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`FluidSF`: A Python package for calculating turbulent flow statistics

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Summary

Fluid systems are everywhere, from small-scale engineering problems to planetary-and-larger-scale systems (atmosphere, ocean, galactic gas clouds). These systems are often turbulent, where motion is chaotic, unpredictable, and can only be characterized through statistical analyses. Structure functions (SFs) are one such statistical analysis technique for turbulence, that require calculation of spatial differences in properties as a function of their separation distance. By combining and then averaging these spatial differences, various types of SF can be constructed to measure physical properties of fluid flow, such as heat and energy transfers, energy density, intermittency etc. However, calculating SFs is often a cumbersome and computationally-intensive task tailored to the specific format of a given fluid dataset. `FluidSF` is a flexible `Python` package that can be used to diagnose and analyze various physically-informative SFs from 1-, 2-, or 3-dimensional fluid data sets.

Statement of need

`FluidSF` can construct an array of traditional and modern structure functions (SFs), and can be easily modified to calculate user-defined SFs that utilize general fluid properties, including scalars (e.g., vorticity, density) and vectors (e.g., velocity, magnetic field). `FluidSF` also includes several tools to process data (e.g., array shifting, binning) and diagnose useful properties (e.g., advection) for SF analysis. The flexibility of this package enables geophysical, astrophysical, and engineering applications such as: quantifying the energy cycles within Earth's ocean (Balwada et al., 2022; J. Pearson et al., 2019), Earth's atmosphere (Lindborg, 1999), and Jupiter's atmosphere (Young & Read, 2017), diagnosing the intermittency of magnetohydrodynamic plasma turbulence (Wan et al., 2016) and the scaling laws of idealized 3D turbulence (Iyer et al., 2020), or measuring the characteristics of ocean surface temperature (Schloesser et al., 2016) or the anistropy of flow over rough beds (Coscarella et al., 2020).

Structure functions are constructed by averaging the correlations between spatial differences of properties. For example, given an arbitrary scalar field (ϕ), we could calculate SFs such as this,

$$SF_{\phi\phi}(\mathbf{r}) = \overline{\delta\phi\delta\phi} = \overline{[\phi(\mathbf{x}+\mathbf{r})-\phi(\mathbf{x})]\,[\phi(\mathbf{x}+\mathbf{r})-\phi(\mathbf{x})]} \tag{1}$$

where $\mathbf{x}$ denotes the position of a data point, $\delta\phi$ denotes the spatial variation of ϕ, and the overline denotes an average over all positions ($\mathbf{x}$). Structure functions depend on the separation vector ($\mathbf{r}$), and are often analyzed with an assumption of isotropic flow statistics [$SF(\mathbf{r}) \rightarrow SF(r = |\mathbf{r}|)$]. There are many types of physically-useful structure functions. The example above is a second-order scalar SF (i.e., it contains 2 δ terms of the scalar ϕ), but additional physical insight can be gained from third- & higher-order scalar SFs (3+ δ terms), SFs that depend on vector fields such as velocity, and SFs that blend information from multiple fields.

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FluidSF can utilize a variety of fluid data, including data sets with 1-, 2-, and 3-dimensional spatial data, and from domains with periodic or non-periodic boundary conditions. In addition to regular Cartesian-gridded data, the software also has some support for non-uniform latitude-longitude grids (1D or 2D) but not for general curvilinear coordinates. When computing SFs that blend information from multiple fields FluidSF assumes all variables are co-located, so care must be taken with staggered grids. Since FluidSF is written in Python, any fluid data intialized and loaded as NumPy (Harris et al., 2020) arrays can be used to calculate SFs. To demonstrate the flexibility of input data, Figure 1 shows several types of SF calculated using FluidSF for a simulation of quasi-geostrophic turbulence in a periodic domain using GeophysicalFlows.jl (Constantinou et al., 2021), while Figure 2 shows SFs calculated from satellite observations of the ocean surface made by the NASA SWOT (Surface Waves and Ocean Topography) satellite mission (Morrow et al., 2018).

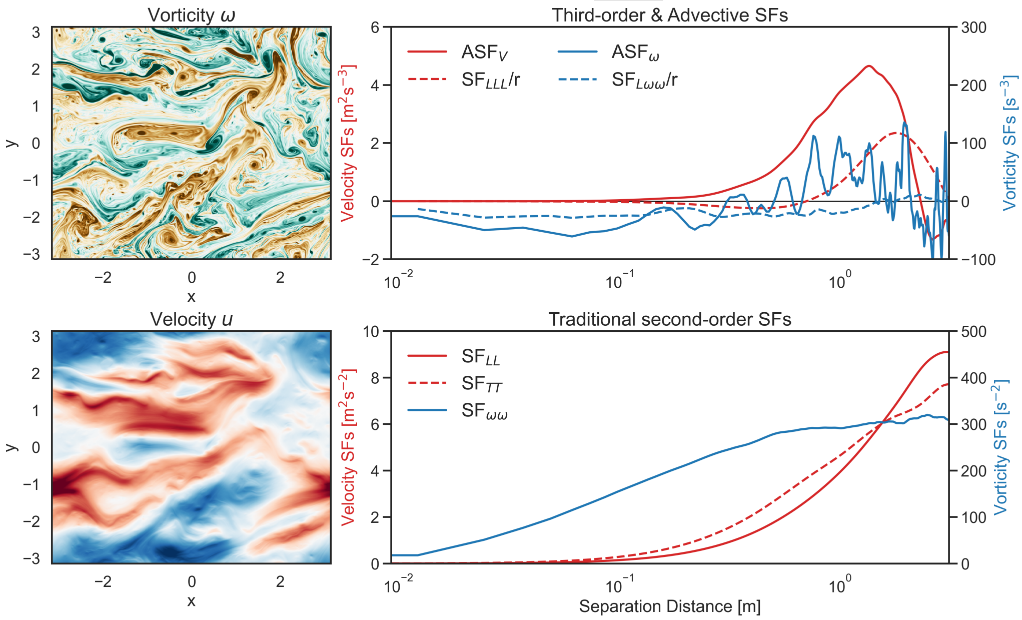

Figure 1: Various structure functions (SFs) calculated from a simulated 2D turbulent flow, visualized through snapshots of the vorticity field (top left) and velocity field (bottom left). The right panels show various SFs based on velocity (red lines) and vorticity (blue lines), including third-order and advective SFs (top right) and traditional second-order SFs (bottom right). The results are from the top layer snapshot of an anisotropic 2-layer quasi-geostrophic simulation conducted with GeophysicalFlows.jl.

As demonstrated in Figure 1 and Figure 2, FluidSF can calculate a wide array of traditional structure functions, including $SF_{\phi\phi}$ (Equation 1; where the scalar field in this case is vorticity ω), second- and third-order SFs of longitudinal velocity ($SF_{LL} = \overline{(\delta u_L)^2}$ and $SF_{LLL} = \overline{(\delta u_L)^3}$; where $u_L = \mathbf{u} \cdot \hat{\mathbf{r}}$) and transverse velocity (SF_{TT} and SF_{TTT}), and blended velocity-scalar third-order SFs ($SF_{L\omega\omega} = \overline{\delta u_L \delta\omega\delta\omega}$), in addition to novel advective SFs of velocity (ASF_V), vorticity (ASF_ω) and scalars (B. Pearson et al., 2021, Under Revision). Advective SFs require fields of the local advection, and FluidSF has a built-in function to compute these advection terms. FluidSF can calculate SFs in specific separation directions (i.e., aligned with the Cartesian co-ordinates, shown in Figure 2), and for 2D data it can diagnose maps showing how SFs vary with the magnitude and orientation of the separation vector $\mathbf{r}$ (Figure 3). FluidSF also includes tools to make the calculation and processing of SFs easier, such as array shifting, diagnosis of the advection terms for novel SFs, decomposition of velocity into longitudinal (along-$\mathbf{r}$; u_L) and transverse (across-$\mathbf{r}$; u_T) components, and data binning based on separation distance.

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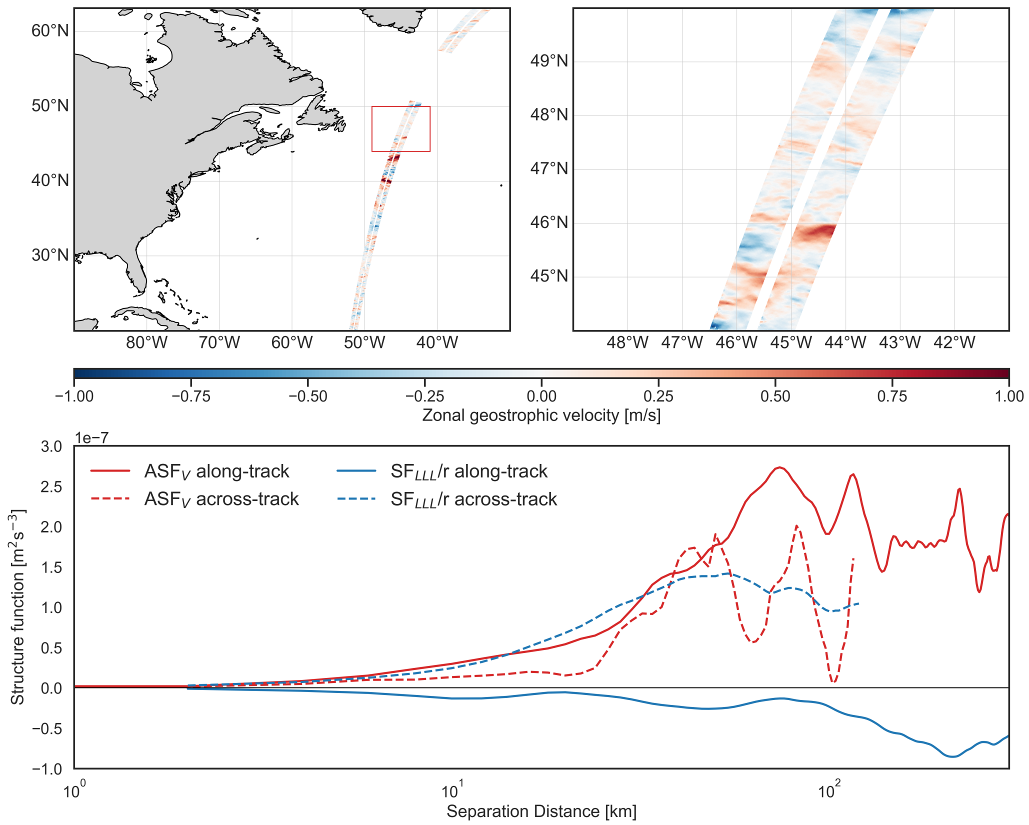

Figure 2: Velocity-based SFs calculated from satellite observations of the ocean surface in the North Atlantic. Maps of the inferred surface velocity from a satellite swath are shown in the top left. The region of data used for SF calculations is indicated by the red box and magnified on the top right. The bottom panel shows the advective (red) and third-order (blue) velocity structure functions calculated with separation vectors across the satellite swath (dashed) and along the swath (solid). Note the velocity fields are estimated from satellite sea surface height measurements assuming geostrophic balance.

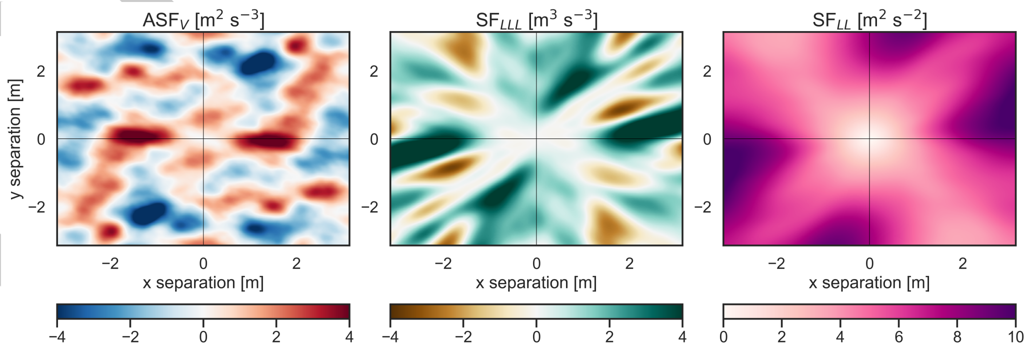

Figure 3: Maps showing the 2D spatial variation of various velocity structure functions. The left panel shows the advective velocity SF, the middle panel is the third-order velocity SF, and the right panel is the second-order velocity SF. These SFs were calculated from the same data as Figure 1.

Related Work

`FluidSF` uniquely contributes to the field through a combination of expanded data support, the ability to diagnose a wide array of structure functions (including advective and blended SFs), and tools for analyzing spatial variations in SFs. `FluidSF` was used to develop new methods for estimating inter-scale geophysical energy fluxes (B. Pearson et al., Under Revision). There are several open source software packages available that calculate aspects of spatial SFs. `fastSF` is a parallelized C++ code designed to compute arbitrary-order SFs of velocity or scalars (but not blended) from Cartesian grids of data (Sadhukhan et al., 2021). Fuchs et al. (2022) created an open source `MATLAB` toolkit that performs a variety of turbulence analysis, including arbitrary-order longitudinal-velocity SFs. A complimentary and alternative method to structure functions for analyzing turbulence data is coarse-graining. `FlowSieve` is a primarily C++ package that uses coarse-graining to estimate ocean and atmospheric turbulence properties from Global Climate Model data (Storer & Aluie, 2023).

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