Topological Dynamics for Fusion Analysis*

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The OFES fusion modeling portfolio has within it multiple discretization methods for the same model, and multiple models representing the same experiment. This coverage is essential in a modeling regime where there is uncertainty in both models and methods. For V&V work the process of converting or cross sampling models or experiments to reconcile these different modeling techniques can be as troublesome as the modeling uncertainty it is meant to uncover. Many of these cross-validation methods can suffer from phase error and resonance effects that can have large impact on transient model comparison but little effect on code dynamics.

Existing visualization methods have focused on point-wise comparison of the fields with L-norm computations and visual examination of tracer streamlines in the field, plus some synthetic instrumentation techniques of modeling data. Modeling practitioners can use some verification techniques within their discretization regime, like convergence studies, but these are not as useful for cross-code and experimental validation.

We argue in favor of a shift to a quantitative analysis of global features of the flow. Specifically, we are interested in topological techniques that allow us to compare different simulations in terms of the global connectivity of their magnetic fields and the distribution of flow structures that appear in the derived scalar fields, as we vary the parameters and the resolution of the simulations.

Flow dynamics analysis. To understand the dynamics of the tracer particles in a magnetic field, we can leverage the existing work on streamline analysis. But instead of visually examining collections of streamlines, we can divide them into equivalence classes by their connectivity. Roughly speaking, one can replace numerical dynamics (the underlying magnetic field) by discrete symbolic dynamics. The latter records which cells of the domain flow into which cells over some fixed period of time. Detecting strongly connected components in the resulting graph identifies *isolating neighborhoods* of the *invariant sets* in the original flow.

We can then use topological methods (specifically, *Conley index theory*) to distinguish between the invariant sets (e.g., to identify attracting vs repelling periodic orbits, to classify different types of fixed points, etc.). Once the invariant sets are identified, one can capture the remaining gradient-like dynamics in *Morse connection graphs*. Naturally, as the dynamics of the simulation changes, as one varies its parameters, so do these topological structures. Relating them across a range of parameters would reveal stable structures in vector fields, stable in the sense that they are present for long ranges of parameters.

Armed with a representation of the topology of vector fields, we can compare different simulations by comparing their global connectivity. For example, we can verify that certain global topological features, such as the large cycles that correspond to the transport around the torus, appear in the results of the simulation, or that they are consistent as we vary the resolution of a simulation.

Scalar field analysis. Another way to understand the topology of the underlying dynamics is to reduce the flow to a scalar field (e.g., by computing the velocity stream function). The chief reason for such a reduction is that the topological analysis of scalar fields is much better understood mathematically.

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Given such a scalar field, one can identify flow structures as either levelsets (isosurfaces) or superlevel sets of the field. We can characterize the topology of these subsets of the domain using *homology theory*: roughly, by counting their connected components, cycles, and voids. We can also quantify the spatial extent of different cycles to distinguish between the large cycles that correspond to the transport around the torus vs small cycles that reflect spurious or transient dynamics.

To make such measurements robust, we can turn to the theory of *persistent homology*, which allows us to compute the distribution of such cycles across all levelset thresholds at once. Moreover, by recording how the cycles relate across multiple such thresholds we can measure their persistence, i.e., how difficult it would be to remove them by perturbing the underlying scalar fields. The distribution of such cycles is summarized in a scatter plot called a *persistence diagram*. Crucially, such scatter plots are equipped with metrics (e.g., bottleneck and Wasserstein distances) that are stable to the perturbations of the underlying scalar field. Accordingly, we can quantitatively compare the topology of the underlying fields across different simulations by measuring the distances between the persistence diagrams. Similarly, we can detect and quantify significant transitions in the dynamics of a single simulation by keeping track of persistence diagrams as they change over time and measuring the distances between consecutive snapshots.

References

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