

Conditional Analysis of DNS Combustion Data Using Local and Global Shape Characteristics

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As high performance computing resources continue to improve, scientists are able to study physical phenomena with unprecedented resolution and complexity. For example, direct numerical simulations (DNS) are first principle, high-fidelity, computational fluid dynamics simulations in which Navier-Stokes equations are numerically solved on a computational mesh in which all of spatial and temporal scales of turbulence can be resolved. These detailed simulations are performed by the combustion science community to study fundamental turbulence-chemistry interactions in an effort to reliably predict efficiency and pollutant emissions for new engines and fuels. Through computing enabled by SciDAC, DOE INCITE and T2O grants, a library of DNS configurations and parametric studies have been performed and archived using S3D, a massively parallel simulation code, developed at the Combustion Research Facility at Sandia National Laboratories. The unique benchmark data generated by S3D is used to glean fundamental insight into combustion processes, and to aid the development and validation of engineering models used in CFD to optimize the design of future combustors.

The data that is output from S3D is extremely large and multi-dimensional and, with increased computational resources, will continue to increase in both size and complexity. Feature identification and characterization in such massive data is challenging and is further complicated by the fact that turbulence is a chaotic phenomenon characterized by a wide range of scales – 4 decades of spatial scales from microns to centimeters and temporal scales from nanoseconds to milliseconds. Feature-based conditional statistical methods are essential for the analysis of this complex, large-scale data. We introduce two shape-based conditional analysis algorithms that can be deployed in complementary settings: local methods are required when the phenomena under study comprises many small intermittent features, while global shape methods are required to study large-scale structures. We present the algorithms in context with their motivating combustion science case studies, but note that the methods are applicable to a broad class of physics-based phenomena.

Conditional Analysis Using Local Shape Characteristics

Motivation: The scalar dissipation rate, χ , is the rate at which scalar fluctuations decay due to diffusive processes. Thin pancake-like regions of locally high χ are created by compressive turbulent strains; whose thickness is assumed to be correlated with length scales of turbulence. In an effort to gain insight into the relationship between mechanical strains and chemical processes in turbulent mixing, one interesting characteristic is the relationship between the thickness and the mean temperature within these structures.

Feature Definition: When many small features exist whose threshold definitions are not known *a priori*, a merge tree efficiently encodes regions of interest

- A merge tree (see Figure 1) represents the merging of contours as isovalues of χ are varied from global maximum to global minimum.
- Each branch of the tree represents a family of contours that continuously evolve without merging as the isovalue is lowered.
- The relevance-based persistence metric (see Figure 2) scales each node in the by its local maximum – the highest in its corresponding subtree.
- Features are defined as the subtree above a user-specified relevance value that lies in $[0, 1]$.

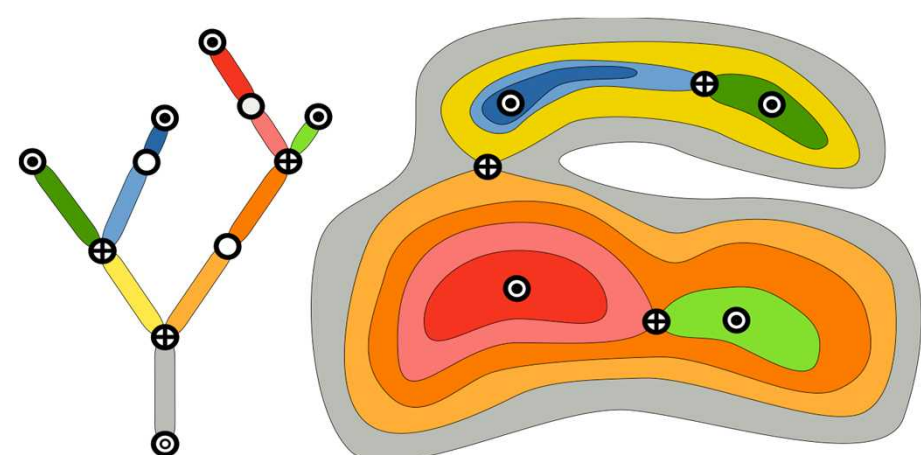


Figure 1: The merge tree provides a complete history of how families of level sets interact as a function is swept from global maximum to global minimum. On the right, a height function is defined on a 2-dimensional plane with associated merge tree shown on the left, with each arc in the tree corresponding to the region with the same color.

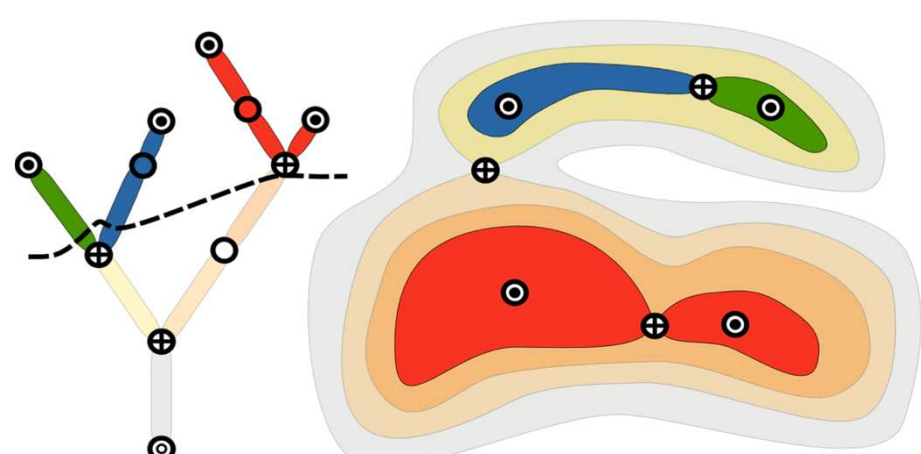


Figure 2: A relevance based segmentation for relevance slightly above 0.2 (slightly below 80% of the local maximum per branch).

Conditional Analysis: We augment the features in the merge tree with various statistics (first- through fourth-order moments, minimal and maximal function values) as well as shape metrics. Statistical summaries, including conditional empirical cumulative density functions, histograms, time-series and parameter studies can be efficiently generating using our data structures.

- For each feature we compute its mean temperature value, temperature variance and first three length scales.
- Length, width & thickness are estimated using a spectral technique in which each shape according to its first non-trivial eigenvector to compute its length, and use the same technique recursively on isocontours of the first eigenvector to compute the width and thickness (see Figure 2).
- The plot in Figure 4 shows the distribution of χ -thicknesses, at a relevance of 0.85, computed for structures grouped by the mean temperature in the segment for four bins, each 250 Kelvin wide. To ensure that the results are not influenced by excessive internal temperature variations, only structures with a low temperature variance (below 5% of the maximum variance) are considered.

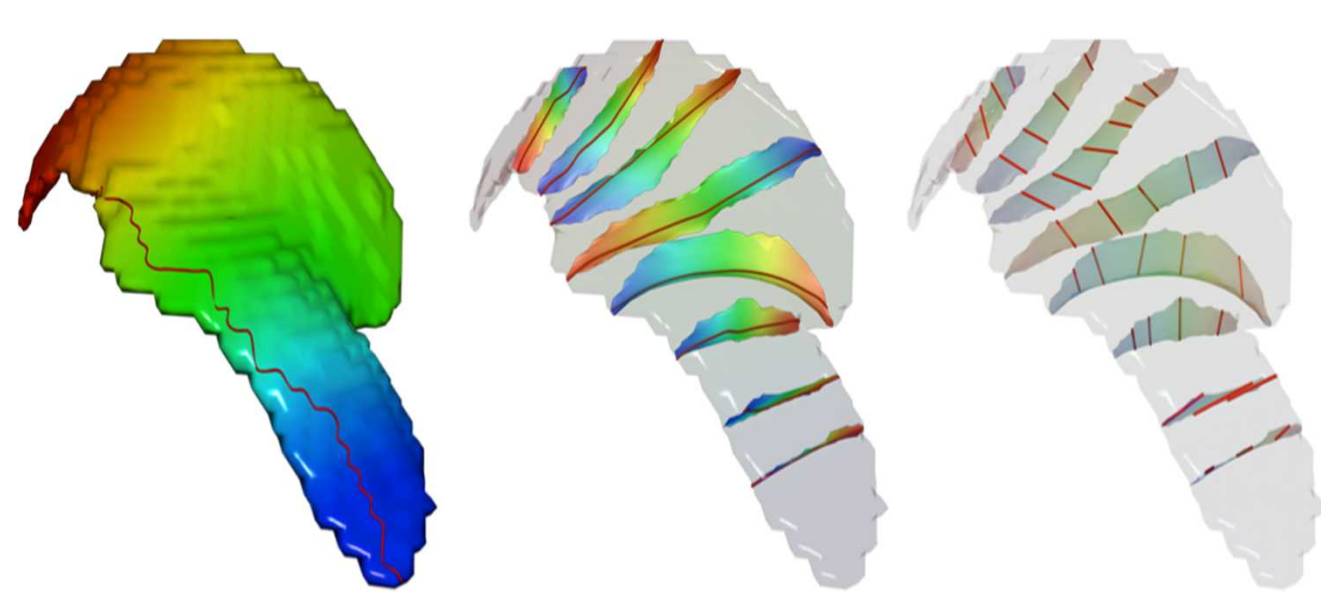


Figure 4: The first three length-scales are estimated using a spectral technique in which each shape is parameterized according to its first non-trivial eigenvector to compute its length. The same technique is performed recursively on isocontours of the first eigenvector to compute the width and thickness.

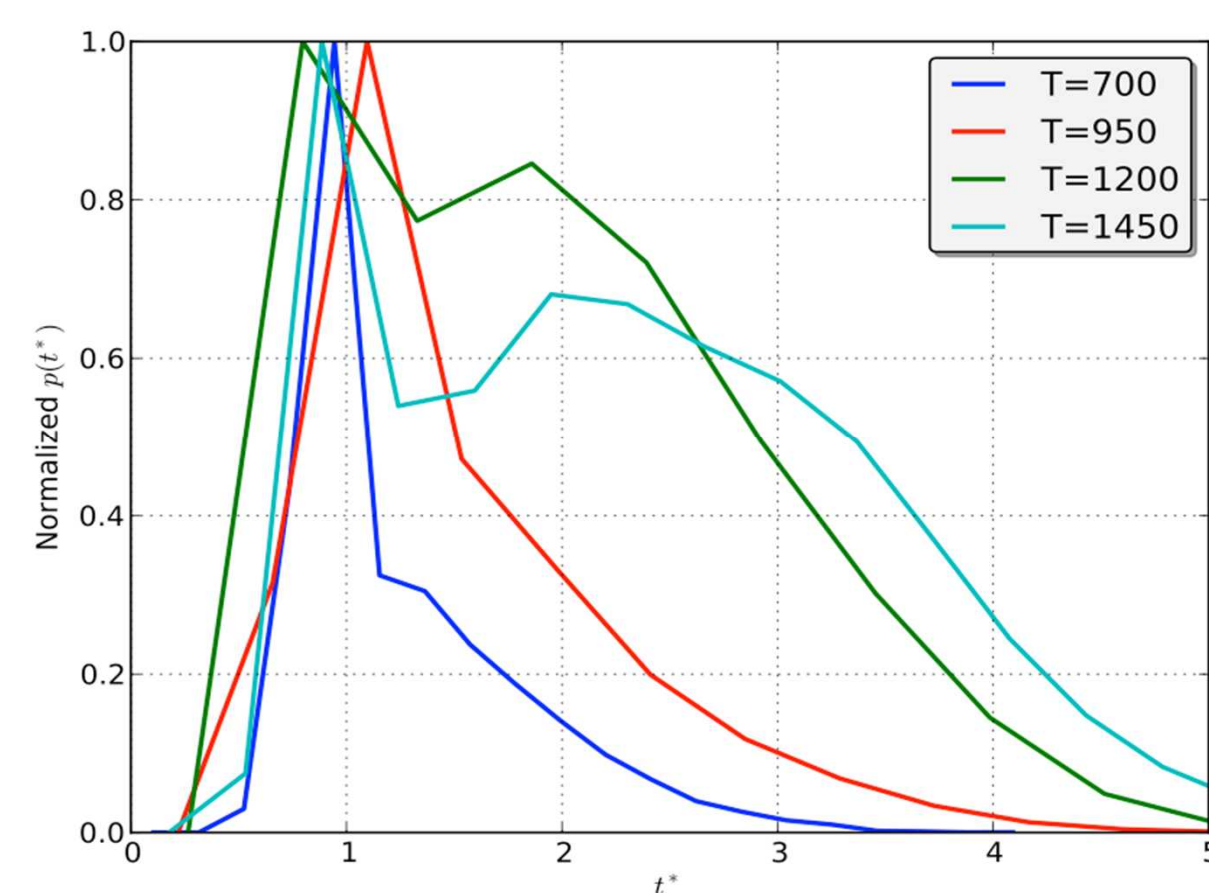


Figure 5: The distribution of χ -thicknesses are computed for segments grouped by the mean temperature in the segment.

Conditional Analysis Using Global Shape Characteristics

Motivation: Characterizing flame stabilization in transverse jets is complicated by the fact that the flame is affected by large-scale boundary layer structures. When aggregating statistics using traditional methods, the large, slow motions induced by the boundary structures require the simulation to be run for prohibitively many time steps in order to guarantee convergence. We introduce a new method for computing statistics conditional on the bulk flame position, in which convergence of statistics takes place with many fewer simulation timesteps.

Feature Definition: Conceptually we want to identify slabs normal to the jet centerline & compute conditional statistics within each slab (see Figure 6).

- Issues with this approach:
 - The centerline is not trivial to define in a rigorous way.
 - The jet is not symmetric around the centerline due to differences in the physics of mixing on the top and bottom of the jet flame.
- Our Solution: we parameterize the jet trajectory and compute statistics based on the resulting coordinate system (see Figure 7).

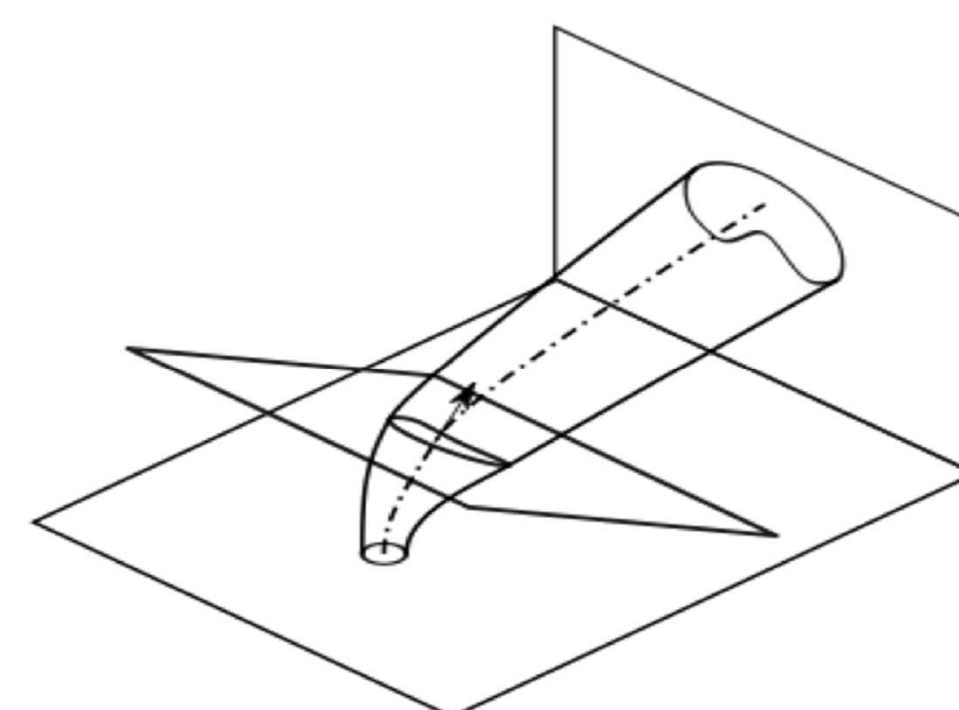


Figure 6: This cartoon depicts a the center line of a flame with a slab indicated by the plane. While this is a nice conceptual notion, in practice it is not easy to define rigorously.

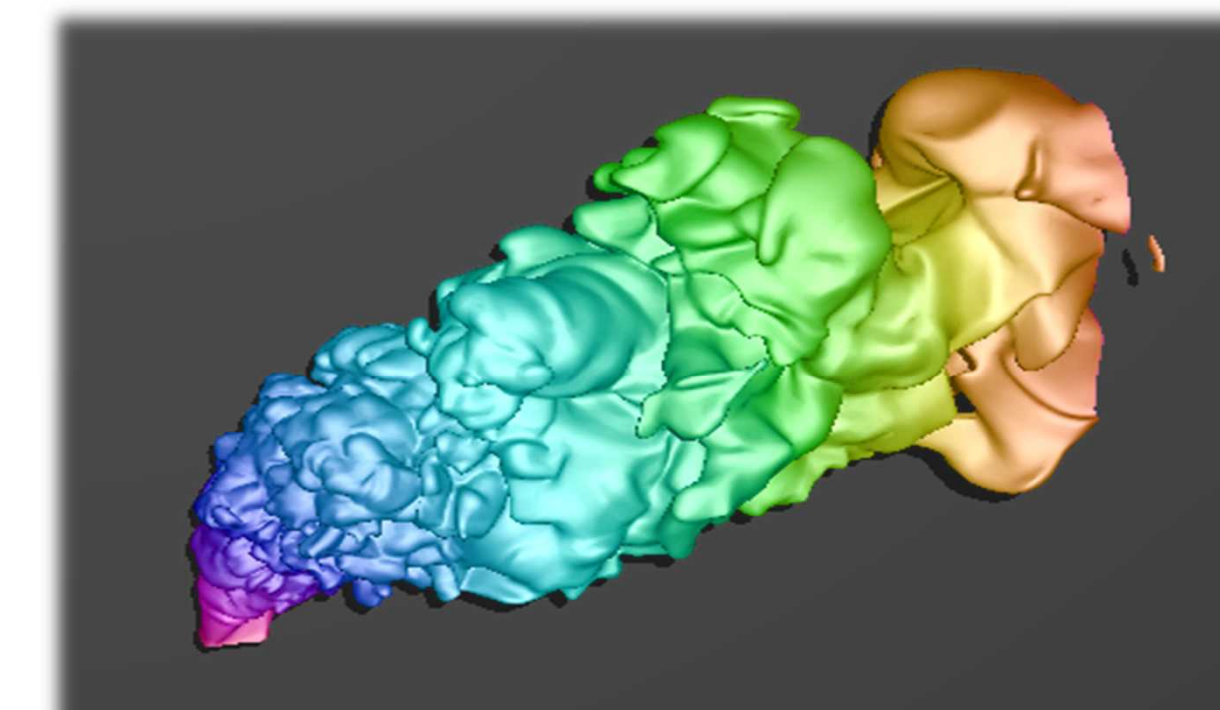


Figure 7: A jet-based coordinate system allows for the aggregation of averages conditioned on bulk flame position.

Conditional Analysis: When there are relatively few large features, a parameterization of the large-scale structure(s) is computed and statistics are aggregated conditional on a coordinate system derived from the shape of the feature itself.

- Parameterization Pipeline:
 - The jet isosurface spans much of the simulation domain and so the resolution of the mesh is reduced using Qslim [<http://mgarland.org/software/qslim.html>].
 - In practice we are able to reduce the size of the mesh many orders of magnitude without degrading the quality of the resulting parameterization.
 - Laplace's equation is solved on the simplified jet surface to capture the trajectory at boundaries and vary these smoothly from entrance to exit.
 - The jet inlet is constrained to zero and the exit boundary is constrained to one.
 - This approach works well even for convoluted surfaces.
 - The interior of the jet is tetrahedralized using TetGen [<http://tetgen.berlios.de/>].
 - The surface parameterization is extended to the interior of the jet by solving Laplace's equation again, providing a four-dimensional point cloud comprised of position and parameter value.
 - The surface solution is used as boundary conditions.
 - Parameter values are computed for all grid points inside the jet.
 - The four-dimensional point cloud is loaded into S3D.
 - Approximate Nearest Neighbors (ANN) code [<http://www.cs.umd.edu/~mount/ANN/>] *in situ* to identify the nearest point cloud neighbor for each grid point.
- Using the parameterization pipeline, scalar quantities are conditionally averaged on the jet path parameter for the jet interior.
 - Figure 8 shows a slice of the velocity magnitude with isolines of the jet path parameter depicted.
 - Figure 9 shows various velocity measures plotted vs the jet path parameter.

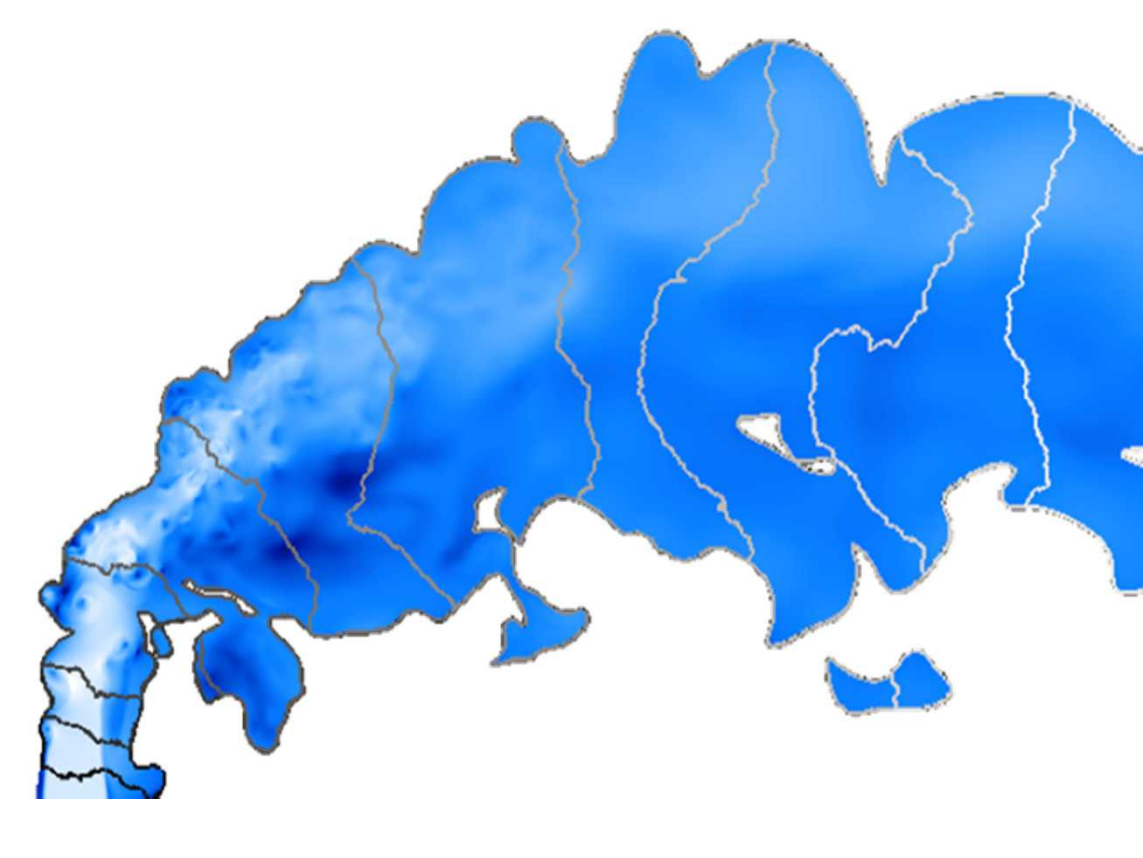


Figure 8: A slice of the velocity magnitude with isolines of the jet path parameter.

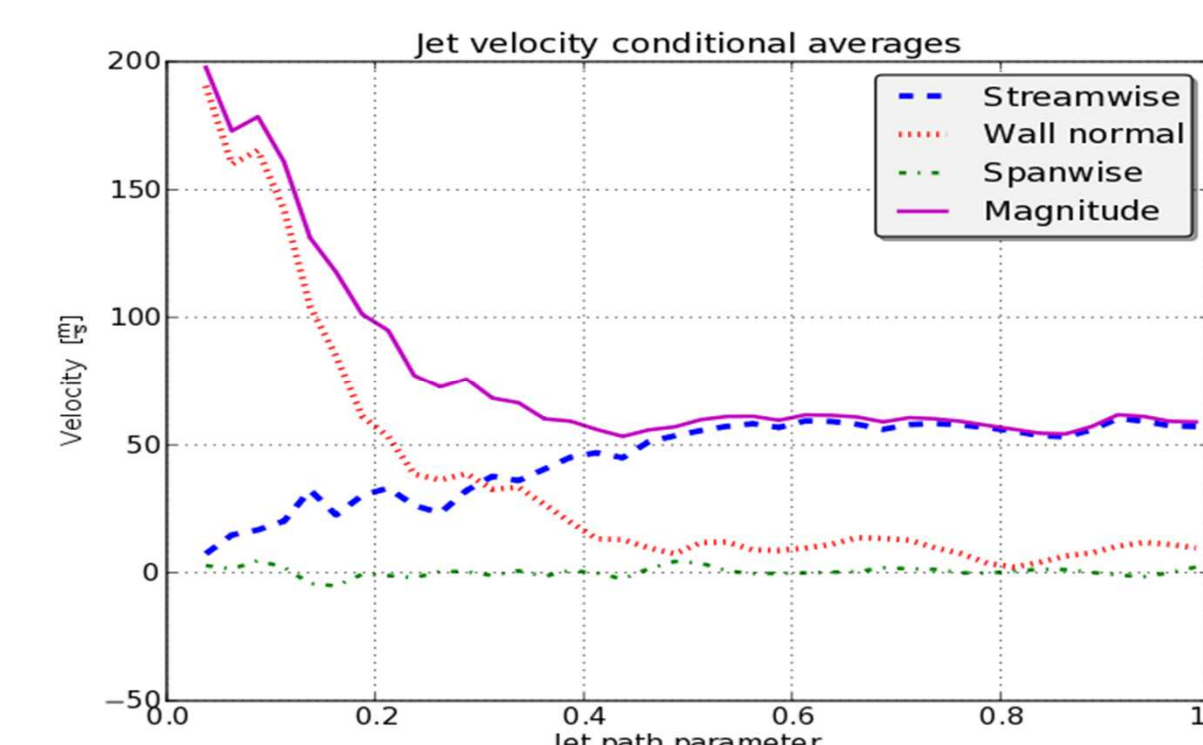


Figure 9: The variation of velocity magnitude and streamwise (left-to-right w.r.t Figure 8b)), wall normal (bottom-to-top) and spanwise (into plane) velocity components are plotted averaged in time and conditioned on the jet path parameter.

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• "Heat Release and Turbulence Statistics From a Direct Numerical Simulation of a Reacting Jet in Cross-Flow Parameterized in a Jet Natural Coordinate System Developed From Scalar Quantities", R. Grout, P.-T. Bremer, A. Gruber, J. Bennett, J. Chen, A. Gyulassy, 13th International Conference on Numerical Combustion, Apr. 2011.

• "A direct numerical simulation study of turbulence and flame structure in a round jet in cross-flow," R. W. Grout, A. Gruber, H. Kolla, J. Bennett, P. T. Bremer, A. Gyulassy, and J. H. Chen, submitted to J. Fluid Mech. 2011.