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Book of Abstracts
Title: Turbulent particle clustering in a fully developed square channel flow
Authors: Laura Villafañe, Andrew Banko, Chris Elkins, John Eaton
Abstract: Particle-turbulence interactions are investigated in a fully developed turbulent channel air flow to determine the gas phase effect on the particle concentration and velocity fields. The experimental apparatus is a vertical channel with square cross section. The bulk channel Reynolds number based on channel width varies between $1 \times 10^4$ and $4 \times 10^4$. The $12$ um nominal diameter nickel particles are smaller than the Kolmogorov length scale and the corresponding Stokes number is between $5$ and $31$. Low volume and mass loading ratios are considered. Under these conditions preferential concentration is expected to be strong while the effect of particles on the gas flow is negligible. The square channel flow contains mean secondary flows not present in high aspect ratio channels studied previously. These will increase transport of particles away from the walls and raise turbulence levels in the central region.

Current experiments are focused on measuring the gas phase turbulence and the statistics of the particle concentration. The particle concentration field is analyzed from high resolution laser illuminated planar images. Box counting methods are used to quantify the degree of preferential concentration of particles by comparison to a random distribution. In agreement with previous studies the test case with Stokes number closest to one shows the strongest preferential concentration. Voronoi tessellations of the instantaneous particle locations are used to identify clusters and voids in the flow. The probability distributions of void and cluster areas exhibit a power law scaling which indicates a scale invariant behavior. By calculating the area and perimeter of particle clusters, it is found that the aspect ratio of clusters increases with the cluster size.

Title: Theoretical and computational analysis of clustering in particle-laden turbulence
Authors: Mahdi Esmaily Moghadam, Ali Mani
Abstract: Interaction of finite-size heavy inertial particles with turbulent flow via Stokes drag is analysed. An asymptotic solution is obtained that quantifies particle clustering in terms of finite-time Lyapunov exponents (FTLE) on a wide range of Stokes numbers (defined based on the Kolmogorov time scale) and flow conditions. The result of our analysis is consistent with the formerly established results at the limit of very small Stokes number, showing that the divergence of particle velocity field is proportional to Stokes number and that the particle-hospitable regions in flow are those with high-shear and low-vorticity. Additionally, our analysis is extended to larger Stokes numbers, showing that the clustering decays as particles become larger. Therefore, our analysis predicts minimal clustering at very small and large Stokes number and maximum clustering at Stokes number order one. These results are validated against numerical simulation of inertial particles in a homogeneous isotropic turbulent flow. This comparison shows that our analysis predicts FTLE correctly at all Stokes numbers, specifically in shorter time periods.

Title: Convergence of Beer's Law for Radiation Transmission in Particle-Laden Turbulent Flows
Authors: Ari Frankel, Rick Rauenzahn, Gianluca Iaccarino, Ali Mani
Abstract: Radiation transmission in particle clouds is a phenomenon of interest in atmospheric physics, remote sensing, and industrial heat transfer applications. Beer's law for radiation transmission is commonly applied to such media. However, the stochastic nature of particle concentration in clouds can produce significant deviations from the exponential attenuation predicted by Beer's law. Though particle-resolved ray tracing models can exactly resolve the transmission, the computational expense of such approaches can be prohibitive in settings involving many particles or in high fidelity numerical simulations requiring the solution of the radiative transfer equation at each time step. In this work we investigate the validity of projecting Lagrangian
particles onto an Eulerian concentration field and using Beer’s law on a local basis. We take particle distributions produced from clustering in turbulent flows and perform both particle-resolved Monte Carlo ray tracing and Beer’s law computations. We show that the error in the calculated transmission decreases as the grid is refined, but that the homogenization error increases rapidly as the grid size approaches the particle diameter.

Title: A novel particle SGS model based on differential filter for LES of particle-laden turbulent flows
Authors: George I. Park, Javier Urzay, Maxime Bassenne, & Parviz Moin
Abstract: When performing large-eddy simulation of particle-turbulence interactions, proper modeling of the effect of subgrid-scale (SGS) fluid motions on the particle dynamics is critical for accurate prediction of particle dispersion. Existing particle SGS models recover the missing SGS fluid velocities required in the particle equation of motion by assuming stochastic evolution of SGS fluctuations seen by particles, or by deconvolving the LES solution with an approximate inverse of the filter. In this study, we investigate the use of the differential filter for deconvolution-based particle SGS modeling. Deconvolution with a differential filter is potentially an attractive alternative to the existing Pade-filter based approximate deconvolution techniques. Exact deconvolution can be done trivially with differential filter, because the filter is defined in the inverse-filter form, and the method can be easily extended to unstructured grids. A dynamic procedure for determining the coefficient related to the nominal filter width has been developed, which imposes a consistency between the actual SGS dissipation produced by the gas phase SGS model and the SGS dissipation implied by the differential filter. The model has been applied to LES of one-way coupled particle-turbulence interaction in isotropic turbulence with a wide range of particle Stokes numbers, where promising results are obtained for predicting particle-clustering related statistics.

Session II – Combustion Processes

Title: High-Energy X-ray Absorption as a diagnostic technique for combustion experiments
Authors: Jared Dunnmon, Sadaf Sobhani, Waldo Hinshaw, Rebecca Fahrig, Matthias Ihme
Abstract: X-ray diagnostics such as X-ray Computed Tomography (XCT) have recently been utilized for measurements of scalar concentration fields in gas-phase flow phenomena. In this study, we apply high-energy X-ray absorption techniques to visualize a laboratory-scale flame via fluoroscopic measurements by using krypton as a radiodense tracer media. Advantages of X-ray absorption diagnostics in a combustion context, including application to optically inaccessible environments and lack of ambient photon interference, are demonstrated. Analysis methods and metrics for extracting physical insights from these data are presented. The accuracy of the diagnostic is assessed via comparison to known results from canonical flame configurations, and the potential for further applications is discussed.

Title: Kinetic rate uncertainty in estimating explosion limits
Authors: Nicolas Kseib, Gianluca Iaccarino
Abstract: In this talk, we will discuss the current state of the art of reporting kinetic uncertainties to show that it is incomplete and only focuses on describing the experimental accuracies and/or uncertainties. For that purpose, we propose a general data-driven statistical framework that bridges the gap between (numerical or laboratory) experimentation, physical modeling and uncertainty quantification. The framework enables the study of uncertainties and biases in physical models estimated from data and it is tested in the context of combustion science and chemical kinetics, specifically on the problem of prediction of explosion limits. We will differentiate between two types of modeling uncertainties and biases, the first one due to physical errors in the models and the second one due to noise introduced by the data-acquisition process. We will demonstrate how
to use our framework to extend the current state of the art and propose a practical technique to report kinetic uncertainties useful for uncertainty propagation in prediction type problems.

**Title:** Regularized Deconvolution Method for Turbulent Combustion Modeling  
**Authors:** Qing Wang, Hao Wu, Matthias Ihme  
**Abstract:** The LES-modeling of partially premixed turbulent combustion remains an outstanding issue. The difficulties introduced in LES are associated with the representation of the turbulent scalar mixing and the turbulence/chemistry interaction. In this work, a regularized deconvolution method (RDM) is developed as unifying closure model for chemical source terms, subgrid stresses, and turbulent scalar mixing. The newly proposed RDM-model is tested using a detailed simulation of a partially premixed flame evolving in decaying turbulence. Comparisons with different deconvolution methods are performed through a-priori analysis, and issues regarding the accuracy of the deconvolution method are examined. Simulations solving explicitly filtered scalars are conducted to examine the performance of RDM, and results are compared with direct numerical simulation (DNS), the conventionally employed approximate deconvolution method (ADM), and direct source-term evaluation.

**Title:** LES of combustion dynamics near blowout in a realistic gas-turbine combustor  
**Authors:** Lucas Esclapez, Peter C. Ma, Jeff O'Brien, Matthias Ihme  
**Abstract:** Driven by increasingly stringent emission regulations, modern gas turbines operate at lean conditions to reduce combustion chamber temperature and NOx emissions. However, as the combustor operates closer to the lean blow-out (LBO) limit, flame stabilization mechanisms are weakened, which increases the risk for complete flame blowout. To better understand the LBO-process and evaluate the fuel effects on the LBO-behavior, large-eddy simulations of the combustion dynamics near blowout are performed in a realistic two-phase flow combustor. An unstructured incompressible Navier-Stokes solver is used in combination with a Lagrangian dispersed phase formulation. Flame dynamics near and at LBO conditions are examined to characterize effects of the fuel properties on evaporation, gaseous-fuel deposition, flame anchoring, and LBO-limits. The LES is shown to capture the progressive reduction of OH* as the LBO-limit is approached. In agreement with experimental studies, it is found that both fuels under consideration exhibit comparable LBO-behavior and the analysis of the LES-results highlights the role of the recirculation zone temperature and position on the evaporation process and the flame stability.

**DAY 2**

**Session III - Fuel Injection and Multiphase Flows**

**Title:** A balanced-force conservative volume-of-fluid method for simulating two-phase flows on unstructured grids  
**Authors:** Christopher Ivey, Parviz Moin  
**Abstract:** A balanced-forced conservative volume-of-fluid method for simulating two-phase flows on unstructured grids is presented. The two-phase Navier-Stokes equations are solved using a median-dual-partitioned collocated node-centered finite-volume discretization and a specialized fractional-step method. Conservative mass and momentum convection fluxes are calculated using a novel volume-of-fluid method. Accurate interface normal and curvature are calculated on the non-convex median-dual mesh using the recently proposed embedded height-function technique. Spurious currents are minimized using a balanced-force algorithm and the continuum-surface force description of surface tension. The results of several two- and
three-dimensional benchmark test cases on various unstructured meshes demonstrate the effectiveness of the proposed two-phase flow solver.

**Title:** Analysis of Fuel Injection and Atomization of a Hybrid Air-Blast Atomizer  
**Authors:** Peter Ma, Lucas Esclapez, Sameer Naik, Matthias Ihme  
**Abstract:** Fuel injection and atomization are of direct importance to the design of injector systems in aviation gas turbine engines. Primary and secondary breakup processes have significant influence on the drop-size distribution, fuel deposition, and flame stabilization, thereby directly affecting fuel conversion, combustion stability, and emission formation. The lack of predictive modeling capabilities for the reliable characterization of primary and secondary breakup mechanisms is still one of the main issues in improving injector systems. In this study, an unstructured Volume-of-Fluid method is used in conjunction with a Lagrangian-spray framework to conduct numerical simulations of the breakup and atomization processes in a gas turbine hybrid air blast atomizer. Results for injection with Cat-A1 aviation fuel are presented and compared to experimental data.

**Title:** Evaporation and Combustion of Multicomponent Fuels  
**Authors:** Pavan Govindaraju, Alessandro Stagni, Lucas Esclapez, Matthias Ihme  
**Abstract:** Current generation fuels are mixtures of hundreds of complicated organic compounds and accurate modeling of their combustion characteristics provides fundamental physical insights which also help in the design of efficient combustors. This however requires accurate simulation of both evaporation and combustion processes. The presentation will elaborate on the assumptions and the framework utilized for evaporation and chemical mechanisms. We also present a comparison between various fuels used in the aviation industry as test cases while highlighting on their pros and cons. The focus of the talk will however be on the physical aspects captured using 1D simulations, i.e., the importance of preferential evaporation and liquid species diffusion on the ignition of multicomponent fuels. We conclude with results related to the ignition of an aviation fuel at conditions of interest in gas turbine engines.

**Title:** A single-fluid multiphase formulation for diffuse-interface modeling of high-pressure transcritical liquid jets  
**Authors:** Lluis Jofre, Javier Urzay, Ali Mani, Parviz Moin  
**Abstract:** High-pressure combustion of liquid propellants is of relevant interest given the current trends that gear design towards higher compression ratios to increase efficiency and performance. In subcritical conditions, atomization involves the rupture of the liquid volume through the competition between aerodynamic shearing and surface tension, such to ensure proper dispersion and mixing of the liquid droplets in the combustion chamber. Under these conditions, liquid-gas interfaces remain sharp, spanning less than a single mean free path. Therefore, two-fluid formulations coupled through appropriate boundary conditions at the interfaces near the injection orifice, along with Lagrangian descriptions for the dilute spray downstream, become natural representations of this regime. In contrast, the classic atomization description becomes inadequate at supercritical conditions when the characteristic temperature and pressure of the gas environment are above the corresponding critical values. In the vicinity of the critical point, the scale separation between the typical size of the bulk phases and the interface thickness is no longer valid and, consequently, the structure and mechanisms of the interfacial transition region must be considered. In that limit, the latent heat of vaporization vanishes and there is virtually no surface tension that prevents rupture of the liquid core and diffusive mixing with the gas environment. In particular, in high-pressure gas turbines the liquid fuel is seldom preheated to supercritical temperatures before injection, and the presence of both subcritical and supercritical conditions in the combustion chamber is warranted. Consideration of the liquid phase is therefore required in addition to the gas phase and the supercritical mixture. A single-fluid multiphase formulation of this problem is presented to investigate mixing and combustion of high-pressure transcritical liquid jets. The
formulation makes use of diffuse-interface concepts facilitated by the relatively larger interface thicknesses at these high pressures.

Session IV – Modeling and Computations

Title: Experimental and modeling study of the flow over a skewed bump
Authors: David Ching, Chris Elkins, John Eaton
Abstract: Three-dimensional separation can have a profound effect on the overall structure of flows as it affects the performance of vehicles, internal flow systems, and propulsion devices. The structure of some separated flows is very sensitive to minor geometric perturbations, and we suspect that the flow over a bump may exhibit such sensitivity. In this study, we examine the flow over a three-dimensional non-axisymmetric bump at various angles by using Magnetic Resonance Velocimetry (MRV). The flow is dominated by coherent vortices that are sensitive to the bump angle. With a symmetric bump, two counter-rotating vortices are formed in the near wake, but in the far wake there is a vortex pair rotating in the opposite sense. With the bump at an angle, one of the vortices is much stronger and overwhelms the other vortex to leave one main vortex downstream of the separation bubble. The shedding frequency in the wake was determined at two bump angles using a spiral magnetic resonance imaging sequence that provides a time series of measurements. The bump was found to have a higher shedding frequency when it is angled. RANS simulations were done to model the cases using the k-e model, and the simulations were found to be fairly accurate in the near wake, but very inaccurate in the far wake. This bump is being used as a test case for a new method of computing pressure from the velocity data.

Title: Single ventricle palliation with the assisted bidirectional Glenn (ABG)
Authors: Jessica Shang, Mahdi Esmaily-Moghadam, Tigran Khalapyan, Richard Figliola, Olaf Reinhartz, Tain-Yen Hsia, Alison Marsden
Abstract: For neonates with single ventricle physiology, a systemic-pulmonary shunt (e.g., a modified Blalock-Taussig shunt (mBTS)) is typically employed as an early-stage procedure in preparation for a later-stage bidirectional Glenn (BDG), which provides a better source of pulmonary blood flow. Mortality rates associated with the mBTS remain high, yet the BDG has poorer outcomes in neonates. The assisted bidirectional Glenn (ABG) proposes to augment the inadequate pulmonary flow associated with early BDG implementation in neonates through an additional shunt between the innominate artery and the superior vena cava (SVC). A nozzle component of the shunt injects high-velocity flow to the SVC and elevates downstream pulmonary pressure. Previous simulations and animal studies indicate that the procedure is feasible and can lead to higher pulmonary flow rates. In numerical simulations, we explore different placements of ABG shunts implanted into a 3D model of the aorta and pulmonary arteries, coupled with a lumped parameter network describing the behavior of the remaining circulatory system for a pre-Glenn patient. We find that the virtual ABG delivers superior pulmonary flow rates (up to 40% increase) and oxygen saturation in an idealized 3D model and in patient-specific models compared to the BDG. The venous pressure and heart load also increased with the ABG. A successful implementation of the ABG would replace the mBTS and BDG procedures and reduce mortality rates in single ventricle patients.

Title: Simulations of a probability density function model of homogeneous turbulence in an Eulerian reference frame
Authors: Alejandro Campos, Karthik Duraisamy, Gianluca Iaccarino
Abstract: The Interacting Particle Representation Model (IPRM) was developed by Kassinos & Reynolds (1996) to simulate the evolution of homogeneous turbulence. With the aim of improving accuracy, the IPRM incorporates additional characteristics of turbulent fluctuations beyond what is described by the Reynolds
stresses (e.g. dimensionality, circulicity). This feature sets it apart from traditional engineering models, whose main focus is the modeling of the Reynolds stresses alone. Later on, Van Slooten & Pope (1997) reinterpreted the IPRM as a Probability Density Function (PDF) model. PDF models are typically solved using particle methods, where a Lagrangian reference frame is employed to follow the evolution of sufficient particles. On the other hand, an alternate solution approach is to solve the evolution equation for the PDF in an Eulerian reference frame. We have developed a solution method for the IPRM that is based on the discretization of one of its marginal PDFs in an Eulerian reference frame. The first step involves the derivation of the marginal PDF in spherical coordinates, which reduces the number of variables that are inputs to the function, and thus the cost of computing its solution. A numerical method based on radial basis functions over a spherical domain is then implemented to discretize the model. The sensitivity of the Eulerian simulations to parameters of the numerical scheme (such as the size of the time step) is analyzed, as well as the stability of the approach based on eigenvalues of the discrete operator. Finally, a comparison between Eulerian and Lagrangian simulations are used to show comparable capabilities between the two approaches.

Title: Rankine-Hugoniot Behavior of Current-Driven Ionization Waves
Authors: Keith Loebner, Thomas Underwood, Mark Cappelli
Abstract: The Rankine-Hugoniot relations describing how flames propagate in combustible gases have been found to bear a striking similarity to how ionization fronts propagate through plasmas. Combustion phenomena ranging from candles to rocket engines are known to exhibit shared dynamics; in this presentation, we show that aspects of these dynamics can also be found in hot, ionized gases (i.e., plasmas) devoid of combustion. High-speed imaging of a pulsed plasma accelerator depicts two distinct types of ionization waves, corresponding to the two analytically-determined branches of the Hugoniot curve. A detailed set of direct immersed-probe measurements further demonstrates the remarkable analogy between the plasma behavior and that seen in combusting gases. These findings provide an important tool to researchers working in a number of fields, including astrophysics and fusion energy, where these ionization fronts appear and play key roles in the system dynamics and behavior.

Session V - Experiments

Title: In Situ Particle Tracking around kW Sized Wind Turbines
Authors: Ian Brownstein, John Dabiri
Abstract: Laboratory studies of model wind turbines are typically unable to match both the Reynolds number (Re) and tip speed ratio (TSR) of full-scale wind turbines. In order to match both relevant parameters, a quantitative flow visualization method was developed to take in situ measurements of the flow around full-scale wind turbines. The apparatus constructed was able to seed an approximately 9mx9mx5m volume in the wake of the turbine using artificial snow. Quantitative results were obtained by tracking the evolution of the snow using particle tracking algorithms. As a step toward full 3D-PTV measurements, results will be presented in which a 2D measurement is taken with a single camera positioned at the base of the turbine looking upward. The resulting tracking is therefore integrated in the span-wise direction. This method is demonstrated through a comparative study of a five-bladed VAWT producing power in different wind conditions at the Field Laboratory for Optimized Wind Energy (FLOWE) in Lancaster, CA. Future work to expand this method to 3D-PTV is also discussed.

Title: Sensitivity of shock boundary layer interaction to weak perturbations
Authors: Ji Hoon Kim, John Eaton
Abstract: Shock-boundary layer interactions (SBLIs) can be sensitive to small changes in the inlet flow and conditions. This sensitivity necessitates robust computational models for accurate predictions. Validation of such models requires a suitable experimental database with well-defined inlet and boundary conditions. To that end, the purpose of this experiment is to systematically document the effects of small geometric perturbations on a SBLI flow to investigate the flow physics and establish an experimental dataset tailored for CFD validation. The facility used is a Mach 2.1, continuous operation wind tunnel set up for particle image velocimetry (PIV) measurements. The SBLI is generated using a 3mm compression wedge placed in the upper wall of the test section; the region of interest is the on the bottom wall boundary layer, where the incident shock impinges and reflects. The geometric perturbations, which are small spanwise rectangular prisms, are introduced on the bottom wall ahead of the compression ramp. Mean streamwise and vertical velocity profiles are taken using high resolution PIV at the reflected/incident shock for 12 different bump locations and 4 different bump heights, resulting in a total of 48 different perturbation configurations. Current results show that the dominant effect of the perturbations is a global shift of the SBLI itself, as evidenced by the shift of the location of the shock crossing point. In addition, the bumps introduce weaker shocks of varying strength and angles, depending on the bump height and location. The results indicate that small uncertainties in scramjet isolator geometry, at the right location, can potentially have large effects on the shock train and engine performance.

Title: Patterns of 3D flow in a rotating cylinder array
Authors: Anna Craig, John Dabiri, Jeffrey Koseff
Abstract: Experimental data are presented for large arrays of rotating, finite-height cylinders, which may provide insight into the flow kinematics of an array of vertical axis wind turbines. These data show that the three-dimensional flows are strongly dependent on the geometric and rotational configurations of the array. Two geometric configurations of the cylinders, each with two rotational configurations, were examined for a total of four arrays. 2D PIV was conducted in multiple intersecting horizontal and vertical sheets at a location far downstream of the leading edge of the array in order to build up a picture of the 3D developed flow patterns. Most notably, a net mean vertical flow from above the array down into the array was found for several configurations. This planform flux is of particular interest as it would bring down into the array high kinetic energy fluid from above the array, thus increasing the energy resource available to turbines far downstream of the leading edge of the array.

Title: New MRI-based diagnostics for temperature and particle concentration
Authors: Daniel Borup, Pablo Vasquez Guzman, Caroline Abbott, Chris Elkins, John Eaton
Abstract: Magnetic Resonance Imaging (MRI) is currently used as a diagnostic tool for measurement of fully 3D, 3-component velocity and scalar concentration fields in turbulent flows. Unlike optical techniques, MRI is well suited for complex applications in which optical access is not possible. Here we present our efforts to extend the suite of MRI techniques to two new applications in water flows: temperature and particle concentration. In the first project (Magnetic Resonance Temperature/Heat Transfer Coefficient or MRT/MRHTC) we aim to leverage existing techniques from the medical arena for the measurement of water temperature. Hydrogen protons in water precess around the strong magnetic field in a clinical MRI scanner; the precession rate is a linear function of temperature, and so the temperature can be obtained by measuring the phase of the protons. Preliminary experiments showed that, for an inclined jet in crossflow, measured temperature compared well with previous scalar measurements after simple corrections were applied to the raw data. Currently, we are preparing a symmetric impingement jet experiment to measure heat transfer coefficient, as well as a thermally conductive version of the inclined jet in crossflow apparatus to allow for an experiment with conjugate heat transfer. In the second project (Magnetic Resonance Particle imaging, or MRP) our goal is to examine the 3D mean concentration field of solid particles in application-relevant geometries such as a turbine blade internal cooling passage. Previously reported work has shown that particles strongly
attenuate signal in MRI, which allowed for qualitative imaging of a particle streak in a turbulent flow. We now understand that a judicious choice of particle size and material can allow for imaging at much lower loadings than originally used. This choice, combined with imaging sequence development, has allowed for rapid and accurate data acquisition at particle concentrations as low as 0.08% by volume.

Session VI - Optimization & Uncertainty Quantification

Title: Fidelity-adaptive combustion simulations using a Pareto-efficient modeling framework  
Authors: Hao Wu, Matthias Ihme  
Abstract: A Pareto-efficient combustion (PEC) framework represents a modeling technique that utilizes combustion submodels at different levels of fidelity for application to complex chemically reacting flows. The model assignment takes into consideration user-specific inputs about quantities of interest, desired simulation accuracy and computational cost. In this work, an extension of this framework to LES of turbulent flames is presented. To this end, an analysis is conducted by performing simulations of a turbulent partially-premixed flame using premixed and diffusion flamelet models. The characteristics of the error estimators with respect to different quantities of interest are examined, and guidance on the model selection is provided.

Title: Dimensional Analysis and Reduction: The Pi Active Subspace  
Authors: Zachary del Rosario, Gianluca Iaccarino  
Abstract: How do we understand a model if the simulation runs for the age of the universe? The study of Dimension Reduction helps us to make impossible problems tractable. This study aims to defray the dreaded Curse of Dimensionality by reducing the number of input parameters, through various strategies. One such strategy to achieve Dimension Reduction is the Active Subspace procedure. Active Subspaces study the gradient of a function, in order to identify linear combinations of parameters that account for variability in some Quantity of Interest. In problems of practical interest, Paul Constantine and his colleagues have found that problems with as many as 50 dimensions reduce to a 1 dimensional Active Subspace - a huge reduction! Though Active Subspaces are powerful, their structure of linear combinations is difficult to interpret - and in some physical systems - not well suited to describe the inputs. Using classical results from Dimensional Analysis - namely, the Buckingham Pi Theorem - we develop an alternative formulation of Active Subspaces. This new formulation, called the Pi Active Subspace, seeks products of parameters and chases down the governing dimensionless parameters of a system.

Title: Data Assimilation and Propagation of Uncertainty in Multiscale Cardiovascular Simulation  
Authors: Daniele Schiavazzi, Alison Marsden  
Abstract: The increasing adoption of computational tools to complement clinical data collection and inform treatment decisions demands a thorough characterization of the confidence in the predicted quantities. This confidence is affected by modeling assumptions as well as variability in clinical data, anatomy, vessel wall material properties and physiological response to surgery. A wide spectrum of pathologies can be investigated using modern computational tools, including complex fluid-structure interaction phenomena (e.g., valve dynamics), multi-scale coupling between 3D Navier-Stokes solvers and 0D boundary circulation models, and growth and remodeling of vascular tissue. However, the challenge of "learning" model parameters from uncertain patient-specific data remains. This is key to our ability to simulate large patient cohorts and to overcome the limitations of operator-dependent and time consuming "manual" tuning often performed for these models. In this context, the ability of constructing condensed model representations is of primary importance to reduce the computational cost of performing iterative parameter estimation and UQ on large multi-scale numerical models. We present a technique based on Relevance Vector Machine regression that provides stable reduced order surrogates of three-dimensional cardiovascular CFD anatomies.
Starting from a characterization of structural and practical identifiability of these reduced representations, we then perform Bayesian parameter learning using adaptive, multi-level MCMC. Finally, forward uncertainty propagation to multi-scale model results is discussed in the context of surgical transition between the first and second stage of palliation in patients with single-ventricle congenital heart disease.

Title: *A multilevel multifidelity technique for Uncertainty Quantification*

Authors: Gianluca Geraci, Michael S. Eldred, Gianluca Iaccarino

Abstract: Numerical studies of any physical phenomenon or engineering device cannot leave aside the quantification of uncertainties on the simulations' outputs. Therefore, Uncertainty Quantification (UQ) has emerged in recent years as a fundamental tool for the scientific computing community. UQ for real-case applications remains challenging due to the presence of discontinuous/high-gradients responses or in general high non-linearity. Very often these features are associated with high dimensionality of the parameter space. In such situations it is very difficult to apply established deterministic UQ approaches, as stochastic collocation or Polynomial Chaos. Despite the improvements obtained in recent years to mitigate the curse of dimensionality associated with these algorithms in high-dimensional spaces, their applicability remains limited. More recently, to deal with high-dimensional parameter spaces, sampling methods gained popularity. In particular, the seminal Monte Carlo (MC) strategy has been generalized to multilevel approaches leading to the so-called Multi Level MC method (MLMC). The MLMC method has been demonstrated to be superior to MC in all possible scenarios, and it is a good candidate for many applications which actually are intractable by other UQ methods. However, the number of simulations required remains high, even if it is more favorable compared to other techniques. In this work we describe a technique aiming to reduce the computational burden through the use of a hierarchy of models. In particular, if it is possible to introduce a low-cost computational model, albeit less accurate, it is virtually conceivable to draw a large number of its realizations to decrease the variability of the MLMC estimator, associated to the high-fidelity simulations, using a control variate approach. We use a 1D heat conduction model problem, for which the stochastic solution is available, to illustrate the features of the new method and demonstrate its efficiency when compared to MC and the standard MLMC method.

Session VII – Large Eddy Simulation

Title: *Towards numerically efficient “enrichment” of LES for stratified Planetary Boundary Layers*

Authors: Aditya Ghate, Sanjiva Lele

Abstract: High Reynolds number wall bounded flows such as the Planetary Boundary Layer (PBL) is characterized by a very wide range of dynamically active scales. Hence, engineering and environmental applications (such as Wind Turbine Fatigue or Pollutant Dispersion) which are inherently sensitive to the spectral resolution of the numerically simulated PBL turbulence, tend to require LES that use very high resolution numerical grids. We will first demonstrate that Kinematic Simulations (Fung et. al., 1992) can be utilized as sufficiently robust surrogates for the high wavenumber content resolved using LES (at high resolutions) through a demonstration for a Stably Stratified PBL. The Gabor Transform is used to formalize this "enrichment" procedure. By invoking the assumption of "quasi-homogeneity", the exact equations that govern the evolution of the "enriched" scales are then solved in Gabor space by modeling the non-linear terms using a spectral viscosity developed using RNG (Ref. Canuto and Dubovikov, 1996) theory. The performance of this simplified approach is appraised using a model problem of the neutrally stratified PBL, and the space-time properties are compared with a recent high resolution LES computed by Stevens, Wilczek and Meneveau (2015). In this model problem, the very largest of scales (~ 200-300 meters) are frozen and advected at a bulk velocity which allows for a comparison with LES that is valid up to moderately large time scales. The results demonstrate excellent agreement between the second order space-time statistics. The computational
efficiency of the algorithm proposed in this talk can potentially make it very feasible to simulate real-world engineering problems such as the PBL-wake interactions and the ensuing fatigue loading in a large wind turbine arrays.

**Title:** LES-based characterization of a suction and oscillatory blowing fluidic actuator  
**Authors:** Jeonglae Kim, Parviz Moin, Avraham Seifert  
**Abstract:** Unsteady turbulent flows within a suction and oscillatory blowing actuator are simulated and characterized to provide better physical understanding of the complex actuator flows. Large-eddy simulation (LES) based upon a novel unstructured-grid technique is used to accurately calculate turbulent flows within the actuator. Simulations are performed for three inlet pressure conditions. Results show good agreement both qualitatively and quantitatively with the experimental measurement. The actuator is characterized by parameters such as pressure ratio, outlet velocity profile, oscillation frequency, suction to total flow rates. The LES-generated data are used to develop a reduced-order model applicable to integrated simulation of aerodynamic flow control as an unsteady boundary condition. Reduced-order modeling based upon dynamic mode decomposition (DMD) is employed to obtain a lower-order representation of the actuator outflows. Using two distinct dynamic modes, a sparsity-promoting variant of the standard DMD algorithm can describe unsteady flow fields at the actuator outlets with good accuracy.

**Title:** Minimum-dissipation models for large-eddy simulation  
**Authors:** Hyunji Jane Bae, Wybe Rozema, Parviz Moin, Roel Verstappen  
**Abstract:** Minimum-dissipation eddy-viscosity models are a class of subgrid scale models for LES that give the minimum eddy dissipation required to dissipate the energy of subgrid scales. The QR minimum-dissipation model [Verstappen, J. Sci. Comp., 2011] gives good results in simulations of decaying grid turbulence carried out on an isotropic grid. In particular, due to the minimum dissipation property of the model, the predicted energy spectra are in very good agreement with the DNS results up to the cut-off wave number unlike other methods. However, its results on anisotropic grids are often unsatisfactory because the model does not properly incorporate the grid anisotropy. We propose the anisotropic minimum-dissipation (AMD) model [Rozema et. al., submitted for publication, 2015], a minimum-dissipation model that generalizes the QR model to anisotropic grids. The AMD model is more cost effective than the dynamic Smagorinsky model, appropriately switches off in laminar and transitional flow on anisotropic grids, and its subgrid scale model is consistent with the theoretic subgrid tensor. Experiments show that the AMD model is as accurate as the dynamic Smagorinsky model and Vreman model in simulations of isotropic turbulence, temporal mixing layer, and turbulent channel flow.

**Title:** A metric for assessing the dynamic content of large-eddy simulations  
**Authors:** Gabriel Nastac, Luca Magri, Matthias Ihme  
**Abstract:** Metrics used to identify the quality of large-eddy simulations commonly rely on a statistical assessment of the solution. While these metrics are valuable, turbulence is inherently a dynamic phenomenon, and a dynamic measure is desirable to characterize the quality of a numerical prediction for capturing such phenomena. To address this issue, a dynamic metric utilizing a form of Lyapunov exponents and error growth rates is proposed and applied to two test cases: homogeneous isotropic turbulence and a turbulent jet diffusion flame. A grid refinement analysis is performed for each test case utilizing this dynamic metric and current results show monotonic trends versus LES filter width. Results for the homogeneous isotropic turbulence provide insights into the effect of LES-resolution on the initial rapid error growth rate; the metric asymptotically approaches a constant as the LES filter width approaches the smallest scales of the system.

Session VIII – Poster Session

**Title:** Parallel implementation and performance of hierarchical fast linear solvers
Authors: Chao Chen, Hadi Pouransari, Kai Yang, Alex Aiken, Eric Darve
Abstract: We present two kinds of hierarchical linear solvers and their parallel implementations. One is based on the hierarchical off-diagonal low-rank (HODLR) structure for dense matrices, which leads to a small number of flops and a small amount of communication. Our algorithm requires only small concurrent matrix solves that take place on a single processor, and matrix-matrix multiplication with data in distributed memory. Our implementation uses a novel runtime system named Legion, which is a data-centric parallel programming system and is very suitable for writing portable high performance programs. We demonstrate the scalability of our HODLR solver on a thousand cores. The other linear solver is based on a different H2 structure for sparse matrices. The algorithm shares some elements with the incomplete LU factorization, but uses low-rank approximations to remove fill-ins. The algorithm also uses multiple levels, in a way similar to multigrid, to achieve fast global convergence. Moreover, only local communication is needed for eliminating boundary nodes on every process. We show preliminary results for the second solver with an implementation using MPI.

Title: Direct Numerical Simulation of turbulent flows over superhydrophobic surfaces: capillary waves on gas-liquid interface
Authors: Jongmin Seo, Ricardo Garcia-Mayoral, (University of Cambridge), Ali Mani
Abstract: Superhydrophobic surfaces present new passive flow control methods for reduction of skin friction on immersed bodies in water; by entrapping gas bubbles in their roughness these surfaces can suppress direct contact between liquid and solid, and thus reduce drag. However, in turbulent flows, gas bubbles can be depleted due to high shear and pressure fluctuations. Our work explores inception mechanisms leading to the gas depletion on superhydrophobic surfaces under overlying turbulent flows. To this end, we perform direct numerical simulations of turbulent flows on superhydrophobic walls with deformable gas-liquid interfaces. The superhydrophobic surfaces are modeled as patterned slip/no-slip conditions on the water boundary. The dynamics of gas-liquid interface is investigated by allowing deformable interfaces through the Young-Laplace equation. Our results show that spanwise-coherent waves develop on the gas-liquid interface as a result of its interactions with turbulence. These waves travel upstream and result in significant pressure fluctuations near the interface. We will show that the traveling waves are well described by a Weber number based on the averaged slip velocity at the interface. In higher Weber number, such capillary waves augment the pressure fluctuations on the gas-liquid interfaces and thus deteriorate the stability of gas pocket.

Title: Uncertainty Quantification on Angle of Impact in Drop-Pool Impact Events
Authors: Seyedshahabaddin Mirjalili, Gianluca Iaccarino, Ali Mani
Abstract: Bubbles of the order of 10 microns known as micro-bubbles are often observed in natural or industrial applications such as oceanic breaking waves, trails of ships, oil aeration and surfactant scavenging. These bubbles can be advected to lower depths, where they can reside for long durations, and thus significantly enhance the gas to liquid mass transfer rate and/or leave a long term bubbly footprint. Experimental observations suggest that entrapment of air films under liquid-liquid impacts can lead to subsequent breakup processes, which can lead to the generation of micro-bubbles. In this study, we consider a canonical setting in which individual liquid drops impact a deep flat pool as a model representative of this phenomena. We present an investigation of the uncertainty in the entrapped air film associated with the angle of impact relative to the interface-normal direction. In practice, this uncertainty can be due to surface waves, wind or measurement errors; understanding this sensitivity might help in incorporating impact models as subgrid scale models in large-scale calculations. We have employed the direct numerical simulations of the Navier-Stokes equations in conjunction with a diffuse interface method to track the phase interface. For UQ analysis, stochastic collocation and quadrature-based non-intrusive polynomial chaos are employed to examine the effect of angle of impact on the characteristics of the thin film at impact time and interfacial profiles at a time after impact respectively. Our investigations showed that normal velocity is the key component in determining the characteristics of the thin film. In other words, keeping the magnitude of drop...
velocity constant while varying the angle resulted in significant variation in film characteristics, whereas changing the angle of impact while maintaining the normal velocity constant was shown to have minimal effects.

Title: Flow Reactor Study of Combustion Characteristics of Jet and Rocket Fuels  
Authors: S. Banerjee, K. Wang, and C.T. Bowman  
Abstract: The development of the next generation of efficient, fuel flexible gas turbine propulsion systems requires the implementation of large eddy simulation (LES) based turbulent combustion models that incorporate a combustion chemistry model for the aviation fuels. Such needs have motivated a significant effort toward the construction of detailed and reduced kinetic models for kerosene fuels. The commercial aviation and federal agencies are looking to further develop next generation fuels, many of which are synthetic biofuel derivatives. Meanwhile, extensive research has not yet been conducted on these types of bio-derivatives. The current study focused on the early stage pyrolytic chemistry of a commercial aviation fuel (Jet A), a rocket fuel (RP2), and a synthetic biofuel (Gevo-ATJ). The experiments were conducted in the Stanford Variable Pressure Flow Reactor at 1 atm pressure and at the intermediate temperature region, ~1100-1200 K. The reaction products were characterized using a micro GC against the residence time of 0-30 millisecond. The major products for the pyrolysis of Jet A and RP2 were found similar, including ethylene, methane, propylene, isobutene, acetylene, ethane, 1,3-butadiene, benzene and toluene. While the Gevo fuel had a significantly different product distribution; a most notable difference was that the Gevo fuel produced much more isobutene than the other two fuels; the formation of the two C3H4 isomers, propyne and allene, were also higher. This may be reflected by the fact that Gevo-ATJ contains significant more isoparaffin (over 99%) than the other two fuels. These observations and pyrolysis data will provide useful insights for the development and validation of combustion models for aviation fuels.

Title: Combustion chemistry modeling of jet fuels  
Authors: Rui Xu, Hai Wang  
Abstract: Jet fuels, conventional or alternative, are multicomponent hydrocarbon mixtures that may contain over thousands of molecular components. The composition can be rather complex and more critically, cannot be defined precisely. Coupled with the high degree of nonlinearity encountered in a combustion process, the advancement of a chemistry model for the combustion behavior of a particular jet fuel has been a daunting task. In the current work, we take an unconventional, new approach to this problem. It is known that in flames almost all large hydrocarbon fuels undergo oxidation in two steps. In the preheat zone of the flame and driven by thermodynamics, the fuel decomposes to about a half dozen of small molecular fragments in an endothermic process, regardless how complex the composition of the initial fuel is. The fragments are dominated by ethylene, propene, butene, butadiene, methane, benzene, toluene and hydrogen. The fragments then enter into the flame zone and are oxidized to combustion products in the second, exothermic step, which is rate limiting. It is through the decoupling of the above two processes, both temporally and spatially, that nature allows hydrocarbon fuels to be stable under ambient temperature while permit them to burn violently once ignited. This understanding allows us to treat the combustion chemistry of a jet fuel by a hybrid chemistry (HyChem) approach: the kinetics of thermal decomposition of the fuel is based on experiments, while the oxidation of the decomposed fragments is described by detailed, fundamental reaction mechanisms and rates. Here, we will show that the hybrid approach is by far the most accurate and efficient to obtain a basic understanding and predictive capability for both conventional and alternative jet fuels.

Title: Uncertainty quantification and minimization of a standard combustion chemistry model of foundational fuels  
Authors: Yujie Tao, Gregory P. Smith, Hai Wang
Abstract: The hierarchical nature of high-temperature oxidation of hydrocarbon fuels requires an accurate and reliable foundational fuel chemistry model. The current effort centers on providing a detailed chemical kinetic model with well-quantified and minimized uncertainty for use as a foundation for the combustion of all hydrocarbon fuels at high temperatures. This foundation model describes the combustion kinetics of hydrogen, carbon monoxide, and C1-4HxOy species. The current version consists of 291 elementary reactions of 33 species up to C2 fuels. The model development effort takes the following steps: trial model compilation in which the reaction pathways were analyzed and their rate constants evaluated, validation against experimental targets, rate constant re-evaluation and target list modification, constrained rate parameter optimization, uncertainty quantification and minimization. A total of 146 targets were selected for model optimization, including laminar flame speed, shock tube ignition delay and species profile of H2, CO, CH4, CH2O and C2H6 oxidation and H2O2 thermal decomposition. Experimental targets were carefully evaluated with special attention placed on the assessment of the uncertainties in the initial conditions and their impact on the simulation of flow reactor and shock tube experiments. Model optimization and uncertainty minimization is based on the Method of Uncertainty Minimization by Polynomial Chaos Expansion (MUM-PCE) [1], with response surfaces [2] generated from Monte Carlo sampling and factorial design. The poster will show the results of the model optimization. Comparisons between the trial and the optimized models will be presented in terms of reaction rate parameters and validation against experimental data, with an assessment of the possible sources of uncertainty and problems in the experimental data.

Title: Gas kinetic theory of nanostructure transport in dilute gases
Authors: Changran Liu, Zhigang Li, Hai Wang
Abstract: Aerodynamic drag force, diffusivity and electric mobility of long-chain molecules, nanorods and nanotubes in fluid media are of great importance to a large range of problems. Such problems include size classification of fibres aerosols, identification of long-chain biomolecules, gas-phase synthesis, processing, characterization of nanotubes and nanorod, and the transport of long-chain alkanes in reacting flows and fuel combustion. These problems are generally far removed from Stokes flow. Historically in the area of reacting and combusting flow simulations, the transport properties of chain-like molecules have been treated with the Chapman-Enskog theory assuming that the interactions of these molecules with the gas media can be treated by isotropic potentials. The validity of this assumption, however, was never examined in detail. Recent molecular dynamics evidence indeed suggests the spherical potential assumption to be inaccurate. This work proposes analytical solutions for aerodynamic drag force on cylindrical nanoparticle in free molecule flow. The derivation is based on the gas kinetic theory and accounts for the effect of intermolecular interactions between the nanoparticle and the gas media. The result of our derivation in rigid body limit agrees with Dahneke’s solution, which has been supported experimentally. Expressions for binary diffusivity of chain-like molecules in common bath gases are also obtained from the drag and the Stokes-Einstein relation. The long chain alkane diffusivities predicted using current theory resolve the experimental and modeling discrepancies previously observed for the extinction strain rates of counterflow, non-premixed n-decane and n-dodecane/nitrogen mixture versus oxygen.

Title: Spontaneous Hydrogen and Electricity Production in a Carbon Fuel Cell
Authors: D.U. Johnson, B.K. Loong, S.M. Stewart, T.M. Gür, R.E. Mitchell
Abstract: At the core of a sustainable future is green and non-polluting electricity production. Towards transitioning into a carbon-free energy future, carbon fuel cells (CFC) offer a great opportunity to achieve significant reduction in carbon emissions by highly efficient conversion of carbonaceous fuel, like coal and biomass, into electricity and/or hydrogen. Furthermore, due to the dense ceramic electrolyte membrane of CFCs, the carbon fuel never mixes with the air stream and therefore, a flue gas highly concentrated in CO2 is produced. Carbon fuel cells are hence ideally suited for integration with CO2 capture and storage technologies. To understand the cell design and system operational trade-offs, we have developed a comprehensive carbon
A fuel cell reactor model. The model includes detailed electrochemistry of the electrode reactions, carbon bed chemistry as well as heat and mass transfer throughout the cell and the reactor. Using the model, we calculate performance metrics such as power density and cell efficiency as well as concentration and temperature distributions within the reactor domain. By exercising the model, we determine how geometric and operational parameters affect these performance metrics. Trace elements contained in coal and biomass, in particular sulfur, is one of the major hurdles to overcome to make carbon fuel cells a practical technology for spontaneous electricity and hydrogen production. Sulfurous species poison the anode catalysts and rapidly degrade fuel cell performance. To overcome this technical problem we are following a two-prong approach. Firstly, we are developing sulfur-tolerant anodes, with a focus on perovskite materials, which are able to maintain their catalytic activity under low sulfur-containing environments. Secondly, we are exploring solid sorbents that can reduce the sulfur gas concentration to electrode-tolerable levels before the sulfur-species reach the anode surface. In this poster, progress in developing a comprehensive carbon fuel cell model and overcoming the sulfur problem is presented.

**Title:** Particle Laden Turbulence in a Duct with Rounded Corners  
**Authors:** Hoora Abdehkakha, Gianluca Iaccarino  
**Abstract:** Aim of this study is to investigate the effects of rounded corner duct on fluid motion and particle distribution. Secondary motion generated in a duct can play a major role in particle preferential concentration, especially near the walls and the corners. In present work, a rounded corner duct and a square duct in high Reynolds number turbulent regime are compared. Comparison shows that stronger secondary motion in rounded corner duct leads particles toward the corners and the walls.

**Title:** The Virtual Inhaler: Particle Inhalation in the Lungs  
**Authors:** Taylor Geisler, Sourav Padhy, Gianluca Iaccarino, Eric Shaqfeh  
**Abstract:** Assessing the human health risks from inhalation of harmful aerosol particle suspensions is often performed by extrapolating experimental data taken using nonhuman primates to humans. Rhesus monkeys in particular are commonly used as substitutes for humans in these studies. Among these numerous in-vivo experimental deposition studies, published results are often coarse measurements of deposition from medical scans or biological dose-response data and don’t provide detailed physical insight into small-scale transport/deposition mechanisms at work. Numerical simulations are proposed as a method to elucidate detailed features of flow and deposition patterns in these animal airways and as a complement the body of experimental data. The “Virtual Inhaler” code has been developed as a robust, scalable, and multi-purpose solver capable of accurately computing both fluid and particle transport equations for an arbitrary airway geometry. The code has been previously used to predict fluid flow and deposition in human lungs, and was validated by comparison to flow through a 3D printed replica lung. In this study, computational studies in a rhesus monkey nasal airway are performed using this framework. Using a CT scan of an adult rhesus monkey head and torso, a computational mesh was created that matched, to millimeter precision, the details of the animal's nasal airway. The simulated nasal airway extends from the nostrils to the end of the trachea, and particle deposition in this region can be seen as filtration before the lower bifurcating regions of the lungs. Micro-particle deposition fractions and locations have been calculated and compared to in-vitro experiments. Additionally, we have investigated asymmetry in particle deposition in a human lung induced by changes in upper-body position, as well as due to the natural asymmetry of the lung. Using these results, we can selectively target aerosol therapeutics from inhalers and predict ways to efficiently deliver inhaled medication to patients.
Title: Laser Characterization of Unsteady Ion Velocity Fields in Hall Thrusters  
Authors: Christopher Young, Andrea Lucca-Fabris, Natalia MacDonald, William Hargus Jr., Mark Cappelli  
Abstract: Time-resolved, two-dimensional (axial/radial) xenon ion velocity fields in a 600 W Hall thruster plume are obtained with a non-perturbative laser-induced fluorescence (LIF) diagnostic. Time resolution is achieved with a parallelized sample-hold approach, partitioning fluorescence signal into discrete measurement gates in time that are synchronized with a specific phase along the strong 48 kHz "breathing mode" current oscillation. Both LIF signal intensity and measured velocity vectors fluctuate on this time scale. This work provides detailed insight into the complex, time-dependent ionization and ion acceleration mechanisms in the channel and near-field plume of the Hall thruster.

Title: The Characterization of a Plasma Deflagration Accelerator For Simulating Fusion Wall Response to Disruptions  
Authors: Thomas Underwood, Keith Loebner, Ben Wang, Mark Cappelli  
Abstract: Transient events in fusion power plants such as DEMO and ITER are known to pose a severe threat to plasma facing components (PFCs) due to melting and erosion after repeated edge localized mode (ELM) loads. In situ experimental testing of potential PFC materials at fusion relevant conditions is difficult and expensive, and as a result plasma devices capable of replicating the desired transient conditions are of increasing interest. At Stanford University, an experimental facility designed to mimic the heat flux, particle fluence, and other key characteristics of ELMs and disruption events in a controlled setting has been developed. A pulsed plasma accelerator operating in the deflagration mode is used to generate high velocity (40-100 km/s) directed plasma jets that are stagnated on target material samples. In this work, we present probe data characterizing the plasma parameters of the accelerated plume using hydrogen as the working gas, as well as preliminary target studies of silicon and copper witness plates exposed to pulses at various total and peak shot energies. Results from the probe analysis indicate achieved energy fluxes and heat flux parameters that are ELM-like, and the observed linearly-correlated damage morphologies on the witness plates indicate that initial surface roughness plays a significant role in the growth characteristics of surface damage patterns.

Title: Electroconvection near the interface of ion-selective membranes and a microchannel  
Authors: Karen Wang, Ali Mani  
Abstract: The transport dynamics of electroconvective flows near ion-selective membranes subject to sidewalls are studied using a direct numerical simulation of the coupled Poisson-Nernst-Planck and Navier-Stokes equations. Previous studies have investigated electroconvective instability near infinitely large flat membranes and have demonstrated their role in significant enhancement of transport via added advection effects. This study demonstrates how the presence of sidewalls from a connecting microchannel can affect the onset of electroconvective flows and also impact the net ion transport rate. We demonstrate that while sidewalls have negligible effect on the onset of instability, they significantly regularize electroconvective vortices resulting in suppression of transport rates. We will discuss the impact of sidewalls on topology of electroconvective vortices and mean ion concentration fields.

Title: Enhancement of Overlimiting Current through an Ion-Selective Membrane via Patterning of Surface Ion-Permeability  
Authors: Scott Davidson, Matthias Wessling, Ali Mani  
Abstract: Electroconvection's ability to enhance transport through ion-selective surfaces provides promising opportunities for improving many diffusion-limited electrochemical and microfluidic systems. We have investigated two sources of electroconvection at ion-selective surfaces, electrokinetic instability and surface-patterning with impermeable stripes and their interactions using direct numerical simulation of the governing equations. We show that despite the reduced surface area available for transport, patterned surfaces can lead
to an up to 80% increase in current density relative to homogeneous surfaces. At applied voltages below the nominal threshold of instability, patterning enhances transport by inducing flow. At higher voltages it does so by regularizing the chaotic electroconvective flows.

Title: Hybrid Analysis of Engine Core Noise  
Authors: Jeffrey O'Brien, Jeonglae Kim, Matthias Ihme  
Abstract: As further reductions in aircraft engine noise are realized, the relative importance of reducing engine core noise increases. In this work, a representative engine flow path is studied to examine the mechanisms by which direct and indirect core noise propagates through the engine and affects the farfield noise emerging from the exhaust. The flowpath consists of a model gas turbine combustor, a single-stage turbine, a converging nozzle, a near field jet, and far-field acoustic radiation. A combination of high-fidelity and low-order simulation techniques are used to represent the development and propagation of disturbances through the flowpath, and a one-way coupling procedure is employed for propagating disturbances from one stage of the calculation to the next. Particular attention is directed to the direct noise calculation in the combustion chamber, as well as LES calculations of the nozzle and its associated near-field jet. Results show changes in both the directivity and spectra of farfield jet noise due to the presence of upstream perturbations. The low frequency portion of the jet's far-field spectrum is amplified by as much as 5 dB at certain angles, which can be attributed to the low frequency direct noise associated with the unsteady combustion occurring upstream. Additionally, the high frequency portion of the spectrum exhibits a slight reduction in SPL and becomes more tonal in nature due to increased vortex pairing attributable to the broadband perturbations. It is clear from these results that core noise can have a meaningful impact on overall aviation engine noise.

Title: Uncertainty Quantification of Nonlinear Electrokinetic Response in a Microchannel-Membrane Junction  
Authors: Shima Alizadeh, Gianluca Iaccarino, Ali Mani  
Abstract: We have conducted uncertainty quantification (UQ) for electrokinetic transport of ionic species through a hybrid microfluidic system using different probabilistic techniques. The system of interest is an H-configuration consisting of two parallel microchannels that are connected via a nafion junction. This system is commonly used for ion preconcentration and stacking by utilizing a nonlinear response at the channel-nafion junction that leads to deionization shocks. In this work, the nafion medium is modeled as many parallel nanopores where, the nano-pore diameter, nafion porosity, and surface charge density are independent random variables. We evaluated the resulting uncertainty on the ion concentration fields as well as the deionization shock location. The UQ methods predicted consistent statistics for the outputs and the results revealed that the shock location is weakly sensitive to the nano-pore surface charge and primarily driven by nano-pore diameters. The present study can inform the design of electrokinetic networks with increased robustness to natural manufacturing variability. Applications include water desalination and lab-on-a-chip systems.

Title: Shock Boundary Layer Interaction and Weak Ignition in Shock Tube Reaction Kinetic Studies  
Authors: Kevin Grogan and Matthias Ihme  
Abstract: Regimes of shock boundary layer interaction are proposed in consideration of shock tube kinetic experiments. For this, we consider three ways that the reflected shock wave interacts with the boundary layer: incipient separation occurs when the shock is just strong enough to subject the flow to an adverse pressure gradient leading to flow reversal; shear layer instabilities manifest after a certain length of time and cause inhomogeneities in the test gas through the ejection of roller vortices from the separated shear layer; and shock bifurcation occurs when the back pressure of the test gas is sufficient to contain the boundary layer fluid within a stagnation bubble causing severe inhomogeneities in the test gas. Theory delineating these regimes is developed, and these delineations are compared to detailed simulations of shock tube experiments as well as experimental data, where reasonable agreement is found. Through the theory applied to the incipient
separation regime, it is determined that boundary layer separation likely occurs in most shock tube experiments; however, separation is unlikely to affect chemical kinetic experiments except at long test times. Additionally, a bifurcation Damkohler is introduced, which is found to perform sensibly well at classifying strong and weak ignition in shock tubes, implying that these combustion phenomena are determined by a competition of physical and chemical timescales. Finally, simulations suggest that tailoring the incident shock Mach number for a given experiment could provide opportunities for mitigating inhomogeneities in the test gas.

**Title:** Photonic Crystal Mode Manipulation with Plasma  
**Authors:** David Biggs and Mark Cappelli  
**Abstracts:** The effect of a low-pressure plasma column on a resonant cavity in a miniature photonic crystal is studied experimentally and computationally. The photonic crystal is created using a square array of alumina rods with the center rod removed to create the resonant cavity. Out of plane radiative losses are minimized by a copper waveguide on either side of the photonic crystal. This geometry creates various resonant modes, some of which are localized to the resonant cavity. The plasma column is formed by a kHz discharge in argon gas at 1 Torr. The bandgap and defect state properties of the photonic crystal with and without a plasma column are measured using a vector network analyzer. The experiments are compared with simulations using a finite difference time domain electromagnetic solver and a simple Drude model of the plasma column.

**Title:** Plasma Metasurface for THz Wave Manipulation  
**Authors:** Roberto A. Colón Quiñones and Mark A. Cappelli  
**Abstracts:** A plasma metamaterial (PM) is an array of plasma structures that interacts with electromagnetic (EM) waves in ways not possible with natural materials. Two-dimensional PMs can be used for generating a band gap, which is a range of wave frequencies in which no waves are transmitted through the structure. Such gap forms when an EM wave travels through a 2D PM of plasma frequency ($\omega_p$) on the order of the frequency of the wave. Until recently, research on PMs has been limited to ($\omega_p < 30$ GHz, which is equivalent to a plasma density of $n_e < 10^{13}$ cm$^{-3}$. Over the last year, PMs of $n_e > 10^{15}$ cm$^{-3}$ have been generated at Stanford through the use of high-power lasers. The PMs are generated by expanding the laser beam from a Q-switched Nd:YAG laser through a Galilean beam expander and subsequently focusing the beam through an optical micro-lens array. The intense photoionization of air that occurs at the focus of the individual lenses leads to the formation of a 2D array of very dense plasma spots. Optical diagnostics show a plasma lifetime of ~500 ns during which the plasma array functions as a PPC, representing a first step towards advancing the field forward into the low THz regime.
Title: Fast linear solvers for variable density turbulent flows  
Authors: Hadi Pouransari, Ali Mani, Eric Darve  
Abstract: In a variety of natural and industrial systems variable density flows are present. Astrophysical flows and flows involved in combustion processes are such examples. For an ideal gas subject to low-Mach approximation, temperature variations can lead to a non-uniform density field. In this work, we consider heated particle-laden turbulent flows as an example application in which density variability is resulted from inhomogeneities heating. Under such conditions, the divergence constraint of the fluid is enforced through a variable coefficient Poisson equation. Inversion of the discretized variable coefficient Poisson operator is difficult using the conventional linear solvers as the size of the problem grows. We apply a novel hierarchical linear solve algorithm based on low-rank approximations. The proposed linear solver could be applied to variety of linear systems arising from discretized partial differential equations. It can be used as a standalone direct-solver with tunable accuracy and linear complexity, or as a high-accuracy pre-conditioner in conjunction with other iterative methods. We present various benchmarks obtained from discretized variable coefficient Poisson equation.

Title: Molecular dynamics of supercritical fluids  
Authors: Dongping Chen and Hai Wang  
Abstract: Next generation of gas-turbine combustors is expected to operate under pressure substantially higher than those in today's engines. The elevated pressure leads to a range of fundamental problems in our ability to predict a range of relevant combustor phenomena, including spray breakup and evaporation, mixing and chemical reactions. The most critical concern is that under the relevant pressure and temperature conditions the multicomponent fluid is supercritical where thermodynamic and transport theories are largely unavailable for mixtures. It is known that supercritical fluids are not homogeneous. They always show some degrees of inhomogeneity at small scales. Such inhomogeneity suggests that for multicomponent mixtures phase separation could occur at the microscopic scale. In this study, we carried out molecular dynamics simulations for supercritical fluids ranging from simple, single-component Lennard-Jones fluid (e.g., argon) to multicomponent mixtures of long-chain hydrocarbons in nitrogen to demonstrate and explore the influence of microscopic inhomogeneity on thermodynamic and transport properties. In agreement with literature findings, a supercritical LJ fluid has a liquid-like region and a gas-like region. The liquid region is characterized by a nearly continuous liquid media in which microscopic “bubbles” are formed dynamically. The gas region is characterized by the formation of molecular clusters due to appreciable intermolecular interactions. The structural and dynamic variations appear to produce interesting phenomena that govern the fluid thermodynamic and transport properties, including the spike in specific heat and failure of the Chapman-Enskog theory to reproduce self-diffusion coefficient. Given the above observations, it is not difficult to understand why special considerations must be made to treat the properties of multicomponent supercritical fluids, as will be discussed in the context of molecular dynamics under a range of conditions.

Title: Assessment of discontinuous Galerkin scheme for high-fidelity simulation of turbulent flows: scheme optimization and comparison to finite-volume solver  
Authors: Yu Lv, Matthias Ihme  
Abstract: The performance of a high-order discontinuous Galerkin method is assessed through direct comparisons against a state-of-the-art finite-volume solver in application to homogeneous isotropic
compressible turbulence. Four different cases are examined to cover a wide range of operating conditions, and an optimal DG-algorithm is formulated to minimize numerical dissipation. Through numerical experiments, it is shown that the preconditioned Roe solver in combination with standard symmetric interior penalty diffusion treatment results in an optimal formulation. To further enhance the solution robustness, the entropy-bounding DG-technique is utilized to achieve numerical robustness, especially for highly compressible flow regimes. Direct comparisons with conventional discretization techniques show that finite-volume schemes hold advantages over DG-scheme on regular hexahedral meshes; however, due to the reduction in the numerical accuracy on unstructured and tetrahedral meshes, the DG-method consistently outperforms finite-volume schemes, as result of the reduction in numerical accuracy.

**Title:** Strategies for improving performance of the Surrogate Management Framework in cardiovascular flow optimization  
**Authors:** Aekanash Verma, Alison Marsden  
**Abstract:** Engineering optimization problems are often limited by the cost of function evaluations. Furthermore, calculation of gradients in such problems can be expensive or even infeasible. Derivative free optimization methods such as variants of the Surrogate Management Framework (SMF) are suitable for such problems and offer a well-established convergence theory. The SMF is comprised of a local search step that is accelerated by a surrogate-based global search. Kriging is typically used for generating the surrogate used in the global search step and pattern search is used for the local or poll step. Traditionally, Kriging-based SMF develop problems during the course of the optimization which affect both global and local search performance. Two such issues are the piling-up of evaluations in a certain region in the design parameter space and improper refinement of the local search grid. We consider the origins of pile-up and improper refinement in view of the SMF algorithm. Then, we propose strategies to alleviate these issues and discuss the performance of these strategies and their mechanisms of improvement. Finally, we apply these strategies to some illustrative problems in cardiovascular blood flow simulations.

**Session X – Multiphysics Simulations**

**Title:** Effects of buoyant forces on chaotic electroconvection  
**Authors:** Elif Karatay, Matthias Wessling, Ali Mani  
**Abstract:** Mass transfer of ions in salt solutions adjacent to charge selective or polarizable surfaces is relevant to a wide variety of systems, spanning from microfluidic separations to large scale desalination systems. The transport of ions is enhanced by induced electroconvection that arise due to electrokinetic instabilities stemming from coupling of hydrodynamics with electrostatic forces. Recent research have presented comprehensive computational analysis of induced electroconvection and have shown the contribution of chaotic multi-scale structures beyond a threshold value of applied electric potential, $\sim \mathcal{O} (1)$ V. However the buoyant forces have been neglected in the existing studies of chaotic electrokinetic flows where the density gradients of salt depletion can become gravitationally stable or unstable depending on the geometric orientation of electrokinetic systems. In this study we thoroughly examine the interplay of gravitational convection and chaotic induced electroconvection in both gravitationally stable and unstable configurations via direct numerical simulations of a model system consisting of a salt solution confined in between two cation selective membranes. Our results reveal that buoyant forces are not negligible and have significant impact on the dominating transport mechanism, even for a millimeter scale gap involving a dilute 1 mM salt solution. When the density gradient of salt depletion is gravitationally stable, the growth of the electrokinetic flow structures are saturated by buoyant forces resulting in diminished mass transfer of ions thereby reduced electric current density. Whereas gravitationally unstable density gradient leads to buoyant flow structures contributing to the mass transfer of ions and thereby enhancing the electric current density.
Our investigations in a wide range of applied potential $\Delta \phi$ and $Ra$ numbers further identifies the asymptotic states where the transport is dominated by either gravitational convection or electroconvection.

**Title:** Simulation of flows involving elastic/plastic deformation of interfaces  
**Authors:** Niranjan S. Ghaisas, Akshay Subramaniam, Sanjiva K. Lele  
**Abstract:** Elastic-plastic large deformations of solids in contact with fluids is of interest in problems such as inertial confinement fusion and manufacturing processes such as metal welding. On account of the large deformations involved, Eulerian, as opposed to Lagrangian, methods are more suitable for these problems. We extend a tenth-order compact finite-difference spatial scheme with fourth-order Runge-Kutta time stepping, previously applied to multi-fluid problems, to problems involving elastic-plastic deformations in solids. Handling large jumps in the solution, such as those encountered in the presence of shocks, requires augmenting the centered finite-difference scheme with artificial fluid properties, such as artificial bulk and shear viscosities, artificial conductivity and artificial mass diffusivity. A method to auto-tune the artificial bulk coefficient based on the material properties and problem parameters is proposed. One and two-dimensional elastic-plastic test problems, including impacts of solids, problems involving shear waves, and the Noh-implosion problem, will be presented. Extension of this method to solid-gas problems is planned in the future.

**Title:** Large Eddy Simulation of Airfoil Self-Noise at High Reynolds Number  
**Authors:** Joseph Kocheemoolayil, Sanjiva Lele  
**Abstract:** Over the past 15 years, significant strides have been made towards using large eddy simulations (LES) for predicting airfoil self-noise. However, they have largely been restricted to canonical configurations at low Reynolds numbers. We summarize the progress made towards extending the scope of LES-based predictions to full-scale Reynolds numbers and non-canonical configurations such as noise generated by flow past an airfoil in the near-stall and post-stall regimes.

The trailing edge noise section of the Benchmark Problems for Airframe Noise Computations (BANC) workshop features five canonical problems at full-scale Reynolds numbers. No first-principles based approach free of empiricism and tunable coefficients has successfully predicted trailing edge noise for the five configurations to date. Our simulations that combine LES with a model for unresolved near-wall turbulence predict trailing edge noise accurately for all five configurations. Successful prediction of noise generated by an airfoil in the near-stall regime will also be demonstrated. Predicting the flow past a wind turbine airfoil in the post-stall regime is a formidable challenge in itself. A novel, large-span calculation that predicts the flow past a wind turbine airfoil in deep stall with unprecedented accuracy is presented. In agreement with a recent theoretical study, our simulation results indicate that the lower lift due to large-scale three dimensionality can be reproduced even in span-periodic calculations as long as the domain size is large enough to contain the stall cells. The simulations are performed using the massively parallel unstructured large eddy simulation framework CharLES provided by Cascade Technologies.

**Title:** Microwave photonic bandgap devices with active plasma elements  
**Authors:** Benjamin Wang, David Biggs, and Mark Cappelli  
**Abstract:** A 3-D alumina rod based microwave photonic crystal device with integrated gaseous plasma elements is designed and characterized. Modulation of the plasma density of the active plasma elements is shown to allow for high fidelity modulation of the output signal of the photonic crystal device. Finite difference time domain (FDTD) simulations of the device are presented, and the functional effects of the plasma electron density, plasma collision frequency, and plasma dimensions are studied. Experimental characterization of the transmission of the device shows active tunability through adjustments of plasma parameters, including discharge current and plasma size. Additional photonic crystal structures with integrated plasma elements are explored.
Session XI - Heat Transfer & Mixing

Title: Thermal Convection from a Minimal Flow Unit to a Wide Fluid Layer
Authors: Curtis Hamman, Parviz Moin
Abstract: In any flow computation, only a portion of the flow is simulated. Boundary conditions separate the flow from its surroundings, but the exclusion of eddies larger than the domain size may distort the flow. In this talk, the use of periodic boundary conditions are examined for thermal convection between rigid walls. Computations of the "minimal channel" by Jimenez & Moin (1991, JFM) provided a conceptual framework and building block from which to study near-wall turbulence driven by mean shear in small computational boxes. Mean buoyancy, in contrast, can sustain a vigorous field of large eddies that extend across many full channel heights. We examine whether a finite periodic array of such structures can predict certain turbulence statistics in thermal convection with and without a mean flow in large-aspect ratio channels.

Title: Heat Transfer and Drag of a Sphere: Variable Density and Buoyancy Effects
Authors: Swetava Ganguli, Sanjiva Lele
Abstract: How do forces acting on a particle change in the presence of significant heat transfer from the particle, a variable density fluid or gravity? We define unit problems isolating subsets of these phenomena and solve them via particle resolved simulations. Our investigations are agnostic to the Boussinesq regime and encompass both, the short time (acoustic) behavior and the subsequent nearly-incompressible flow field that is established. Defining $\lambda$ as the ratio of the initial particle-fluid temperature difference to the far-field fluid temperature, we observe that the particle size affects the acoustic response whereas $\lambda$ and Re affects the low-Mach response. The heating of the fluid near the particle affects the acoustic response whereas $\lambda$ and Re affects the low-Mach response. The heating of the fluid near the particle affects the drag significantly which is studied in a parameter space where Re, $\lambda$ and the Grashof number are varied. In the isothermal case, the drag computed numerically matches the drag correlation of Clift-Grace-Weber. For heated particles, using the density of the fluid at the particle surface in the correlation under-estimates the drag (e.g. by 30% when $\lambda = 1$), using the dynamic viscosity of the fluid at the particle surface over-estimates the drag (e.g by 17% when $\lambda = 1$) and using both still over-estimates the drag (e.g. by 13% when $\lambda = 1$). The deviations increase as $\lambda$ increases.

Title: Turbulent Scalar Flux Modeling for Inclined Jets in Crossflow: an Optimization Approach
Authors: Pedro Milani, Kevin Ryan, John Eaton
Abstract: Turbulent mixing for jets in crossflow is important in numerous applications. Reynolds-averaged models for turbulent scalar transport are usually based on the gradient diffusion hypothesis (GDH), with a scalar eddy diffusivity calculated from the model eddy viscosity. Such models are not accurate in the near jet region causing poor prediction of the scalar concentration distribution. We use 3D mean velocity and concentration data acquired using magnetic resonance imaging to infer improved diffusivity models. The transport equation is solved using the experimental velocity data and a prescribed functional form for the scalar diffusivity. An evolutionary algorithm then optimizes the model constants to minimize the difference between the calculated and measured scalar concentration fields. Tests of multiple model forms for seven different jet in crossflow configurations provide insight into the required characteristics of advanced models. The GDH with a weakly anisotropic diffusivity is very accurate beyond 4 hole diameters downstream of the injection point. However, standard turbulent diffusivity models overestimate turbulent mixing in the separation region; in most cases, the optimization procedure inferred counter-gradient diffusion in this region. New models that adjust automatically depending on the characteristics of the mean velocity and concentration fields are under development.

Title: Numerical Simulation of Multi-Material Mixing in an Inclined Interface Richtmyer-Meshkov Instability
Authors: Akshay Subramaniam, Sanjiva Lele

Abstract: The Richtmyer-Meshkov instability arises when a shock wave interacts with an interface separating two fluids. In this work, high fidelity simulations of shock induced multi-material mixing between nitrogen and carbon-dioxide in a shock tube are performed for a Mach 1.55 shock interacting with a planar material interface that is inclined with respect to the shock propagation direction. In the current configuration, unlike the classical perturbed flat interface case, the evolution of the interface is non-linear from early time onwards. Our previous simulations of this problem at multiple spatial resolutions have shown that very small 3D perturbations have a large effect on vortex breakdown mechanisms and hence fine scale turbulence. We propose a comparison of our simulations to the experiments performed at the Georgia Tech Shock Tube and Advanced Mixing Laboratory (McFarland et al., 2014).

Results before and after reshock of the interface will be shown including TKE, Reynolds stress anisotropy and turbulent mass flux. Simulations shown are conducted with an extended version of the Miranda solver developed by Cook et al (2007) which combines high-order compact finite differences with localized non-linear artificial properties for shock and interface capturing.