Analysis and Exploration of High Dimensional Landscapes of Simulation Ensembles for Uncertainty Quantification

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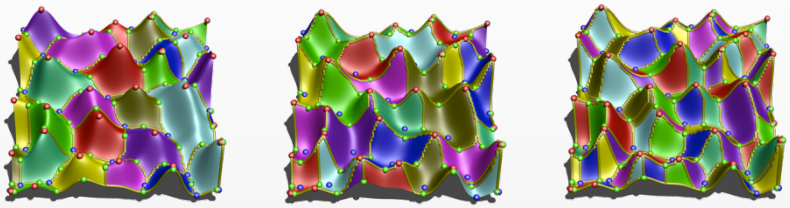
One important aspect of uncertainty quantification is to understand the impact various user select inputs have on the outcome of a simulation. Using a variety of merit functions this problem can be reduced to the analysis of a high dimensional function. We present a new topology-based framework to explore, analyze, and illustrate the global structure of such functions. Based on the Morse-Smale complex, an abstract representation of the topology structure, we have developed a multi-scale framework supporting both local and global analysis, as well as structure preserving regression and sensitivity analysis. Furthermore, by combining topological and geometric information we provide an intuitive visualization that enables interactive exploration to gain new insights from otherwise abstract data.

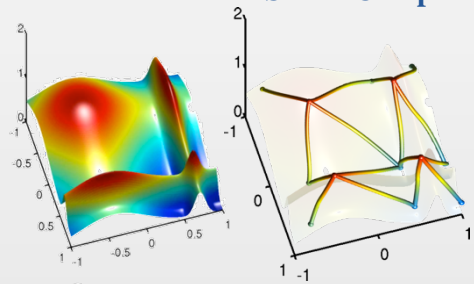
Topology as High Level Data Abstraction



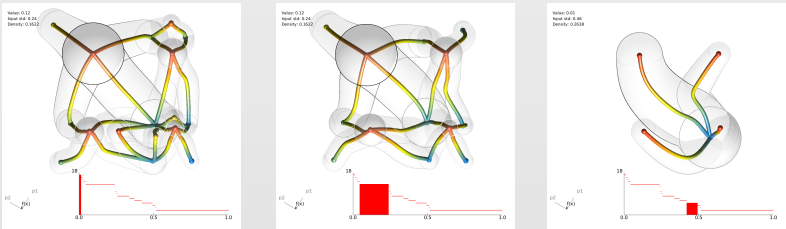
(a) (b) (c)

We analyze functions by computing their Morse-Smale complex, the segmentation of the domain into regions of uniform gradient flow. The intersection of the stable manifolds (a) around maxima and the unstable manifolds (b) around minima form, the Morse-Smale complex (c). All gradient lines within a Morse-Smale cell start at the same minimum and end at the same maximum.

Hierarchical Morse-Smale Complexes in High Dimensions

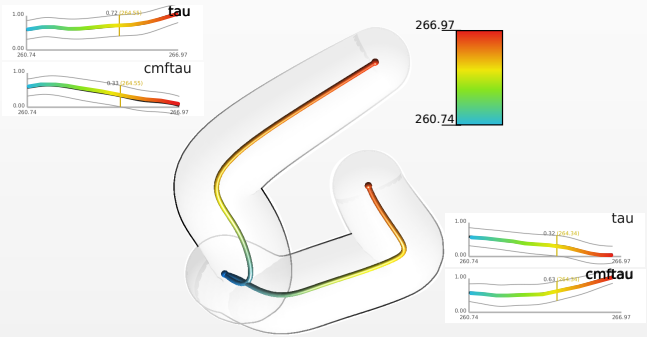


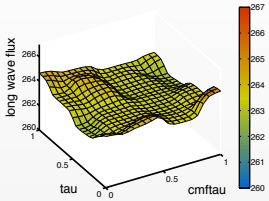
In high dimensions we approximate the Morse-Smale complex using a new graph based algorithm. By representing each cell as its centerline connecting its minimum with its maximum we create a topology preserving and dimension agnostic representation.



By simplifying the Morse-Smale complex using persistence as metric we create a hierarchical representation which corresponds to L-infinity optimal simplifications. This enables us to identify and remove noise as well as to analyze features at different scales.

Upward Clear Sky Flux in a CAM Ensemble

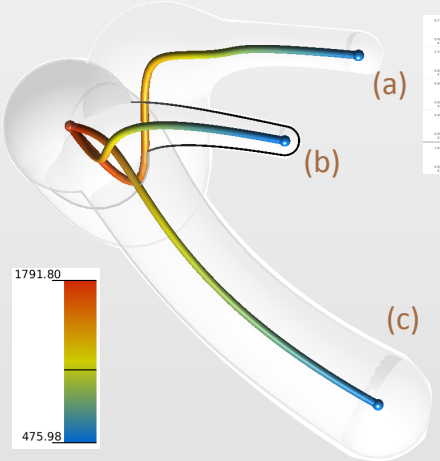


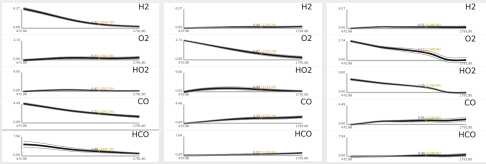


A kernel regression of the flux on cmftau and tau does not show a strong influence of either even with a small kernel bandwidth.

Average upward clear sky flux in a 21 dimensional CAM ensemble. There exist two strong maxima and a global minimum. The insets show the inverse regression of the flux with respect to two of the 21 parameters on a per-crystal basis. The two crystals show an inverse relation of tau and cmftau which govern deep and shallow convection respectively. Note, that the same relation is not apparent in a standard kernel regression.

Heat Release in Turbulent Combustion





(a) (b) (c)

Chemical composition in relation to heat released in a temporal jet simulation of a turbulent C0/H2-air flame. There are ten chemical species forming the domain of this high dimensional PDF four of which are shown in the insets. The three distinct minima correspond to pure fuel, pure oxidizer, and extinction/re-ignition. The insets shown graphs of chemical composition plotted against temperature for the crystals corresponding to pure fuel (a), pure oxidizer (b), and extinction/re-ignition.

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