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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 anistropy 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, iregularly-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 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 delta terms of the scalar ϕ), but additional physical insight can be gained from third-order SFs (3 deltas), SFs that depend on other scalar or vector fields, and SFs that blend information from various scalar/vector fields.

`FluidSF` calculates SFs from 1D-, 2D-, and 3D-data with periodic and non-periodic boundary conditions. Regular Cartesian (1D, 2D, 3D) and non-uniform latitude-longitude gridding (1D, 2D) are supported. Since FluidSF is written in `Python`, any data intialized and loaded as `NumPy` arrays can be used.

`FluidSF` is the first software pacakage that calculates novel advective SFs, a type of SF that depends on velocity advection and does not assume an isotropic flow field (B. C. Pearson et al., 2021). Therefor FluidSF also computes advection for 2D and 3D data. It supports blended SFs, i.e. a combination of longitudinal and transverse velocity SFs, whereas other software only supports purely longitudinal or transverse SFs.

To explore spatial variations in SFs, FluidSF computes 2D polar maps of SFs that vary in separation distance and separation direction.

Related Work

`FluidSF` uniquely contributes to the field through a combination of expanded data support, the ability to diagnose a wide array of SF types, and tools for analyzing spatial variations in SFs. There are a small number of open source software available that calculate structure functions. `fastSF` is a parallelized C++ code designed to 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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