearly ideal solution for the efficient transfer and dissipation of heat. Unlike traditional heat pipes, however, the performance of thin heat pipes is heavily dependent on detailed internal parameters, including the vapor core geometry and structural mechanics characteristics. In this study, the development and testing of a new computational modeling and optimization tool for the design of thin heat pipes is presented. The computational model is described in detail and includes parameters that define properties of the liquid wick, vapor core, and structural case. This model is coupled to a gradient-based optimization procedure that minimizes a multi-objective cost function expressed as a weighted sum of the total temperature drop, maximum heat dissipation, mass, and structural deflection for a range of operating conditions. The model is then used to optimize the design of a copper-methanol flat heat pipe applied to a small satellite mission. The flat heat pipe design is optimized with respect to both cold and hot orbital conditions.

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Direct Numerical Simulation of Unsteady Mixing in Direct Contact Membrane Distillation Systems with Membrane Spacers

Jacob Johnston, *Mechanical Engineering, Colorado School of Mines*
Jincheng Lou, *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 spacers play a significant role in these processes by affecting fluid flow and reducing flux limiting phenomena such as concentration polarization and temperature polarization. To date, computational fluid dynamics studies of spacers have been limited by the fact that most commercial computational fluid dynamics software uses body-fitted grids to simulate spacer surfaces. Such grids are time consuming to build, and limit the number of spacer geometries that can be considered. Thus motivated, we leverage recent advances in immersed boundaries to develop a method of simulating spacers without body-fitted grids. Rather, the method uses simple Cartesian grids that nevertheless recover the same order of accuracy as traditional grids. We show that the method accurately simulates not only the no-slip condition for the fluid flow, but also the advection of heat and salts near the spacer surface interface, which are often tricky to simulate. Using our method, we simulate heat and mass transport in a direct-contact membrane distillation system with spacer elements in both the feed and distillate channel.

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On a Class of High-Order, Low-Cost Time Integrators for the Navier-Stokes Equations

Mokbel Karam, *Chemical Engineering, University of Utah*
Tony Saad, *Chemical Engineering, University of Utah*

Pressure projection methods are used to enforce mass conservation for the incompressible Navier-Stokes equations by decoupling the velocity from the pres- sure using a predictor-corrector technique. This technique consists of two steps: first, advance the momentum equations in time without satisfying mass conservation, then correct the resulting velocity field by finding a pseudo pressure that enforces continuity. The correction step results in a Poisson equation for the pressure whose solution requires the use of a global linear solver. In the context of high-performance computing, the use of global linear solvers is known to be detrimental to parallel performance and scalability due to the global communication requirements across compute nodes. One strategy to hide the communication cost of linear solvers is to increase computation to achieve higher arithmetic intensity (ratio of computation to data transfers). Increased arithmetic intensity can be achieved by increasing time accuracy. For fluid flow simulations, this entails embedding projection methods within high-order integrators such as Runge-Kutta schemes. However, these necessitate solving the Poisson equation at each intermediate stage of the Runge-Kutta integrator, which in turn increases communication and defeats the intended purpose. In this work, we propose a time-accuracy analysis framework that enables us to rationally reduce the number of Poisson solves within a time-step while maintaining a formal order of accuracy. For example, we will show that with a proper combination of pressures from previous time-steps, one pressure Poisson equation is needed for second and third-order Runge-Kutta schemes. This results in savings of up to 50% in the cost of a single time-step. We also evaluate the impact of skipping projections on stability and show that there is a fine balance between stability and computational cost.

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Towards a Reduced Biogeochemical Flux Model for Large Eddy Simulations of the Upper Ocean

Skyler Kern, *Mechanical Engineering, University of Colorado, Boulder*
Katherine Smith, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*
Marco Zavaterelli, *Physics and Astronomy, University of Bologna*
Nadia Pinardi, *Physics and Astronomy, University of Bologna*

We are unable to simulate the entire global climate system due to limitations on our computational abilities. Current Earth System Models (ESMs) have to parameterize small scales, which can not be resolved. An important area of investigation is the interaction between upper ocean dynamics and biogeochemical processes that occur on these parameterized scales. The problem is current biogeochemical models have been developed primarily for ESMs and therefore are not ideal for coupling with small scale physical models. To confront this issue a new Biogeochemical Flux Model with 17 state variables (BFM17) has been developed by reducing the full Biogeochemical Flux Model. To reduce the computational cost and focus on open ocean settings, the full BFM was reduced by eliminating certain processes - including benthic, silicate, and iron influences- and parameterizing others, such as the bacterial loop. BFM17 was coupled with the one-dimensional Prince Ocean Model (POM1D) for calibration and validation against observational data from the Sargasso Sea. A sensitivity study and optimization were performed with BFM17 + POM1D. The results generally showed better correlations between model results and observational data and smaller errors compared to previous attempts.

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Efficient Simulation of Complex Fire Phenomena

Caelan Lapointe, *Mechanical Engineering, University of Colorado, Boulder*
Nicholas Wimer, *Mechanical Engineering, University of Colorado, Boulder*
Jeff Glusman, *Mechanical Engineering, University of Colorado, Boulder*
Amanda Makowiecki, *Mechanical Engineering, University of Colorado, Boulder*
John Daily, *Mechanical Engineering, University of Colorado, Boulder*
Greg Rieker, *Mechanical Engineering, University of Colorado, Boulder*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

Wildland fires are an increasingly dangerous and costly phenomena, motivating studies focused on wild fire mitigation and suppression. However, large-scale experiments can be infeasible, making computational studies appealing. However, computational studies of wild fire can be difficult in part due to physical scale separation; length scales range from the fine scales of reactions and turbulence (sub-milimeter scale) to large scales characteristic of topographical variation and the atmospheric boundary layer (kilometer scale). Novel computational techniques are required to make computational studies tractable. In this talk, we use adaptive mesh refinement (AMR) to increase fidelity in regions of interest (e.g. a propagating flame front) and concentrate power where it is needed. Capability for efficient simulation of turbulent diffusion is demonstrated, and progress towards simulation of kilometer-scale fire spread is highlighted.

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Combustion and Droplet Behavior of JP-8 Surrogates in a Two-Phase Reacting Flow

Stephen Lucas, *Mechanical Engineering, Colorado State University*
Bret Windom, *Mechanical Engineering, Colorado State University*
Radi Alsulami, *Mechanical Engineering, Colorado State University*

Typical jet fuels can have hundreds of individual hydrocarbon species with varying physical and combustion properties; thus, computational modeling of jet fuel combustion is not currently feasible. Surrogate fuels containing mixtures of 3 - 4 species have been developed to emulate the behaviors of the parent fuels, but these surrogates are typically developed using either thermophysical properties or gas-phase combustion properties, without accounting for the two-phase combustion present in most real applications of jet fuel combustion. This work explores the ability of published surrogate fuels to emulate the behavior of the parent JP-8 fuel in an annular co-flow spray burner. Basic behaviors such as flame liftoff and lean blowout are compared to the parent at the same flow conditions. In addition, using a combination of CH* radical fluorescence imaging and Mie scattering, droplet distribution both with and without combustion is analyzed in order to determine whether the surrogates will reasonably emulate real two-phase combustion of the parent fuel.

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Fluid Dynamic Forces Affect the Spatial Distribution of Cellular Injury During the Progression of Ventilator-Induced Lung Injury

Courtney Mattson, *Bioengineering, University of Colorado, Anschutz*
Kayo Okamura, *University of Colorado, Denver*
Matthew Kiselevach, *University of Colorado Denver*
Bradford Smith, *Bioengineering, University of Colorado, Denver*

Acute respiratory distress syndrome (ARDS) is characterized by airspace edema fluid, surfactant insufficiency, and alveolar collapse. ARDS requires mechanical ventilation (MV) to maintain proper gas exchange. MV exacerbates ARDS through fluid-mechanical forces within the lung via ventilator-induced lung injury (VILI). In order to reduce the 40% mortality rate of ARDS, we must understand the temporal evolution of injury during VILI progression. We hypothesize that injury and edema will start in high stress locations; these injured areas will create stress foci that make proximal areas highly susceptible to further injury. Mechanically ventilated mice were prepared for microscopy; injured cells were labeled with propidium iodide. Animals were ventilated until respiratory system elastance increased to three predetermined levels. Whole-slide imaging used in combination with customized cell detection algorithms yield high-resolution maps detailing the locations of all injured cells. Various metrics, including voronoi tessellations and radial density functions were used to determine the spatial dependence of injury. Our metrics inform us that injury tends to form in initially small clusters that expand as VILI progresses. Heterogeneous distribution of injury is affected by the heterogeneous distributions of strains throughout the lung tissue. Fluid accumulation and increased surface tension in injury foci cause inhomogeneous distributions of air, which influence the strain distribution.

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Synthetic Turbulence Generation Method to Simulate Turbulence Generating Plates

Michael Meehan, *Mechanical Engineering, University of Colorado, Boulder*
Ankit Tyagi, *Mechanical and Nuclear Engineering, Pennsylvania State University*
Jacqueline O'Connor, *Mechanical and Nuclear Engineering, Pennsylvania State University*
Peter Hamlington, *Mechanical Engineering, University of Colorado, Boulder*

In many practical engineering applications, turbulence plays a large role in flow development, such as boundary layers, heat transfer processes, and intermittent phenomena. Understanding and predicting these changes as a result of turbulence is of utmost importance to constructing more effective, efficient, and innovative devices. To quantify changes as a result of turbulence, experimental techniques have been developed to increase turbulence intensities, most notably the use of turbulence generating plates where perforated sheets are installed inside the experimental apparatus. This methodology has been found effective in many situations, but the analyses could be enhanced by complimentary simulations that have access to the full three-dimensional field and the ability to explore a wider variety of parameters that may be extremely difficult experimentally. Here, we implement a technique in a block-structured adaptive mesh code that approximately represents the turbulence generated by the perforated sheets without requiring an explicit simulation of the internals of the experiment. The technique relies on the fact that turbulence approximately decays exponentially spectrally and temporally. Computational data is compared directly with experimental data of a slot jet.

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Azeotrope Formation During the Evaporation Process of Fuel Blends

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The transportation sector is currently the largest source of greenhouse gas emissions in the United States primarily due to the usage of petroleum-derived gasoline and diesel fuels. In response, researchers are studying various fuel blends to determine feasible alternatives to traditional petroleum-based blends. Several potential fuels include high percentages of ethanol. Ethanol has a higher octane number than gasoline, and therefore, greater knock resistance. The increased knock resistance of ethanol has the potential to improve the efficiency and performance of future direct-injection spark-ignition engine designs. The presence of ethanol in fuel blends, however, has tended to correlate with greater particulate matter emissions in previous research, though there is a lack of understanding of the cause of this phenomenon. A hypothesis is that ethanols high heat of vaporization (HOV) relative to gasoline, and the fact that it forms a highly non-ideal solution with hydrocarbons, are slowing the evaporation of heavy aromatics in gasoline leading to increased particle formation in the resulting fuel-rich regions of the fuel-air charge. The objective of this research is to examine how ethanol and other alcohols impact the evaporative process of various fuel blends including how the formation of azeotropes impacts the evaporation rate and the heat of vaporization. Mass spectrometry was

also used to study the evaporation of fuel components. The results of this research are pending.

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New Fluid Flow Data Assimilation Formulations Using Perceptual Loss Networks

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A common problem in fluid dynamics is inferring a flow field that balances sparse observations and a forward model with simplified physics. Typical approaches to solving this problem involve Bayesian inference or gradient-based optimization of a regularized loss function. Here we introduce a new data assimilation approach that includes a perceptual loss network (PLN) as an additional regularization term in the objective function. Perceptual loss networks are pretrained deep convolutional neural networks that identify a sophisticated hierarchy of features in a given dataset. These PLNs can be used to identify the "style or "content of input fields from activations at different layers in the network. For data assimilation, we use the PLN to add a style to our inferred velocity field that reflects physical properties not explicitly incorporated in the forward model but observed elsewhere, e.g. higher fidelity models. In this talk we present the formulation of this new data assimilation problem and discuss challenges and implications of this approach. We also provide preliminary results for inferring a wind farm flow field that incorporates sparse observations, a Reynolds-Averaged Navier Stokes (RANS) forward model, and a large eddy simulation (LES) style.

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Inflow Boundary Conditions for Scale Resolving Simulations

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While it is possible to compute transition using Direct Numerical Simulation (DNS) of the Navier-Stokes equations, the cost to reach Reynolds numbers of practical interest is very high. To reduce the cost and/or extend DNS to high Reynolds numbers motivates the investigation of unsteady inflow boundary conditions that circumvent the need to compute transition. It is important that these boundary conditions will admit physically realistic behavior some short development length downstream. A particular implementation of the synthetic turbulence generator (STG) method for unsteady inlet conditions is described. Furthermore, results from the application of this STG method to a DNS of a zero pressure gradient flat plate turbulent boundary layer are discussed. The successes obtained on flows in the incompressible regime motivates the extension of STG to compressible, high Mach number boundary layers

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Fine-Wire Sensor Calibration System for Low Velocity Flows at Stratospheric Conditions

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An open-circuit wind tunnel, developed to calibrate balloon-borne hot-wire anemometers and cold-wire thermometers, is described. The fine-wire instruments are designed to measure velocity and temperature fluctuations associated with turbulence through the middle to upper stratosphere. The system is designed to reproduce thermodynamic conditions for sensor calibration over an approximate altitude range of 20-40 km, with a pressure range of approximately 5,500 Pa (41.3 Torr) to 275 Pa (2.06 Torr), and with a minimum air temperature of 210 K (-63.2 C) achieved to date. The fine-wire instruments are lofted on balloons with measurements taken during a slow descent from the maximum altitude at speeds targeted between 2 m/s and 10 m/s. The velocity profile in the tunnel calibration plane was predicted analytically for fully-developed, axisymmetric Poiseuille flow and is currently being verified using a factory-calibrated 5

μm hot-wire anemometer. Numerical simulations of the flow field were used to quantify distortions in the velocity profile due to probe blockage effects. The accuracy of the flow velocity at the calibration plane is calculated as a function of test conditions and discussed in addition to the operating modes of the system.

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Capturing a Blade Tip Vortex

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Blade-resolved simulations of wind power plants will allow engineers better understanding of the ramifications of design decisions, like a proposed control strategy or turbine arrangement. The blade tip vortex is an important dynamic in wind power plant models, as it affects the wake, which may impact the power production or fatigue damage of downstream turbines. In this study, we simulate a rectangular and untwisted NACA 0015 wing using the Nalu-Wind computational framework and compare our results to a wind tunnel experiment. We examine the sensitivity of the computed tip vortex dynamics to the turbulence modeling approach, experimenting with the Menter Shear Stress Transport Reynolds-Averaged Navier-Stokes model, implicit large eddy simulation, and detached eddy simulation, which is a blend of large eddy simulation with the Menter model.

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Numerical Simulations of the Supercritical Carbon Dioxide Round Turbulent Jet

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We explore the fundamental connection between properties of a supercritical fluid and observed behavior of the flow by comparing simulations of a supercritical carbon dioxide (sCO2) round jet to canonical simulations using an ideal gas model. sCO2 has desirable behavior that can improve power density compared to traditional fluids for applications involving closed-cycle gas turbines, heat transmission, and hydraulic fracturing while facilitating carbon sequestration. While literature exists focusing on the prospects of sCO2 in various industries, the quantities of interest studied tend to be application specific whereas our investigation generalizes across multiple applications. The Soave-Redlich-Kwong equation of state is utilized to close our system of equations; we use a second order finite volume method in conjunction with adaptive mesh refinement as implemented in PeleC. The jet is at $p = 10$ MPa and $T = 600$ K in order to maintain a single-phase fluid. Quantities of interest for this study include the mean axial velocity and Reynolds stresses.

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Sparse Identification of Non-linear Dynamics for an Unsteady Pitching Wing Section

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Stall flutter is a cyclical aeroelastic phenomena created by the geometric coupling of structural and aerodynamic forces experienced by an unsteady pitching airfoil. A experimental model has been developed to

study this behavior through mimicking the dynamic response of a elastic wing. This system, described as ”cyber-physical”, is composed of a solid wing section driven by a closed-loop controlled motor that utilizes angular encoder information to command the model to act as a rotational single degree of freedom system. It was noticed that the response of the wing had discrepancies compared to its prescribed performance. This investigation used a linear regression technique as well as the method of Sparse Identification of Non-linear Dynamics (SINDy) to quantify and compare the experimental response to that for an ideal second order linear system. This analysis identified significant over-damped behavior due to non-linear friction in the mechanical components of the system. This insight has helped inform a redesign of the model to improve accuracy in future experimental flutter investigations.

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Transient, High Pressure Oil-gas Dilution Study

Jesse Schulthess, *Mechanical Engineering, Colorado State University*
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Natural gas, to be a useful commodity, must be transported hundreds or sometimes even thousands of miles from the well site to the consumer. This transmission process requires the use of compressors which must be lubricated to prevent wear of their moving parts. The lubricants used in these compressors have a tough job as they are exposed to natural gas which is highly soluble in common, oil-based lubricants. As natural gas components dissolve into the lubricant, the lubricant experiences a decrease in viscosity necessitating the use of more lubricant. This study is investigating the time it takes for natural gas to dilute different lubricants under varying conditions. This measure of the viscosity decease over time will be used to optimize lubrication rates for natural gas compressors.

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Mechanics and Efficiency of Zebrafish 30HPF Heart

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Deborah Garrity, *Biology, Colorado State University*
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The heart is the first organ to function in vertebrates, initiating contractions shortly after heart tube fusion. Immediately after formation, the valveless heart tube is able to drive blood forward throughout the embryonic body through a series of contractions initiated by a confluent monolayer of myocardial cells. This layer compresses a layer of cardiac jelly that is sandwiched by the myocardium and endocardium. The valveless pumping mechanism at this stage has received significant attention over the past decade where studies have investigated the potential of peristalsis or impedance pumping, by studying contractile mechanics and blood flow. However, mechanical properties of this stage are rarely considered, limiting the ability to identify the pumping mechanism. Here, we have developed a computational Multiphysics model to study the interplay between mechanical properties, contraction, and blood flow. We validate our results through experiments involving a zebrafish heart (30 hpf).

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Simulation of Low-Temperature Helium Flow in a Heated Microchannel

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Helium is a natural cryogenic material that acts as a refrigerant in various superconducting applications

such as quantum computers, superconducting electronics and magnets, and shielding of magnetic fields. At cryogenic temperature, properties such as density, viscosity, and specific heat varies significantly within 3 K. Initial simulations in the supercritical fluid regime are preformed using the PeleC computational fluid dynamics code with Soave-Redlich-Kwong (SRK) equations of state. These results are used as baseline results for the effects of property variations. We perform these simulations of the laminar flow of liquid hydrogen in rectangular microchannels at the standard pressure while decreasing the temperature to approach the "lambda point (2.17 K). The hydraulic diameters of our microchannel are in the range of 100 - 1000 μm. Future simulations will incorporate the NIST REFPROP package to improve the accuracy of properties beyond the SRK equation of state.

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An Efficient Proper Orthogonal Decomposition Algorithm for Adaptively Refined Meshes

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Michael Meehan, *Mechanical Engineering, University of Colorado, Boulder*
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Proper orthogonal mode decomposition (POD) is used to reduce the order of a dynamical model by decomposing its spatio-temporal data into orthonormal basis functions, or modes, that are optimal in capturing the most amount of variance in the fewest number of modes. In the study of turbulence, POD can be used to identify coherent structures or develop reduced-order models. We develop an algorithm that computes POD on block-structured adaptively refined meshes that have been interpolated to uniform meshes using nearest neighbor interpolation. This new algorithm leverages the repeated solution values to reduce the number of operations performed. We present the performance results of this algorithm on synthetically generated data to demonstrate the strengths and weaknesses of the algorithm and establish criteria for its optimal use on real simulation data.

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A Microfluidic Model of Bleeding to Probe the Fluid Mechanics and Biochemistry of Bleeding Disorders

Matt Sorrells, *Hematology / Oncology, University of Colorado, Anschutz*

Hemophilia and Von Willebrands disease are two common bleeding disorders that affect roughly 1% of the worlds population. Both of these disorders are issues in hemostasis the stoppage of blood flow out of an injury to a blood vessel. These diseases arise from the deficiencies of certain proteins that are critical to hemostasis. Though the primary causes of these diseases are well known, other variations in biophysical and biochemical parameters make predicting bleeding risk for patients with mild to moderate deficiencies near impossible. Microfluidics offer a highly controlled environment to study hemostasis in, where the biochemistry and fluid mechanics relevant to certain clotting events can be reproduced and finely controlled manner. However, to date most microfluidic models used for these purposes model thrombosis, or the buildup of a blood clot in a closed vessel akin to a heart attack or a deep vein thrombosis (DVT). Here we have developed a microfluidic model of hemostasis that mimics the fluid mechanics observed in bleeds associated with hemophilia and VWD and demonstrates physiologically accurate hemostatic behavior. We incorporated a novel use of flow meters to track the flow of blood across our hemostatic device, allowing us to obtain real time measurements of the hydraulic permeability of blood clots forming under flow. Finally, we used a genetic algorithm coupled with a hydraulic circuit model to successfully design an advanced generation of hemostatic models, in which we can precisely manipulate device designs to finely the effect of key biophysical parameters.

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Physics-Informed Super-Resolution of Climatological Wind Data

Karen Stengel, *Complex Systems Simulation and Optimization, National Renewable Energy Laboratory*
Andrew Glaws, *National Renewable Energy Laboratory*
Ryan King, *National Renewable Energy Laboratory*

Many aspects of modern societyincluding agriculture, transportation, emergency preparation, and resource planningrely on high resolution (HR) weather and climate data. However, due the complex nature of weather and climate models, HR meteorological data is only available at local scales and even low resolution (LR) global climate models (GCM) are extremely computationally expensive. In this work, we apply a deep learning image transformation technique, known as super-resolution (SR), to enhance GCM wind velocity data. Our model, based off of the SRGAN model, is trained on coarsened wind velocity data from the Wind Integration National Dataset (WIND) Toolkit. Wind resource planning would greatly benefit from having GCM data at a comparable resolution to the WIND Toolkit. The model successfully increased the spatial resolution of the data 50x while preserving the underlying physics. When applied to the global wind velocity data from the National Center for Atmospheric Researchs Community Climate System Model (CCSM), our trained model was able to generate perceptually-realistic and physically-consistent wind velocity data fields at 2km resolutions from the original 100km resolution that preserve a number of turbulent flow physics like energy spectra and velocity gradients.

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Detonation Initiation by Compressible Turbulence Thermodynamic Fluctuations

Colin Towery, *Mechanical Engineering, University of Colorado, Boulder*
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Theory and computations have established that thermodynamic gradients created by hot spots in reactive gas mixtures can lead to spontaneous detonation initiation. However, current theory and models are restricted to the prediction of detonations in quiescent gases with isolated hot spots formed on timescales shorter than chemical and acoustic timescales. In this work, we adapt current theory in order to predict spontaneous detonation initiation by thermodynamic gradients resulting from compressible turbulence fluctuations. Compressible turbulence forms non-monotonic temperature fields with tightly spaced local minima and maxima that evolve over a range of timescales, including those much larger than chemical and acoustic timescales. We examine the utility of the adapted hot-spot scaling laws through direct numerical simulations of compressible isotropic turbulence in premixed hydrogen-air reactants for a range of conditions. We find strong evidence of spontaneous detonation initiation due to turbulence-induced thermodynamic gradients in a regime similar to that predicted by established theory for isolated laminar hot spots.

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Computational Fluid Dynamics of a Heavy Hydrocarbon Direct Injected Unmanned Aerial Vehicle

Miguel Valles Castro, *Mechanical Engineering , Colorado State University*
Siddhesh Bhoite, *Mechanical Engineering, Colorado State University*
Bret Windom, *Mechanical Engineering, Colorado State University*
Anthony Marchese, *Mechanical Engineering, Colorado State University*

The US military has identified heavy hydrocarbon fuels like JP-8 as viable candidates to meet their Single-Fuel Policy (SFP). However, by implementing JP-8, into a traditional gasoline Unmanned Aerial Vehicle engine, abnormal combustion with knocking and pre-ignition are significant issues due to its higher reactivity and reduced volatility compared to gasoline. Stratified combustion presents a possible solution to reduce the probability of engine knock by promoting conventional combustion propagation from the point of ignition down to the piston without autoignition of the end-gas. Stratified combustion is achievable by modifying and shortening the duration of a fuel injector. Through CFD modeling, a computational study was carried out to demonstrate unstable combustion with premixed JP-8 fuel in the 3w-28i engine and to test the potential for stratified combustion to mitigate knock. With a spray pattern of four injections at a 20μm droplet size with low pressure, a reasonable reduction in knock was observed. This work shows that novel fuel injector technology may be able to promote optimized stratified combustion and help reduce the severity of knock with JP-8 in small UAV combustion platforms.

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Fluid Mechanical Forces in a Sepsis Mediated Model of Ventilator-Induced Lung Injury

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

The surface tension of the alveolar lining fluid is lowered by pulmonary surfactant so that the alveoli may inflate and deflate without collapsing. Acute respiratory distress syndrome (ARDS) is characterized by pulmonary edema and high surface tension and, as such, mechanical ventilation is a necessary lifesaving therapy. However, ventilator-induced lung injury (VILI) occurs when mechanical ventilation generates or exacerbates lung injury. VILI is caused by fluid-mechanical forces that damage the delicate cells that line the airways and alveoli, resulting in alveolocapillary barrier injury and accumulation of proteinaceous fluid in the airspace. This instigates a positive feedback mechanism of leak, surfactant inactivation, deranged mechanics, and VILI. To study VILI in the context of sepsis-mediated ARDS, healthy mice were exposed intratracheally to endotoxin (ETX) to elicit an inflammatory response. One day post-exposure, mice were mechanically ventilated to cause VILI. Lung mechanics were evaluated with the forced oscillation technique (FOT) before and after the ventilation period. The FOT applies a sinusoidal waveform to analyze resulting pressure and volume signals, ultimately revealing mechanical information about the lung. These sensitive measurements are not enough to distinguish the ETX from control group. However, disruption of the microscale stress balance in the ETX exposed lungs causes leak, inflammation and elevated bronchoalveolar protein that is not present in untreated controls. As such, the ETX exposed mice are more susceptible to the fluid-mechanical stresses of VILI.

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Simulation of Bluff-Body-Stabilized Flames Using PeleC, a Combustion Code for Exascale Computing

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

Flame stabilization is important for maintaining steady combustion in gas turbines. However, computational combustion models do not capture the dynamic complexity of stabilized flames with sufficient generality, limiting attempts to improve turbine performance. To understand this complexity and provide validation data, we adapt PeleC, an exascale compressible combustion code, to Blue Waters to develop direct numerical simulations of stabilized reacting and non-reacting flows surrounding a triangular bluff body, currently under experimental investigation. Adaptive mesh refinement (AMR) is incorporated via the AMReX block-structured framework to locally resolve the physics of interest at reduced cost compared to static mesh approaches. We show results of a convergence study for the non-reacting case and preliminary work from the reacting case, in which heat release interacts with shear-layer instabilities and vortex formation in the wake. AMR is necessary to accurately resolve the interactions among shear-layer, vorticity dynamics, reaction-rate chemistry, and flame formation at a computationally manageable cost.

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Simulation of High Rayleigh Number Natural Convection Flows using a Central Moment Lattice Boltzmann Method on a Rectangular Grid

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

Numerical simulation of flows with heat transfer efficiently has gained much recent attention with the need to enhancing the performance in engineering applications. In this work, we will develop and employ an effective lattice Boltzmann (LB) approach to simulate natural convection flows at high Rayleigh numbers. We will present a LB scheme based on central moments and multiple relaxation times on a two-dimensional, nine velocity (D2Q9) rectangular lattice for flows with heat transfer. In this regard, we will extend the equilibrium moments by including corrections that restore the isotropy in correctly recovering the Navier-Stokes equations and the energy equation for LB simulations on a stretched grid. A consistency analysis is

performed and the model parameters are derived via a Chapman-Enskog multiscale expansion. Preliminary results of natural convection in a square cavity at Rayleigh number up to 109 are presented.

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Updating High Temperature Methane Absorption Models Using Dual Comb Spectroscopy Data

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The presence of methane in exoplanetary atmospheres is considered a potential biomarker in the search for extraterrestrial life. Proper identification of methane and characterization of thermodynamic properties from exoplanet transit spectra (when exoplanets pass in front of a star and imprint their atmospheric absorption fingerprint on the starlight) requires accurate lineshape models. Currently, there are near-infrared methane bands in commonly used linelist models such as HITRAN that still need to be validated with experimental data that span temperature ranges useful to exoplanetary research. This presentation will present experimental spectra taken with dual frequency comb spectroscopy (DCS) in the 6770 - 7190 cm-1 region. DCS is an emerging form of laser absorption spectroscopy that can cover large spectral regions with an extremely stable frequency axis resulting in highly accurate, high bandwidth spectra. DCS light was sent through a furnace containing a cell of high purity methane at temperatures spanning room to 770 K and pressures from 18 torr to room. Linelist parameters were then updated using a multispectral fitting procedure. Results will be presented with an emphasis on updated lower state energies, line strengths, and self-broadening parameters.

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