

FluidSF: A Python package for calculating turbulent fluid 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. Spatial 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.

Statement of need

FluidSF is a flexible Python package for calculating spatial structure functions (SFs) from general fluid datasets that describe spatial variations in one-, two-, or three-dimensions. The package can construct an array of traditional and modern SFs, and can be easily modified to calculate user-defined SFs that utilize general fluid properties, including scalars (e.g., vorticity, density) and/or vectors (e.g., velocity, magnetic field). The package also includes several tools to process data and diagnose useful properties. 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 anisotropy of flow over rough beds (Coscarella et al., 2020).

Paragraph on package capabilities & limitations. Regularly-gridded data, Lat-lon gridded data, track/directional sampling, 1D-data, evenly-spaced, irregularly-spaced (what are limitations), binning, bootstrapping(?), local advection terms (B. C. Pearson et al., 2021), Bessel function examples(?) (Xie & Bühler, 2018) examples of time-averaging, SWOT application. What are limitations (can it take 2D data in a vector rather than array format? Can it calculate 2D or 3D maps of SF rather than just a function of $|r|$ magnitude?). Perhaps these don't need to be mentioned, or can be stated as future developments.

Spatial SFs are constructed by averaging the correlations between spatial differences of properties. For example, given an arbitrary scalar field (ϕ), we could calculate a structure function,

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

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

40 separation vector (\mathbf{r}), and are often analyzed with an assumption of isotropic flow statistics
41 [$SF(\mathbf{r}) \rightarrow SF(r = |\mathbf{r}|)$]. There are many types of physically-useful structure functions. The
42 example above is a second-order scalar SF (i.e., it contains 2 δ terms of the scalar ϕ), but
43 additional physical insight can be gained from third- & higher-order SFs (3+ δ terms), SFs
44 that depend on other scalar or vector fields, and SFs that blend information from various
45 scalar/vector fields.

Some basic structure functions from a simulation of anisotropic 2D or QG turbulence: (a)
Snapshot of the vorticity field used for SF calculations, (b) various Zonally- and
meridionally-separated SFs, including third-order velocity, advective, and vorticity SFs from 2D
turbulence simulation, (c) Inter-scale fluxes inferred from structure functions and diagnosed
directly from the simulation

Figure 1: Some basic structure functions from a simulation of anisotropic 2D or QG turbulence: (a)
Snapshot of the vorticity field used for SF calculations, (b) various Zonally- and meridionally-separated
SFs, including third-order velocity, advective, and vorticity SFs from 2D turbulence simulation, (c)
Inter-scale fluxes inferred from structure functions and diagnosed directly from the simulation

Structure functions calculated from satellite observations of the ocean surface:

Figure 2: Structure functions calculated from satellite observations of the ocean surface:

Map of the 2D spatial variation of the (a) 3rd-order longitudinal and (b) advective velocity
SFs from the same data set as Figure 1:

Figure 3: Map of the 2D spatial variation of the (a) 3rd-order longitudinal and (b) advective velocity
SFs from the same data set as Figure 1:

46 FluidSF can utilize a variety of fluid data, including data sets with 1-, 2-, and 3-dimensional
47 spatial data, and from domains with periodic or non-periodic boundary conditions (Figure
48 1). In addition to regular Cartesian-gridded data (1D, 2D or 3D), the software also has
49 some support for non-uniform latitude-longitude grids (1D or 2D). Since FluidSF is written
50 in Python, any fluid data initialized and loaded as NumPy arrays can be used to calculate SFs.
51 To demonstrate the flexibility of input data, Figure 1 shows SFs calculated by FluidSF for a
52 simulation of quasi-geostrophic turbulence in a periodic domain using GeophysicalFlows.jl
53 (?), while Figure 2 shows SFs calculated from satellite observations of the ocean surface made
54 by the SWOT (Surface Waves and Ocean Topography) mission (Morrow et al., 2018).

55 FluidSF can calculate a wide array of traditional and novel structure functions, including
56 $SF_{\phi\phi}$ (Eq. 1), second- and third-order SFs of longitudinal and transverse velocity, blended
57 velocity-scalar third-order SFs, and advective SFs of velocity, vorticity and scalars (B. C. Pearson
58 et al., 2021). FluidSF can calculate these SFs in specific directions (i.e., aligned with the
59 Cartesian co-ordinates), and for 2D data it can diagnose a map showing how the SFs vary with
60 the magnitude and orientation of the separation vector \mathbf{r} (as shown in Figure 3). FluidSF
61 also includes tools to make the calculation and processing of SFs easier, such as array shifting,
62 diagnosis of the advection terms for novel SFs, decomposition of longitudinal and transverse
63 velocities, and bin data based on separation distance.

64 Related Work

65 FluidSF uniquely contributes to the field through a combination of expanded data support,
66 the ability to diagnose a wide array of SF types (including novel and blended SFs), and tools
67 for analyzing spatial variations in SFs. There are a small number of open source software
68 available that calculate structure functions. fastSF is a parallelized C++ code designed to
69 compute structure functions 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 structure functions. An 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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