Rocky Mountain Fluid Mechanics Research Symposium 2017: Technical Program

Sustainability, Energy and Environment Complex (SEEC)
University of Colorado Boulder
August 11$^{\text{th}}$, 2017

Keynote Presentation

Dr. P.K. Yeung, (8:45 AM - 9:45 AM)
Turbulent Mixing and High Performance Computing

Presentation Schedule

Session 1A: Geophysical and Astrophysical Fluid Dynamics
10:15 AM - 12:00 PM (Room A)

10:15 AM Joe Werne (NorthWest Research Associates, CoRA Office, Boulder, CO)
Instability, Evolution, and Mixing in Stratified Shear Flow as a Function of Richardson Number

10:30 AM Amrapalli Garanaik (Colorado State University, Fort Collins, CO)
Assessment of Small Scale Anisotropy in Stably Stratified Turbulent Flows

10:45 AM Scott Wieland (University of Colorado, Boulder, CO)
Background Stratification Effects on the Compressible Rayleigh-Taylor Instability

11:00 AM Stefano Maffei (University of Colorado, Boulder, CO)
Multiscale Numerical Simulations of Magnetoconvection at Low Magnetic Prandtl and Rossby Numbers

11:15 AM Warren Smith (University of Colorado, Boulder, CO)
The Role of Radiation in Accelerating the Genesis of Atlantic Hurricane Matthew

11:30 AM Scott Bachman (National Center for Atmospheric Research, Boulder, CO)
Parameterizing the Ocean Boundary Layer Beyond 1D

11:45 AM Katherine Smith (University of Colorado, Boulder, CO)
Effects of Langmuir Turbulence on Upper Ocean Carbonate Chemistry

Session 1B: Wings and Jets
10:15 AM - 12:00 PM (Room B)

10:15 AM Ethan Culler (University of Colorado, Boulder, CO)
The Influence of Second Harmonic Phase and Amplitude Variation in Cyclically Pitching Wings

10:30 AM Riccardo Balin (University of Colorado, Boulder, CO)
A Comparison of RANS Modeling Strategies for High-Lift Systems

10:45 AM Daniel Bateman (University of Colorado, Boulder, CO)
Design and Qualification of an Unsteady Wind Tunnel

11:00 AM Owen Brown (University of Colorado, Boulder, CO)
Nonreacting Buoyant Jet Validation Case

11:15 AM Siddharth Nigam (University of Colorado, Boulder, CO)
Sensitivity Analysis for an Open Catalytic Burner

11:30 AM Jason D. Christopher (University of Colorado, Boulder, CO)
Inlet Fuel Quantity Estimation for a Turbulent Buoyant Jet Using Approximate Bayesian Computation

11:45 AM Lucas Droste (University of Colorado, Boulder, CO)
Design and Qualification of an Axisymmetric Jet for Preforming Probe Calibrations

Session 2A: Optimization, Uncertainty, and Data Driven Approaches
1:00 PM - 3:00 PM (Room A)

1:00 PM Caelan Lapointe (University of Colorado, Boulder, CO)
Topology Optimization for Compressible Internal Flows

1:15 PM Steven Isaacs (University of Colorado, Boulder, CO)
Computational Modeling and Optimization of Thin Flat Heat Pipes

1:30 PM Julian Quick (National Renewable Energy Laboratory, Golden, CO)
Optimization Under Uncertainty for Wind Power Plant Wake Steering Strategies

1:45 PM Ashley Montalvo (University of Colorado, Boulder, CO)
Uncertainty Quantification from Measures of Divergence in 2D PIV Data

2:00 PM Ryan W. Skinner (University of Colorado, Boulder, CO)
Multi-Fidelity Modeling Efficiency in a Parametric Study of NACA Airfoils

2:15 PM Jolene Britton (University of California, Riverside)
Covariance computation for active subspaces applied to a wind plant surrogate model

2:30 PM Olga Doronina (University of Colorado, Boulder, CO)
Parameter Estimation for Eddy-Viscosity Model Using Approximate Bayesian Computation

2:45 PM Christiane Adcock (Massachusetts Institute of Technology, Cambridge, MA)
Data-Driven Wind Plant Flow Modeling for Atmospheric Stability

Session 2B: Fuels, Combustion, and Reacting Flows
1:00 PM - 3:00 PM (Room B)

1:00 PM Bahareh Abdollahipoor (Colorado State University, Fort Collins, CO)
Blending Effects of Hydrous and Anhydrous Ethanol on Gasoline Properties

1:15 PM Mangesh Dake (Colorado State University, Fort Collins, CO)
Considerations for CFD Simulations of a Refueling Pump Nozzle with Application to the Computer aided Engineering of a Vehicle Refueling System

1:30 PM Tianzhu Fan (University of Colorado, Boulder, CO)
Numerical Design of a Novel Microreactor to Study Short Residence Time Combustion

1:45 PM Anthony Draper (University of Colorado, Boulder, CO)
Design and Evaluation of a High-Temperature and High-Pressure Spectroscopic Cell

2:00 PM Mohammad J. Rahimi (National Renewable Energy Laboratory, Golden, CO)
Computational Fluid Dynamics Study of Industrial-Scale Aerobic Bioreactors for Biofuel Production

2:15 PM   Samuel H.R. Whitman (University of Colorado, Boulder, CO)
Dependence of Intermittency on Turbulence Intensity and Simulation Fidelity in Premixed Reacting Flows

2:30 PM   Ryan Darragh (University of Colorado, Boulder, CO)
Lagrangian Analysis of Enstrophy in Turbulent Premixed Flames

2:45 PM   Colin A.Z. Towery (University of Colorado, Boulder, CO)
Lagrangian Analysis of Premixed Autoignition in Compressible Turbulence

Session 3A: Fluid Dynamics in the Environment
3:30 PM - 5:00 PM (Room A)

3:30 PM   Aaron True (University of Colorado, Boulder, CO)
Classical and Fractal Grid Turbulence Characteristics in a Liter-Scale Oscillating Grid Tank

3:45 PM   Jian Zhou (Colorado State University, Fort Collins, CO)
Gravity Currents Propagating over a Submerged Array of Cylinders

4:00 PM   Aseperi Oladapo (Colorado State University, Fort Collins, CO)
Dynamics of Flows in River Bends

4:15 PM   Yang Guo (Colorado School of Mines, Golden, CO)
Colloid Transport In A Microfluidic Soil Analog: Population Dynamics And Single Particle Trajectories

4:30 PM   Shaken Kenzhekhanov (Colorado School of Mines, Golden, CO)
Processes During Hydraulic Fracturing Well Interference

4:45 PM   Nicholas T. Wimer (University of Colorado, Boulder, CO)
Direct Numerical Simulation of Wildland Fires at Small Scales

Session 3B: Biology, Surfaces, and Droplets
3:30 PM - 5:00 PM (Room B)

3:30 PM   Carlos Quiroz-Arita (Colorado State University, Fort Collins, CO)
Computational Study of Turbulence and Mixing in Algae Raceway Ponds: Implications of Fluid Mechanics in Algae-based biofuels Growth Models

3:45 PM   Nicholas Danes (Colorado School of Mines, Golden, CO)
Toward a Mathematical Model of Hemostasis

4:00 PM   Anudeep Pendurthi (Colorado State University, Fort Collins, CO)
Fabrication of Nanostructured Omniphobic and Superomniphobic Surfaces with Inexpensive CO_2 Laser Engraver

4:15 PM   Matthew Cackovic (Colorado State University, Fort Collins, CO)
Droplet Manipulation on a Surface using the Triboelectric Effect

4:30 PM   Eduard Benet (University of Colorado, Boulder, CO)
Deformation and Transport of Soft Colloidal Particles in Confined Networks

4:45 PM   Tong Shen (University of Colorado, Boulder, CO)
Phoretic Motion of Soft Vesicles and Droplets

Keynote Presentation

Professor P.K. Yeung[1] **(8:45 AM - 9:45 AM)**

[1] Schools of Aerospace and Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA

Turbulent Mixing and High Performance Computing

A fundamental property of turbulence is efficient mixing, which occurs via the action of velocity fluctuations breaking up large-scale non-uniformities into smaller fragments, subsequently to be smeared out by molecular diffusion. The basic physics depends on the geometry, the Reynolds number, as well as the Schmidt number which is the ratio of fluid kinematic viscosity to the molecular diffusivity of the transported substance or property. Depending on the application, the Schmidt number can vary from of order 0.01 to nearly 1000. The regime of Schmidt number of order unity is most easily studied in the laboratory, but detailed results at both very low or high Schmidt numbers are much less available. In this talk I will begin with an overview of some of the numerical and theoretical aspects of turbulent mixing, followed by a detailed discussion of recent work in the regime of very high Schmidt number. This latter regime also brings about unique challenges for direct numerical simulations which can provide rich physical insights if formulated carefully and conducted efficiently. In particular I will describe the development of a new parallel algorithm which computes velocity and scalar fields on grids of different resolution, implemented using a hybrid programming strategy which includes both distributed and shared memory parallelism, as well as graphical processor units in a heterogeneous system environment. Some thoughts about the future of high-performance computing, from Petascale to Exascale, will be offered for discussion.

Speaker Biography:
Professor P.K. Yeung joined the faculty at Georgia Tech in 1992, after post-doctoral appointments at Queen's University at Kingston (Canada) and at Pennsylvania State University. Professor Yeung's primary interests are in the use of high-resolution direct numerical simulations to study the fundamental behavior of turbulent flows with a view towards collaborative efforts in simulation and modeling, and in massively-parallel computing and Cyberinfrastructure. Topics investigated have included basic issues in Reynolds number dependence and similarity scaling, mixing with molecular diffusivity effects over a wide range of Schmidt numbers, Lagrangian fluid particles acceleration and dispersion, and the effects of uniform solid-body rotation. Current simulations, with 64 grid points and scaled up to 131072 parallel processors, are among the world's largest and are conducted on some of the world's largest supercomputers supported by the National Science Foundation (NSF) and the U.S Department of Energy (DOE). Professor Yeung has published over 50 archival journal articles, which have been cited more than 1600 times in total. He leads a four-institution Petascale Applications project supported by NSF, and served as lead organizer of an NSF Cyber-Fluid Dynamics workshop held in July 2007. He is also an Adjunct Professor in the Division of Computational Science and Engineering at Georgia Tech. He is a Fellow of the American Physical Society (elected 2006).

Presentation Abstracts

Session 1A: Geophysical and Astrophysical Fluid Dynamics
10:15 AM - 12:00 PM (Room A)

10:15 AM - Joe Werne[1] and B.A. Pettersson-Reif[2]

[1] NorthWest Research Associates, CoRA Office, Boulder, CO
[2] Forsvarets Forskningsinstitutt (FFI), NO-2027, Kjeller, Norway

Instability, Evolution, and Mixing in Stratified Shear Flow as a Function of Richardson Number

Results are reported for high-resolution direct numerical simulations of the Kelvin-Helmholtz instability and ensuing turbulence for four different values of the Richardson number: $Ri = 0.05, 0.10, 0.15$, and 0.20. Flow morphology and evolution are found to depend strongly on Ri. Whereas the lowest Ri (i.e., the least stable) case exhibits coherent KH billows, whose round cross-section and rapid solid-boy rotation stabilizes them and delays the onset of turbulence in the billow cores, perhaps ironically the highest Ri (or most stable) case displays flatter billows which transition to turbulence immediately upon billow formation, with turbulence initiated in the cores and migrating laterally as time progresses. In marked contrast, the lowest Ri, least-stable case exhibits a much more complex transition to horizontally homogeneous turbulence, characterized by a sequence of distinct steps that include 1) layered billow formation, 2) secondary instability of billow edges, 3) vigorous turbulence in the braid region between billow cores, and 4) development of turbulence in the cores. Nevertheless, despite the dramatic differences in the flow evolution and dynamics, the final states exhibit nearly identical mid- layer stability profiles and shear/buoyancy timescale ratios, N/S, providing useful guidance for layer parameterization. Here N is the Brunt-Vaisala frequeny and S is the velocity strain rate. Time evolution, flow dynamics and morphology, final layer depth, and vertical mixing are all significantly affected by Ri and will be discussed.

All simulations are initiated using a $U(z) = U_o \tanh(z/h)$ velocity profile (z is the vertical coordinate and h characterizes the initial layer depth) and a linear $T(z) = \beta z$ temperature (or density) profile. Calculations are performed using a highly accurate pseudo-spectral numerical method in which all field variables are represented by three-dimensional Fourier series. Lateral boundaries are periodic, while top and bottom boundaries are fixed-temperature, impenetrable, and stress free, and the domain size is $4\lambda \times 2\lambda \times 2\lambda$, where λ is the most-unstable KH wavelength. Derivatives are computed efficiently by wavenumber multiplication in spectral space, and non-linear terms are handled via multiplication in physical space. Time advance employs the 3rd-order Runge-Kutta time- stepping algorithm of Spalart, Moser, and Rogers. Simulations were computed using as many as $3000 \times 1500 \times 1500$ spectral modes.

10:30 AM - Amrapalli Garanaik[1] and Subhas K. Venayagamoorthy[1]

[1] Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO

Assessment of Small Scale Anisotropy in Stably Stratified Turbulent Flows

We have analyzed small scale turbulent structures and statistics in stably stratified flows using direct numerical simulations for the assessment of widely used Kolmogorov's hypothesis of small scale isotropy. Direct measurement of the small scale turbulent quantities such as the rate of dissipation of turbulent kinetic energy and the rate of dissipation of temperature variance requires nine mean square velocity gradients and three mean square scalar gradients respectively. Oceanographers measure dissipation quantities from just one gradient component for both and by invoking Kolmogorov's small scale isotropy hypothesis. Though the use of the isotropic assumption at small scales in oceanic flows is both tempting and necessary, such an assumption is likely to result in an over- or under estimation of small scale turbulent quantities for two main reasons. First, the Reynolds number for oceanic flows is not always sufficiently high enough to justify isotropy at small scales. Second, oceanic flows are strongly influenced by stable vertical stratification resulting in large scale anisotropy. In this study we have revisited the

small scale isotropy assumption in stably stratified flows and provide an estimation of departure from isotropy.

10:45 AM - Scott Wieland[1,2], Scott Reckinger[3], Peter E. Hamlington[1], and Daniel Livescu[2]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

[2] Los Alamos National Lab, NM

[3] Montana State University, Bozeman, MT

Background Stratification Effects on the Compressible Rayleigh-Taylor Instability

The Rayleigh-Taylor instability (RTI) occurs when a more dense fluid is suspended above a less dense fluid in the presence of an accelerative body force resulting in the acceleration and density gradient having opposite directions. The evolution of the classical incompressible case is well understood and researched, but investigations into the compressible case still remain incomplete. To further study the compressible RTI, wavelet based direct numerical simulations have been completed. For these simulations, an initially hydrostatic background state must be defined, but this leaves a seemingly infinite number of different conditions that could be used. To better understand the physics of the problem, it was chosen to isolate any variables possible, and thusly the initial states investigated were the isothermal, isentropic, and isopycnic states, all at a variety of stratification strengths. It was found that the isothermal stratification had the greatest impact on the instability growth and acts to slow the growth of the instability which, when the strength of the stratification is high enough, results in the instability being completely suppressed. The isentropic stratification also acts to suppress the growth of the instability, and while it does not reach complete suppression, it does lead to an exaggerated asymmetry in the comparison of the upwards and downwards motion of the RTI. Finally, the isopycnic case leads to an increased acceleration of the growth that intensifies as the strength of the background stratification is increased. These results can be understood through an exploration of the vortex dynamics occurring in the system.

11:00 AM - Stefano Maffei[1], Michael Calkins[1], Keith Julien[2], and Philippe Marti[2,3]

[1] Department of Physics, University of Colorado, Boulder, CO

[2] Department of Applied Mathematics, University of Colorado, Boulder, CO

[3] Institute of Geophysics, ETH Zurich, Switzerland

Multiscale Numerical Simulations of Magnetoconvection at Low Magnetic Prandtl and Rossby Numbers

The dynamics of the Earth's outer core is characterized by low values of the Rossby, Ekman and magnetic Prandtl numbers. These values indicate the large spectra of temporal and spatial scales that need to be accounted for in realistic numerical simulations of the system. Current direct numerical simulation (DNS) are not capable of reaching this extreme regime, suggesting that a new class of models is required to account for the rich dynamics expected in the natural system. Here we present results from a quasi-geostrophic, multiscale model based on the scale separation implied by the low Rossby number typical of rapidly rotating systems. In particular, we investigate a plane layer geometry where convection is driven by an imposed temperature gradient and the hydrodynamic equations are modified by the presence of a large scale magnetic field. Analytical investigation shows that at values of thermal and magnetic Prandtl numbers relevant for liquid metals, the energetic requirements for the onset of convection is not significantly altered even in the presence of strong magnetic fields. Results from strongly forced nonlinear numerical simulations show the presence of an inverse cascade, typical of 2-D turbulence, when no or weak magnetic field is applied. For higher values of the magnetic field the inverse cascade is quenched.

11:15 AM - Warren Smith[1] and Melville Nicholls[1]

[1] Cooperative Institute for Research in Environmental Sciences, Department of Atmospheric and Oceanic Sciences, University of Colorado, Boulder, CO

The Role of Radiation in Accelerating the Genesis of Atlantic Hurricane Matthew

Despite active study, much remains unknown about the mechanisms behind the transformation from a tropical disturbance into a tropical depression, a process known as tropical cyclogenesis. Several recent studies have found that the presence of radiation in numerical models has a very pronounced effect on accelerating tropical cyclogenesis in both idealized models and case study simulations. In idealized simulations this appears to be primarily due to a weak nocturnal transverse circulation brought about from differential heating between the cloudy disturbance and the surrounding cloud-free region. This process creates a positive feedback, thus providing a favorable environment for tropical cyclogenesis. Hurricane Matthew was a Category 5 storm that made devastating landfall in Haiti, Cuba and South Carolina in October 2016. Results will be presented from a WRF case study simulation of Hurricane Matthew's genesis near the Lesser Antilles and its early intensification. Two simulations will be considered that are identical except that one contains longwave and shortwave radiation schemes while the other does not. A comparison of these simulations will illustrate that radiation plays a critical role in the development of the tropical cyclone. Because of the socioeconomic impact of tropical systems like Matthew, it is worthwhile to understand the processes that lead to their formation and intensification so that we may improve the predictability of their track and intensity.

11:30 AM - Scott Bachman[1]

[1] National Center for Atmospheric Research, Boulder, CO

Parameterizing the Ocean Boundary Layer Beyond 1D

Next-generation ocean models are expected to routinely resolve dynamics at 1/4 degree or smaller, offering new challenges in modeling subgridscale physics. These models are entering a regime where the unresolved turbulence is less constrained by planetary rotation, requiring a paradigm shift in the way modellers construct turbulence closures. Of particular importance is the representation of submesoscale turbulence, occupying $O(1\text{-}10)$ km scales, which plays a leading role in setting the stratification of the surface mixed layer and mediating air-sea fluxes. This talk will introduce the submesoscale parameterization problem by presenting a few extant parameterizations, and will focus on a special type of fluid instability for which no parameterization has previously been developed: symmetric instability (SI). The theory and dynamics of SI will be discussed, from which a new parameterization will be proposed. This parameterization is dependent on external forcing by either surface buoyancy loss or down-front winds, which reduce potential vorticity (PV) and lead to conditions favorable for SI. Preliminary testing of the parameterization using a set of idealized models shows that the induced vertical fluxes of passive tracers and momentum are consistent with those from SI-resolving Large Eddy Simulations.

11:45 AM - Katherine Smith[1], Peter E. Hamlington[1], Kyle Niemeyer[2], Baylor Fox-Kemper[3], and Nikki Lovenduski[4]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[2] School of Mechanical, Industrial and Manufacturing Engineering, Oregon State University, Corvallis, OR
[3] Department of Earth, Environmental, and Planetary Sciences, Brown University, Providence, RI
[4] Institute of Arctic and Alpine Research, Department of Atmospheric and Ocean Sciences, University of Colorado, Boulder, CO

Effects of Langmuir Turbulence on Upper Ocean Carbonate Chemistry

Reactive tracers such as carbonate chemical species play important roles in the oceanic carbon cycle, allowing the ocean to hold 60 times more carbon than the atmosphere. However, uncertainties in regional

ocean sinks for anthropogenic CO_2 are still relatively high. Many carbonate species are non-conserved, flux across the air-sea interface, and react on time scales similar to those of turbulent processes in the ocean, such as small-scale Langmuir turbulence. In order to more accurately model the biogeochemistry of the ocean in Earth system models (ESMs), a better understanding of the fundamental interactions between these reactive tracers and relevant turbulent processes is required. In this talk, results from large eddy simulations of carbonate chemical species in the presence of realistic mixed layer ocean turbulence are presented. The simulations explore the effects of wave- driven Langmuir turbulence by solving the wave-averaged Boussinesq equations with an imposed Stokes drift velocity. Comparisons are made between simulations with time dependent chemistry, equilibrium chemistry, and no chemistry. Additionally, strength of the Langmuir turbulence is varied in order to determine a relationship between the degree of enhancement (or reduction) of carbon that is fluxed across the air-sea interface due to the presence of Langmuir turbulence. By examining different reaction chemistry and surface forcing scenarios in these simulations, the coupled turbulence-reactive tracer dynamics are connected with spatial and statistical properties of the resulting tracer fields. These results along with implications for development of reduced order reactive tracer models will be discussed.

Session 1B: Wings and Jets
10:15 AM - 12:00 PM (Room B)

10:15 AM - Ethan Culler[1] and John Farnsworth[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

The Influence of Second Harmonic Phase and Amplitude Variation in Cyclically Pitching Wings

From wind tunnel testing of a cyber-physical wing model, it has been found that the pitch trajectory for stall flutter is described by an array of higher harmonic frequencies with decaying energy content. These frequencies distort the stall flutter motion from that of a pure sinusoidal oscillation in pitch and can have a significant effect on the resulting force production. In order to understand how these higher harmonic frequencies contribute to the overall pitching moment characteristics of a wing in stall flutter, a rigid finite span wing model, with aspect ratio four, was pitched in the wind tunnel. The prescribed motion of the pitch cycle was varied by changing the amplitude ratio and phase of the second harmonic of the oscillation frequency. The second harmonic represents the second highest energy mode in the pitching cycle spectra. Pitching moment and planar particle image velocimetry data was collected. From these pitching trajectories, a significant dependence of pitching moment on both the phase and amplitude of the prescribed waveforms was found. Specifically, for the same amplitude ratio, variations in the phase produced changes of approximately 30 percent in the phase averaged pitching moment.

10:30 AM - Riccardo Balin[1], Scott Worst[1], Ryan Skinner[1], and Kenneth E. Jansen[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

A Comparison of RANS Modeling Strategies for High-Lift Systems

When performing numerical simulations of complex, fully three-dimensional, high-lift systems, the preferred turbulence modeling approach is Steady RANS (SRANS). In addition, there are two common selections for the initial conditions of the computation; 1) using free stream conditions or 2) using the solution of the flow obtained at a smaller angle of attack. SRANS computations were carried out with the PHASTA solver adopting both approaches for a series of angles of attack with the JAXA Standard Model (JSM) high-lift geometry. The results obtained indicate that the first approach can lead to more significant over-prediction of flow separation. By contrast, more accurate flow predictions were obtained restarting simulations from a smaller angle of attack. The second approach, however, suffers from the drawback of being computationally expensive if the configurations of interest are those at large angles of attack around the location of maximum lift and stall. Unsteady RANS (URANS) computations were performed of a post-stall condition for the JSM geometry using free stream initial conditions. The flow solutions obtained are of comparable accuracy of those predicted with SRANS and the second approach, however for a fraction of the computational cost.

10:45 AM - Daniel Bateman[1] and John Farnsworth[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

Design and Qualification of an Unsteady Wind Tunnel

A new upstream louver system was designed and installed on the low-speed research wind tunnel within the Experimental Aerodynamics Laboratory at the University of Colorado Boulder to dynamically impose longitudinal variations in the freestream velocity. The system consists of ten airfoil vanes, geared in five counter-rotating pairs, that are located upstream of the wind tunnel inlet. Through opening and closing the louver system, the inlet area to the wind tunnel can be rapidly varied from approximately 0 to 90% blocked area. A quasi-static evaluation of the system is being performed to determine the relationship between the reduction in inlet area and the decrease in the test section velocity. Following the quasi-static qualification, the wind tunnel response will also be assessed under dynamic operation of the

louver system, where both periodic and discrete disturbances will be studied. The velocity response of the tunnel is being measured using multiple single component hotwire anemometers to quantify both the temporal profile and spatial variation of the disturbances; as well as the speed at which they propagate through the test section. Finally, the novel unsteady wind tunnel facility will be operated in both open and closed test section configurations to impart both convectively and globally propagating disturbances. The performance of the wind tunnel system will be compared to established results from other unsteady wind tunnel facilities.

11:00 AM - Owen Brown[1] and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Nonreacting Buoyant Jet Validation Case

The Sandia National Laboratories Simple Jet case provides an experimental baseline to validate the computational fluid dynamics (CFD) solver CONVERGE. The three dimensional, non-reacting, turbulent, buoyant jet is an elementary flow case that is ideal for observing fundamental fluid characteristics. The computational results, which include detailed statistical analysis of mean and RMS fluctuations in density, are compared against experimental data at several axial and radial locations. This serves as a preliminary case for future endeavors concerning advanced energy efficient transportation technologies and systems involving the use of propane and other fuels.

11:15 AM - Siddharth Nigam[1], Caelan Lapointe[1], Jason D. Christopher[1], Nicholas T. Wimer[1], Torrey R. S. Hayden[1], Gregory B. Rieker[1], and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Sensitivity Analysis for an Open Catalytic Burner

Catalytic burners are widely used in industrial applications but their vertical temperature profiles are difficult to simulate due to the proprietary nature of catalysts. Additionally, these simulations are difficult to validate with experimental results because of the chemistry involved in the combus- tion and because the simulations often assume complete combustion of the fuel (methane) within the burner. Experimental results showed higher values in the temperature profile above the burner when compared to the simulations. In this study, high fidelity two-dimensional (2D) large eddy simulations (LES) of the region above a catalytic burner are used to characterize the tempera- ture profile in the domain with increasing amounts of unreacted methane coming out of the burner. Through advanced chemistry models, it is possible to track species of interest such as H2O and OH that help understand the trends seen experimentally. Initial single-step-reaction simulations show that the temperature profile is very sensitive to small amounts of methane. Advanced-chemistry- model simulations (41 step, 16 specie model) show that methane is likely not the sole reason for the increase in temperature fields above the catalytic burner.

11:30 AM - Jason D. Christopher[1], Caelan Lapointe[1], Nicholas T. Wimer[1], Torrey R. S. Hayden[1], Siddharth Nigam[1], Ian Grooms[2], Gregory B. Rieker[1], and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[1] Department of Applied Mathematics, University of Colorado, Boulder, CO

Inlet Fuel Quantity Estimation for a Turbulent Buoyant Jet Using Approximate Bayesian Computation

Approximate Bayesian Computation (ABC) is a powerful tool that allows sparse experimental or other "truth" data to be used for the pre- diction of unknown model parameters in numerical simulations of real- world engineering systems. In this presentation, I first introduce the ABC approach. I then use ABC to predict unknown inflow conditions in simulations of a three-dimensional (3D) turbulent, high-temperature reacting-flow buoyant jet. For this test case, truth data are obtained from an experimental

laser diagnostic technique. Using spatially-sparse H_2O concentration statistics from the experimental data, specifically the vertical height of the peak H_2O concentration, I estimate how much additional CH_4 would be required to increase the amount of H_2O observed in the computational domain. ABC method proves a robust tool to accurately predict unknown parameters. The success of the ABC approach in the present test suggests that ABC is a useful and versatile tool for engineering fluid dynamics research containing combustion.

11:45 AM - Lucas Droste[1], Ryan Aronson[1], and John Farnsworth[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

Design and Qualification of an Axisymmetric Jet for Preforming Probe Calibrations

The calibration of hot-wire anemometers and multi-hole pressure probes is an expensive necessity that also delays the progress of field and wind tunnel experiments. Previously researchers in the Ann and H.J. Smead Aerospace Engineering Sciences Department at the University of Colorado Boulder relied upon external companies for manufacturing and calibrating these devices. To alleviate these costs and delays in future research, a small stand-alone calibration jet was designed and manufactured. The calibration jet was designed in a simple modular fashion to allow for modifications in the future. The mass-flow through the calibration jet is supplied by the building air system at approximately 550 kPa and the mass flow rate is precisely controlled by an ALICAT Scientific MCR-1500SLPM-D Flow Controller. Initial testing of the calibration jet with a pitot static probe showed a linear correlation between the commanded mass flow rate and exit airspeed. Additional tests were then conducted to map the jet profile in the radial and axial directions to determine the spatial limits for probe calibration. In future tests, the turbulence intensity will be measured, and an externally calibrated five-hole pressure probe will be used to fully validate the capabilities of the calibration jet.

Session 2A: Optimization, Uncertainty, and Data Driven Approaches
1:00 PM - 3:00 PM (Room A)

1:00 PM - Caelan Lapointe[1] and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Topology Optimization for Compressible Internal Flows

The adjoint method is an attractive way to calculate gradients in a cost functional for gradient-based optimization because its expense scales only with the dimension of the objective function. A novel solver using the discrete adjoint method for gradient-based topology optimization of internal compressible flows has been developed in OpenFOAM. Impermeable material is then added to or removed from the domain subject to this sensitivity, resulting a new, optimal domain once the solver converges on a solution. Constraints on material addition have been implemented to more accurately mimic an additive manufacturing process. In this talk, solver performance will be demonstrated for sonic test cases with turbulence modeling. These test cases are designed to be straightforward with an easily anticipated solution that (i) demonstrates solver functionality and (ii) increases confidence in solver capability.

1:15 PM - Steven Isaacs[1,2] and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[2] Roccor, LLC., Longmont, CO

Computational Modeling and Optimization of Thin Flat Heat Pipes

Small scale heat pipes are a promising solution for a variety of thermal management solutions ranging from mobile electronic devices to defense electronics. This study introduces a reduced order model of a flat heat pipe and validates results with an experimental prototype. This prototype was a flat copper heat pipe with woven mesh liquid wick and vapor core structure. A maximum effective thermal conductivity of 2,140 W/mK was measured with a maximum heat transport capability of 15 W. The reduced order model was coupled with a gradient-free optimization method in order to optimize the design of the liquid mesh. Additionally, a high fidelity CFD model was constructed to accurately predict flow characteristics within a simple heat pipe vapor core. This model showed close agreement with published data and model results. By considering the basic dimensions of the vapor core, this CFD model was coupled with a gradient-based optimization method in order to minimize the pressure drop along the length of the vapor core. The total pressure drop was reduced by 20% using this approach.

1:30 PM - Julian Quick[1,2], Jennifer Annoni[2], Ryan King[2], Paul Fleming[2], Andrew Ning[3], and Katherine Dykes[2]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[2] National Renewable Energy Laboratory, Golden, CO
[3] Brigham Young University

Optimization Under Uncertainty for Wind Power Plant Wake Steering Strategies

The current paradigm in designing wind turbine control strategies is to control the wind turbine to maximize its power. Recently, researchers have started to look into plant-level turbine control strategies, controlling turbines to maximize power plants total energy output. One of these strategies is referred to as "wake steering," where some turbines offset their yaw position from the incoming wind to "steer" the wake away from downstream turbines, reducing the offset turbines' power and increasing the power of waked turbines. This control strategy requires forecasting how offsetting turbines' yaws will impact the behavior of turbines' wakes. There are several sources of uncertainty when forecasting this impact: the future behavior of the atmosphere is challenging to predict, engineering models do not fully represent reality, and the instruments used to measure the state of the wind power plant are imperfect. In this

study, we examined how uncertainty in the turbines' yaw positions and the inflow speed and direction affects the performance of wake steering strategies, and how these strategies can be explicitly designed to perform well when there is uncertainty in these values.

Wind power plants present fluid scientists with new and interesting problems, including forecasting the behavior of wakes behind turbines. The FLOw Redirection Induction and Steady-state model (FLORIS) approximates the behavior of wind turbine wakes as curved cones, assuming, among other non-physical parameters, a "wake expansion coefficient," a metric of how quickly the wake expands. These non-physical synthetic variables were tuned using a large eddy simulation of two wind turbines.

We examined the influence of wind speed and direction and turbine yaw position uncertainty on a simple two-turbine case and a utility-scale wind power plant. In both cases, we examined the benefits of designing wake steering strategies using optimization under uncertainty (OUU), performing Monte Carlo simulations of possible realizations of the uncertain variables during each optimization iteration and optimizing a statistic describing the range of possible scenarios. We compared the performance of OUU strategies to the deterministic wake steering formulation, which assumes perfect knowledge of the simulation parameters, and to the baseline strategy, where no turbine's yaw are offset.

We found that introducing uncertainty significantly affects the expect power production resulting from wake steering strategies. Generally, it is optimal to steer less when there is more uncertainty. In some cases, the deterministically formulated strategy performed slightly worse than the baseline. We found that, when accounting for inflow speed and direction and yaw misalignments, the OUU solution produced 2.9% and 0.8% more annual energy than the baseline and deterministic strategies respectively, in the utility-scale wind power plant model. In addition, the OUU strategy generally has less extreme yaw offsets than the deterministic strategy. This induces less wear and tear on the turbines.

This OUU used 150,000 spares-grid Monte Carlo simulations in each of 1,000 optimization iterations. While the FLORIS model requires little computer time, the computational requirements would be much greater for a higher fidelity mathematical model that more accurately describes the affects of wind turbine wakes. Potential solutions include:

- Quantifying the model-form uncertainty of the FLORIS model, learning a discrepancy function to anticipate the overall model-form uncertainty and/or generating probability distributions in synthetic parameters like the wake expansion coefficient

- A multifidelity OUU approach, using FLORIS (or any wake model that is inexpensive to run) to capture trends in the high-fidelity model and incorporating the uncertainty in mapping the FLORIS output to the high-fidelity simulation output in the statistics being optimized

- Using adjoint gradients to optimize a high-fidelity steady-state simulation.

Wind power plant control is an exciting new application of fluids science. Explicitly considering uncertainty when designing wake steering strategies increases their efficacy.

1:45 PM - Ashley Montalvo[1], Ethan Culler[1], and John Farnsworth[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

Uncertainty Quantification from Measures of Divergence in 2D PIV Data

Particle image velocimetry (PIV) is subject to various sources of uncertainty that can lead to erroneous velocities in the derived vector fields. In recent years, significant effort has been focused on developing methods to quantify this uncertainty. In general, these methods calculate uncertainty from the raw PIV images and the quality of the cross correlation. This project has been initiated to develop a method for quantitative data quality assessment using vector fields alone. This approach utilizes the fact that for incompressible flows, erroneous vectors will result in non-zero divergence. The presented work focuses on quantifying the relationship between uncertainty and divergence. Planar PIV measurements were taken in the wake of a NACA 0015 airfoil at four angles of attack and uncertainty was calculated using the correlation statistics method implemented in the LaVision DaVis software. Correlations were then made between the divergence and uncertainty fields through methods of cross-correlation and covariance. A

correlation of approximately 50 percent was found for the raw fields; however, this value is sensitive to data filtering and noise floor levels.

2:00 PM - Ryan W. Skinner[1], Alireza Doostan[1], Eric L. Peters[1], John A. Evans[1], and Kenneth E. Jansen[1]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO

Multi-Fidelity Modeling Efficiency in a Parametric Study of NACA Airfoils

Multi-fidelity modeling offers substantial efficiency gains for optimization and design space exploration, reducing total cost by offloading some high-fidelity (HF) work onto low-fidelity (LF), approximate simulations. Typical multi-fidelity approaches either require a moderate number of HF simulations to map the design space, or a low number of HF simulations to identify a single optimum configuration. Here, we evaluate a new multi-fidelity model, which offers a full map of the design space with only O(10-20) HF simulations. Accuracy hinges on (a) the HF system being low-rank, and (b) the LF system capturing the HF system's qualitative response to parametric variation. Our physical system is a 2D NACA 4412 airfoil with +/- 20% geometric variation and 0-6 degree angle of attack at Re = 1.52M. Grid-independent and coarse-mesh RANS constitute our HF and LF models, respectively. We are able to achieve 2.5% error in Cp prediction along the airfoil surface with a 50x cost-reduction, and less than 1% error with more than 16x cost-reduction.

2:15 PM - Jolene Britton[1,2], Mathew Reynolds[2], and Ryan King[2]

[1] University of California, Riverside
[2] National Renewable Energy Laboratory, Golden, CO

Covariance Computation for Active Subspaces Applied to a Wind Plant Surrogate Model

The method of active subspaces is an effective means for reducing the dimensions of a multivariate function f. This method enables experiments and simulations that would otherwise be too computationally expensive due to the high-dimensionality of f. By using a covariance matrix composed of the gradients of f, we can find the directions in which f varies most strongly, i.e., the active subspace. The current standard for estimating these covariance matrices is the Monte Carlo estimator. Due to the slow convergence of Monte Carlo methods, we propose an alternative algorithmic approach utilizing a separated representation of f. Such representations have well-defined sampling strategies and allow for the analytic computation of entries of the covariance matrix. Experimental results demonstrate how Monte Carlo methods compare to our proposed alternative approach as applied to approximating a function f that depends on the solution to a simple elliptic PDE problem. Furthermore, the two methods are compared when applied to a function f representing power output of a wind turbine that depends on the solution to Reynolds Averaged Navier Stokes flow model.

2:30 PM - Olga Doronina[1] and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Parameter Estimation for Eddy-Viscosity Model Using Approximate Bayesian Computation

Autonomic closure is a new technique for achieving fully adaptive and physically accurate closure of coarse-grained turbulent flow governing equations, such as those solved in large eddy simulations (LES). Although autonomic closure has been shown in recent a priori tests to more accurately represent unclosed terms than do dynamic versions of traditional LES models, the computational cost of the approach makes it challenging to implement for simulations of practical turbulent flows at realistic Reynolds numbers. The optimization step used in the approach, in particular, introduces large matrices that must

be inverted and is highly memory intensive. In order to reduce memory requirements, here we propose to use approximate Bayesian computation (ABC) in place of the optimization step, thereby yielding a computationally-efficient implementation of autonomic closure that trades memory-intensive for processor-intensive computations. The latter challenge can be overcome as co-processors such as general purpose graphical processing units become increasingly available on current generation petascale – and next generation exascale – supercomputers. In this work, we outline the formulation of ABC-enabled autonomic closure and present initial results demonstrating the accuracy and computational cost of the approach.

2:45 PM - Christiane Adcock[1,2] and Ryan King[2]

[1] Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA
[2] National Renewable Energy Laboratory, Golden, CO

Data-Driven Wind Plant Flow Modeling for Atmospheric Stability

Atmospheric stability substantially affects wind turbine wake propagation and therefore wind plant power output. However, accurately modeling wakes in different stability conditions remains a persistent challenge. In this talk, we present a framework for assimilating lidar remote sensor and meteorological tower data into an existing flow model to better predict the effects of atmospheric stability on wakes. The model, WindSE, is a 2D, steady-state, RANS flow model which previously assumed neutral stability, and neglected the effects of stable or unstable conditions that suppress or enhance mixing. We assimilate the data by finding the turbulent eddy viscosity fields that produce optimal agreement with lidar observations during stable, neutral, and unstable conditions. We use gradient-based optimization and an adjoint formulation to find the high-dimensional gradients required to solve this problem. To validate our model, we compare the performance of the original and updated WindSE models against an accurate, but computationally expensive large eddy simulation in stable, neutral, and unstable conditions.

Session 2B: Fuels, Combustion, and Reacting Flows
1:00 AM - 3:00 PM (Room B)

1:00 PM - Bahareh Abdollahipoor[1] and Bret Windom[1]

[1] Department of Mechanical Engineering, Colorado State University, Fort Collins, CO

Blending Effects of Hydrous and Anhydrous Ethanol on Gasoline Properties

Bio-ethanol obtained from fermentation contains water and cannot be separated with distillation at the azeotrope point and needs expensive and energy intensive methods for further water removal. Thus, hydrous ethanol at the azeotrope point can be used to reduce the cost and improve energy balance. In this effort, blends of gasoline with 10%, 15% and 30% by volume of anhydrous and hydrous ethanol were studied and named E10, E15, E30, H10, H15, and H30, respectively. Hydrous ethanol refers to a mixture of 96 vol. % anhydrous ethanol and 4 vol. % deionized water. In order to compare effect of anhydrous and hydrous ethanol on gasoline properties, following parameters were measured: distillation curve, Reid vapor pressure, vapor lock index, viscosity, density, copper strip corrosion, haze and phase separation points, and lower heating value. Negligible differences in properties between anhydrous and hydrous blends especially at low and mid-levels confirmed that blends of gasoline with hydrous ethanol can be potentially used as a drop-in fuel.

1:15 PM - Mangesh Dake[1], Bret Windom[1], Joe FitzWilliam[1], Matthew Swanson[2], Joshua Shaw[2], and Marc Henderson[3]

[1] Department of Mechanical Engineering, Colorado State University, Fort Collins, CO
[2] Honda R&D Americas Inc., Raymond, OH
[3] Honda R&D Americas Inc., Denver, CO

Considerations for CFD Simulations of a Refueling Pump Nozzle with Application to the Computer Aided Engineering of a Vehicle Refueling System

This study aims to validate CFD simulations which predict the fluid dynamics through a refueling gasoline pump nozzle. Evaporative hydrocarbons from vehicle fuel systems are a pollution source. Because the engineering development of a fuel system is expensive and resource intensive, a CAE model, which could predict performance of fuel system's effectiveness, would be a valuable tool. Other performance issues inherent to the refueling process such as premature click-off and spit-back also warrant the need for such a model, as both would be cause for redesign. To create an adequate computer model, this study first focuses on modeling the flow through and out of a gasoline-refueling gun, as this is a key inlet condition of a refueling system. A commercial CFD software was used to model gasoline flow through two different nozzle geometries. The CAD geometries used to construct the CFD domain were created from dimension measurements taken of the physical nozzles. Nozzle spray patterns were measured and compared to the CFD simulation results. A mesh and time-step independence study is conducted, as well as, an investigation of different inlet techniques to simulate the air entrainment process within the nozzles responsible for the auto shut-off behavior.

1:30 PM - Tianzhu Fan[1], Cory Rogers[1], John W. Daily[1], Barney Ellison[2], and Nicole Labbe[1]

[1]Department of Mechanical Engineering, University of Colorado, Boulder, CO

Numerical Design of a Novel Microreactor to Study Short Residence Time Combustion

Microreactors have historically been used as powerful tools to understand the early time pyrolytic behavior of fuels, especially when coupled with photoionization mass spectrometry (PIMS) or Fourier transform infrared spectroscopy (FTIR) diagnostics. However, current systems are often limited in scope of systems that may be studied due to the lack of consistency in profiles for reactor temperature, pressure, and velocity. Furthermore, these reactors are often made of silicon carbide, which is eroded under oxidative

conditions, limiting use to pyrolytic conditions. In this work, we aim to redesign these microreactors to address the aforementioned challenges through computational fluid dynamics simulations (CFD). 2D steady-state simulations were run with ANSYS Fluent to screen possible geometries for the new microreactor. The addition of a converging nozzle to the microreactor was identified as the best reactor geometry and the influence of the microreactor structure (microreactor body length; converging nozzle length and exit diameter) on centerline reactor properties has been explored to identify the optimum reactor design. Finally, transient simulations were performed to explore the effects of using a puled valve configuration, rather than a continuous pumping configuration, on the centerline temperature, pressure, and velocity profiles. As a direct result of this work, the redesigned microreactor is being fabricated and installed for experimental testing.

1:45 PM - Anthony Draper[1], Ryan Cole[2], Paul Schroeder[2], and Greg Rieker[2]

[1] Department of Aerospace Engineering Sciences, University of Colorado, Boulder, CO
[2] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Design and Evaluation of a High-Temperature and High-Pressure Spectroscopic Cell

Infrared absorption spectroscopy offers unique capabilities for nonintrusive measurements of combustion and exoplanetary systems, but rely heavily on accurate molecular absorption models. The most widely used absorption model databases, HITRAN and HITEMP, are known to be inaccurate when extrapolated to temperatures or pressures beyond 1 atm at 296 K. Work by our group and others have explored either higher temperature or higher pressure regimes separately, however the spectroscopic investigation into the combination of the two is largely unexplored. To overcome this, we designed and constructed a spectroscopic system allowing measurements to be taken in a 45.7 cm quartz cell at high pressure and temperature simultaneously. The tube-in-tube design that permits these measurements employs a pressure vessel with sapphire optical access windows surrounding a custom furnace to contain the quartz sample cells in the center. This system, together with our dual frequency comb spectrometer capable of large spectral bandwidth, dense point spacing, will be used to enhance databases and knowledge of molecular behavior in harsh environments. Here we present the design of the system along with the first spectra collected at 50 atm and 773 K.

2:00 PM - Mohammad J. Rahimi[1], Hariswaran Sitaraman[1], David Humbird[2], and Jonathan J. Stickel[1]

[1] National Renewable Energy Laboratory, Golden, CO
[2] DWH Process Consulting, Centennial, CO

Computational Fluid Dynamics Study of Industrial-Scale Aerobic Bioreactors for Biofuel Production

Bubble column and airlift bioreactors are widely used systems, mainly in pharmaceutical industry for large-scale production of high value products. Scaled-up aerobic reactors in the context of lower value products such as biofuels have not been explored and little information exist about their operability and cost. We present reacting multiphase CFD simulations using OpenFOAM to better understand the complexity of these reactors and characterize important parameters such as gas-liquid mass transfer and hold-up. The reacting multiphase model includes transport equations for chemical species in liquid and gas phase along with interphase mass transfer and an oxygen uptake model representing the aerobic bioreaction. Essential multiphase physics such as wall lubrication, turbulent dispersion forces and bubble-induced turbulence are also included in our model. The geometry of the simulation is based on a projected large-scale bioreactor with 5 m diameter and 25 m liquid height. In this study, hydrodynamics, gas hold-up, and oxygen transfer rates in different bioreactor designs are compared and insights regarding reactor performance and aeration rates are obtained.

2:15 PM - Samuel H.R. Whitman[1], Colin A.Z. Towery[1], Alexei Y. Poludnenko[2], and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[2] Department of Aerospace Engineering, Texas A&M University, College Station, TX

Dependence of Intermittency on Turbulence Intensity and Simulation Fidelity in Premixed Reacting Flows

Intermittency is an important metric for determining the likelihood of extreme fluctuating quantities in turbulent premixed flames. Such extreme quantities may lead to flow-altering events including extinction, auto- and re-ignition, and deflagration to detonation transitions. Here we analyze intermittency of enstrophy (i.e., vorticity magnitude) and temperature gradient magnitude fields based on data from direct numerical simulations (DNS) of stoichiometric premixed hydrogen-air flames in unconfined domains. The DNS are performed for different turbulence intensities, for single- and multi-step chemistry models, for varying spatial resolution, and for temperature-dependent and constant viscosities. These simulations thus enable the study of physical effects on intermittency, as well as the study of effects based on simulation fidelity. We show that intermittency in the temperature gradient magnitude varies with the chemistry model but has little dependence on viscosity, while enstrophy intermittency varies with the viscosity model, but has little dependence on the fidelity of the chemistry.

2:30 PM - Ryan Darragh[1], Colin A.Z. Towery[2], Peter E. Hamlington[2], and Alexei Y. Poludnenko[3]

[1] Smead Aerospace Engineering Sciences Department, University of Colorado, Boulder, CO
[2] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[3] Department of Aerospace Engineering, Texas A&M University, College Station, TX

Lagrangian Analysis of Enstrophy in Turbulent Premixed Flames

Turbulent combustion is a multi-scale and multi-physics problem depending upon both chemical and fluid dynamic processes. These processes are often examined using an Eulerian framework, but recently the Lagrangian framework, a long-time tool in non-reacting flow research, has become increasingly common for the study of turbulent combustion. The two analysis frameworks are in fact equivalent, with the only difference being a change in reference frame. In this study, a Lagrangian fluid parcel tracking algorithm is used to analyze the enstrophy (i.e., vorticity magnitude) dynamics in turbulent premixed reacting flows. The analysis of vorticity dynamics in the premixed flame case is based on data from a three dimensional direct numerical simulation of a premixed stoichiometric hydrogen- air flame in an unconfined domain. Vorticity budget terms are tracked along Lagrangian trajectories as fluid parcels travel through the flame, with particular focus on understand- ing the dynamical causes of turbulence variations through the flame preheat and reaction zones.

2:45 PM - Colin A.Z. Towery[1], Ryan Darragh[2], Alexei Y. Poludnenko[3], and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO
[2] Department of Aerospace Engineering Sciences, University of Colorado, Boulder, CO
[3] Department of Aerospace Engineering, Texas A&M University, College Station, TX

Lagrangian Analysis of Premixed Autoignition in Compressible Turbulence

Autoignition plays a fundamental role in high-speed combustion systems, such as scramjet engines, where combustion occurs at large Karlovitz numbers and the turbulence can be highly compressible, with turbulence Mach numbers $Ma_t > 0.1$. The effects of compressible turbulence on the ignition delay time and intermittency of autoignition in high-speed combustion are investigated here using direct numerical simulations of three-dimensional, reactive, homogeneous isotropic turbulence with single-step Arrhenius reaction kinetics. Probability distributions of the fuel mass-fraction and reaction rate reveal large increases in intermittency and small-scale structure between the linear and non-linear compressibility regimes, with eddy shocklets appearing at $Ma_t > 0.4$. Detailed time histories of fluid parcel pathlines

analyzed in the Lagrangian reference frame for $Ma_t = 0.2$, 0.4, and 0.6 indicate that, at the turbulence Mach numbers expected in high-speed combustion systems, compressibility significantly shortens ignition delay time, and that both subsonic and supersonic autoignition waves can be formed simultaneously in both the linear and nonlinear compressibility regimes.

Session 3A: Fluid Dynamics in the Environment
3:30 PM - 5:00 PM (Room A)

3:30 PM - Aaron True[1], Jeanette Wheeler[2], and John Crimaldi[1]

[1] Department of Civil, Environmental, and Architectural Engineering, University of Colorado, Boulder, CO
[2] Institute for Environmental Engineering, ETH Zurich

Classical and Fractal Grid Turbulence Characteristics in a Liter-Scale Oscillating Grid Tank

Producing turbulent flows in the laboratory that mimic in situ conditions is important for the study of microscale biological-chemical-physical interactions in aquatic ecosystems. These studies are often uniquely constrained to experimental volumes on the order of one liter. To this end, we have designed and built a one liter, dual oscillating grid turbulence tank. We use planar particle image velocimetry to characterize turbulence as a function of grid stroke (10, 15, and 20 mm), frequency (0.5, 1, 2, and 4 Hz), and geometry (parameter- matched classical and fractal square grids). Turbulence intensity (rms velocity fluctuation), turbulent kinetic energy (TKE) dissipation rate, Kolmogorov microscales, and mean flow and isotropy are quantified throughout the parameter space, revealing a wide range of turbulence characteristics from low intensity, high mean flow to high-intensity, near zero-mean flow conditions. TKE dissipation rates and Kolmogorov microscales span a range of conditions similar to oceanic turbulence. Under identical forcing (stroke and frequency), fractal grids produce turbulence with enhanced TKE dissipation rates and smaller dissipation scales when compared to classical grids. Going forward, we will investigate turbulence characteristics for cases where the grid phases are decoupled and the forcing frequency and duration are randomized; we hypothesize that this will improve turbulence homogeneity and isotropy.

3:45 PM - Jian Zhou[1], Claudia Cenedese[2], Subhas K. Venayagamoorthy[1], Roger Nokes[3]

[1] Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO
[2] Department of Physical Oceanography, Woods Hole Oceanographic Institution, Woods Hole, MA
[3] Department of Civil and Natural Resource Engineering, University of Canterbury, New Zealand

Gravity Currents Propagating over a Submerged Array of Cylinders

In this study, the propagation of lock-exchange gravity currents in a horizontal channel containing a submerged array of cylindrical obstacles are investigated using laboratory experiments and large eddy simulations. Excellent agreement on the flow structure and front velocity between the experimental and numerical results is found. A thorough parametric study is performed in which the array density is varied from 0 (flat-bed) to 1 (solid-slab), and the submergence ratio is varied from 1 (emergent) to 10 (deeply submerged). A decomposition of the array density into a new two-dimensional parameter space consisting of a streamwise array density and a spanwise array density is proposed to provide a more quantitative and unambiguous description of the current propagation dynamics. The various flow regimes arising from the current-array interaction and their mutual transitions are investigated in detail. Two possible current acceleration mechanisms are identified with the underlying physics interpreted. Funded by the Office of Naval Research and the National Science Foundation.

4:00 PM - Aseperi Oladapo[1] and Subhas K. Venayagamoorthy[1]

[1] Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO

Dynamics of Flows in River Bends

Rivers are vital for water supply, navigation, and transport of pollutants and nutrients. These benefits among others are only available and sustainable when river systems function optimally; since the flip side is flooding, loss of lives and property. Natural rivers and manmade channels are common conveyance

systems that typically have meandering (curved) geometries. A better understanding of the flow dynamics as well as the associated complex flow structures in river bends is critical for developing improved engineering design methods for protecting such conveyance systems against failure due to erosion. This research is aimed at contributing towards fundamental understanding of the flow structure in river bends using computational simulations.

4:15 PM - Yang Guo[1], Jingwei Huang, Xiaolong Yin, Keith Neeves, Ning Wu

[1] Department of Chemical and Biological Engineering, Colorado School of Mines, Golden, CO

Colloid Transport In A Microfluidic Soil Analog: Population Dynamics And Single Particle Trajectories

Abstract: Low solubility contaminants such as heavy metals and radionuclides can adsorb onto mobile colloids and travel with underground water in soils over kilometers. However, the detailed flow pathway and rate-limiting transport mechanism of colloids in soils are largely unknown. To study these phenomena we developed a microfluidic soil analog to measure both population dynamics and single particle trajectories of model colloids. The soil analog consists of an $O(1 \text{ mm}^2)$ chamber filled with packed 15 μm polystyrene beads. Comparisons between measured and estimated hydraulic permeability from Lattice Boltzmann Method (LBM) simulations suggest a pseudo-two dimensional packing with $\sim$50% of beads displaced from the bottom of the channel. A T-junction at the exit of soil analog allowed for encapsulation and enumeration of several thousand colloids per experiment to give population dynamics. Single particle trajectories of 0.5, 1, and 3 μm colloids were captured by fluorescence microscopy within the soil analog at Peclet numbers of 1600-9600. Tortuosity calculated from these trajectories and comparison with LBM simulations using point particles revealed that pore-scale transport of colloids was influenced by the size exclusion effect. The innovative features of this device provide a means to link microscale transport properties like particle trajectories, which are difficult to measure in natural soils, to macroscale transport properties like dispersion, which can be measured in column and field-scale experiments. This device will enable future studies to connect micro- and macroscale colloid transport and to measure the effect of chemical heterogeneities that mimics those found in natural soils.

4:30 PM - Shaken Kenzhekhanov[1], Martin Lozano[1], Keith B. Neeves[1], Xiaolong Yin[1], and Tao Huang[2]

[1] Colorado School of Mines, Golden, CO
[2] China University of Petroleum, East China

Invasion-Flowback Processes During Hydraulic Fracturing Well Interference

Technology development in horizontal drilling and multistage fracturing unleashed the energy potential of shale and low permeability reservoirs that have not been previously considered as feasible. The main mechanism that enables higher recovery rates of hydrocarbons from such reservoirs is to maximize contact with reservoir rocks by horizontal well bore and hydraulic fractures. The capacity of reservoir rocks to flow fluids (permeability) in such reservoirs is very low, therefore the drainage area of a well follows the trajectory of the wellbore and the fractures. It is a challenge to space wellbores and fracturing stages optimally, without significant well interference and yet not leaving much unstimulated reservoir volume behind. As such, well interference is quite common and has been widely observed in the field using diagnostic tools, such as microseismic imaging, pressure monitoring, chemical tracers, and fiber-optic sensors.

Conventional wisdom suggests that as two well's hydraulic fracture network overlap, the fracturing fluid of the new well entering the fracture network of the old well should negatively affect the performance of the old well. However, field data suggest that sometimes the influence on the interfered wells can be positive. While there have been several numerical studies on this issue, experimental studies that can lead to a fundamental understanding of physical mechanisms of positive and negative well interferences are few. This study focuses the consequence of a new well's fracturing fluid entering an existing well's fracture network. We used microfluidic porous media micromodels directly visualize invasion of

hydraulic fracturing fluid into a porous matrix and flowback. To mimic the interaction between the hydraulic fracturing fluid and the matrix in the case of well interference, two invasion-flowback cycles were carried out. The first invasion flowback cycle's purpose is to simulate the hydraulic fracturing of the old well and establish the corresponding saturation state. The second invasion-flowback cycle simulates fluid invasion from the new well into the old well's fracture network and its interaction with the matrix. Through micromodels experiments, we found that most of the time invasion of hydraulic fracturing fluid of a new well should damage the production of the old well. However, if the new well's fracturing fluid contains surfactant and the old well's fracturing fluid does not, surfactant can reduce the water saturation in the porous matrix after the second invasion-flowback cycle. The invasion-flowback experiments using NOA81 micromodels demonstrated that visual analysis of multiphase flow and fluid-fluid interactions could provide a valuable information in well interference phenomena. The fluid saturation profile of invasion-flowback processes also could be used to investigate important parameters, such as relative permeability, capillary forces, wettability, that affect the hydrocarbon recovery.

4:45 PM - Nicholas T. Wimer[1], Amanda W. Mackoweicki[1], John W. Daily[1], Gergory B. Rieker[1], and Peter E. Hamlington[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Direct Numerical Simulation of Wildland Fires at Small Scales

Preliminary results are presented from a new research effort focused on understanding and characterizing wildland fire spread at small scales (roughly 1m-1mm) using direct numerical simulations (DNS). The simulations are intended to directly resolve, with high physical accuracy, all small-scale fluid dynamic and chemical processes relevant to wildland fire spread. Simulation of wildland fires is an incredibly complex and challenging problem due to the vast difference in scales associated with the problem. An understanding is needed not just of the burning of fuel, but also of the atmospheric conditions, weather patterns, topography, and turbulence-flame dynamics. This work is focused on the sub-meter scales associated with wildland fire; in particular, the dynamics of small-scale diffusion flames. Here, preliminary results are presented for DNS of centimeter-scale gaseous pool fires coupled with multi-step chemical reaction mechanisms. The results are connected to the fundamental structure and spread of wildland fires, and an outlook is provided for the future expansion of these DNS studies.

Session 3B: Biology, Surfaces, and Droplets
3:30 PM - 5:00 PM (Room B)

3:30 PM - Carlos Quiroz-Arita[1,2], Patricia E. Gharagozloo[1], Myra L. Blaylock[1], Ryan Davis, Thomas H. Bradley[2,3], Thomas Dempster[4], and John McGowen[1]

[1] Sandia National Laboratories, Thermal/Fluid Science & Engineering, Livermore, CA

[2] Department of Mechanical Engineering, Colorado State University, Fort Collins, CO

[3] Sandia National Laboratories, Bioscience, Livermore, CA

[4] Arizona Center for Algae Technology and Innovation and the Algae Testbed Public Private Partnership, Mesa, AZ

Computational Study of Turbulence and Mixing in Algae Raceway Ponds: Implications of Fluid Mechanics in Algae-based biofuels Growth Models

A dynamic algae growth model is coupled to a Computational Fluid Dynamic model based on a raceway pond affiliated with the ATP3 collaboration. Our dynamic model solves a set of ordinary differential equations consisting of growth functions which are dependent on incident radiation, temperature, and nutrients availability. Our model also incorporates dynamic losses due to dark and photo-respiration. The novelty of this model is the coupling of the dynamic algae bioprocesses with 3D turbulence mixing, based on Reynolds Average Navier Stokes equations which impact in the light regimes and respiration losses that algae experience and the resultant productivities in these raceway systems. Two main sources of model uncertainty have been identified as the velocity inlet profile and the turbulence intensity, which shows the importance of 3D turbulence characteristics to the model accuracy. The biomass productivity predicted by the 1D dynamic algae growth model, where well-mixed conditions are assumed, has a relative error of 13.86% with respect to the ash-free dry weight of Nannochloropsis oceanica, of 0.476 g.l-1 (+/- 0.021), observed in open raceway ponds at AzCATI during the ATP3 Unified Field Studies. The model error suggests that 3D mixing rates may impact the light fluctuations experienced by algae in these systems. Our research demonstrates that the appropriate selection of turbulence mixing models coupled with algae growth models is critical in the accuracy of algae biomass productivity predictions.

3:45 PM - Nicholas Danes[1], Rogier Schoeman[2], Keith Neeves[2], and Karin Leiderman[1]

[1] Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden, CO

[2] Department of Chemical Engineering, Colorado School of Mines, Golden, CO

Toward a Mathematical Model of Hemostasis

Hemostasis is the process by which a blood clot forms to prevent bleeding. The formation time, size and structure of a clot depends on the local hemodynamics and the nature of the injury. Extravascular injuries, those which occur outside the vessel, have not been extensively modeled or understood. To understand such injuries, both experimental and computational models of hemostasis must be simultaneously developed from the ground up. Here we develop and validate a computational model against analogous experimental results for the fluid dynamics inside a microfluidic bleeding chip. Future steps to further communicate the experimental and computational models are also presented for modeling the transport and reactions of the platelet populations.

4:00 PM - Anudeep Pendurthi[1], Sanli Movafaghi[1], Wei Wang[1], Soran Shadman[1], Azer P. Yalin, and Arun K. Kota[1,2]

[1] Department of Mechanical Engineering, Colorado State University, Fort Collins, CO

[2] School of Biomedical Engineering, Colorado State University, Fort Collins, CO

Fabrication of Nanostructured Omniphobic and Superomniphobic Surfaces with Inexpensive CO_2 Laser Engraver

Super-repellent surfaces can be broadly classified as superhydrophobic surfaces (i.e., surfaces that are

extremely repellent to high surface tension liquids like water) and superomniphobic surfaces (i.e., surfaces that are extremely repellent to both high surface tension liquids like water and low surface tension liquid like oils). Superomniphobic surfaces (i.e., surfaces that are extremely repellent to both high surface tension liquids like water and low surface tension liquids like oils) can be fabricated through a combination of surface chemistry that imparts low solid surface energy with a re-entrant surface texture. Recently, surface texturing with lasers has received significant attention because laser texturing is scalable, solvent-free, and can produce a monolithic texture on virtually any material. However, to the best of our knowledge, there are no reports of superomniphobic surfaces fabricated via laser texturing. Further, most reports of superhydrophobic surfaces fabricated via laser texturing have employed expensive nanosecond or femtosecond lasers. In this work, we fabricated nanostructured omniphobic and superomniphobic surfaces with a variety of materials using a simple, inexpensive and commercially available CO_2 laser engraver. Further, we demonstrate that our simple, inexpensive, scalable, and solvent-free laser texturing technique allows fabrication of superomniphobic (or omniphobic) surfaces, gradient wettability surfaces, and droplet manipulation tracks with a wide variety of materials.

4:15 PM - Matthew Cackovic[1], Wei Wang[1], Hamed Vahabi[1], Rui Jang[1], and Arun Kota[1]

[1] Department of Mechanical Engineering, Colorado State University, Fort Collins, CO

Droplet Manipulation on a Surface using the Triboelectric Effect

Discovered over two thousand years ago in ancient Greece, triboelectrification is the phenomena in which two surfaces to acquire charges of opposite signs through contact-induced surface charging. The triboelectric series (i.e., a list of materials ranked based on their tendency to become positively or negatively charged) interestingly do not contain any liquid, even though the contact electrification of liquids with both high (e.g., water) and low (e.g., n-hexadecane) dielectric constants) after they contact a solid surface has been observed in the past century. Liquid droplets can be moved via external stimuli that allows controlled manipulation and complex functionalities on a surface. In this work, for the first time, we demonstrate the controlled manipulation of liquid droplet with both high (e.g., water) and low (e.g., n-hexadecane) dielectric strengths on a smooth, slippery surface via triboelectric effect. Most current droplet manipulation methods such as magnetic fields, electric fields, light, vapor, wettability gradients, and morphing of surface topography usually have drawbacks such as complex fabrication of manipulation platform, low droplet motility (i.e., long response time), expensive actuation system and lack of precise control. Our method is simple, facile and portable methodology enables on-demand, precise manipulation of droplets using solely the electrostatic attract or repulsion force, which is exerted on the droplet by a simple charged actuator. We envision that our triboelectric effect enabled droplet manipulation methodology will open a new avenue for droplet based lab-on-a-chip systems, energy harvesting devices and biomedical applications.

4:30 PM - Eduard Benet[1], Guillaume Lostec[1], John Pellegrino[1], and Franck J. Vernerey[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Deformation and Transport of Soft Colloidal Particles in Confined Networks

The transport of micron-size particles such as bacteria, cells or synthetic lipid vesicles through the porous spaces is a relevant process in drug delivery, separation processes or detection to cite a few. Often, the motion of these particles depends on their ability to squeeze through small constrictions in the porous medium to move through, making their capacity to deform an important factor to their permeation. To better understand and control these processes, it is therefore critical to predict how either the design of the particle or that of the porous medium affects the transport and eventual jamming of particles. We are particularly interested in two quantities: (a) the network topology and size and (b) the particle size, shape, stiffness, and surface. Using the principles of percolation theory, we address this problem by showing that these microscopic properties of the system can be connected to the macroscopic behavior of the porous media. We further validated the applicability of this method against a coarse-grained model of the particle transport. The results show that there is a nonlinear relationship between the particle

flux and the overall applied pressure, whose profile is well explained by the microscopic properties of the system. Furthermore, we isolated the effect of individual magnitudes such as particle size, surface tension, or pore shape, which are often the target in designs trying to achieve a unique objective, like the separation of two similar particles.

4:45 PM - Tong Shen[1] and Franck Vernerey[1]

[1] Department of Mechanical Engineering, University of Colorado, Boulder, CO

Phoretic Motion of Soft Vesicles and Droplets

Self-propelled droplets and vesicles have drawn much attention since they not only help reveal the mechanism of bio-locomotion, but also have potential for practical applications in drug delivery and chemical machinery. The mechanism of such self-propulsion can be classified into two categories, the Marangoni effect and diffusiophoresis. For the former, the surface tension of a droplet is altered by the chemical or temperature gradients in the surrounding fluid, generating a driving force for motion. For the latter, the droplet chemically interacts with solute and generates an active slip flow on its surface that drives motion. While tremendous efforts have been devoted to theoretically understand these two mechanisms, numerical study is limited due to the difficulty in handling the discontinuous slip flow on the droplet surface. In this presentation, we introduce a computational framework that is based on the extended finite element method (XFEM) that naturally address this issue by introducing the enriched tangential degrees of freedom for the fluid velocity across the interface. This model is then applied to study three interesting phoretic problems: suspension of a water droplet in oil via the Marangoni effect; the self-propulsion of a deformable droplet via diffusiophoresis; spontaneous motion of a droplet in an initially isotropic solute concentration.