Direct Numerical Simulations of Turbulence in Python: Development, Scaling, and Analysis Using **Entropy Measures** and **Gradient Pattern Analysis** Techniques

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Abstract

In the context of fluid dynamics, turbulence is characterized by irregular and chaotic fluid flow, with fluctuations in parameters such as velocity and pressure. The Reynolds number, a dimensionless quantity based on the fluid viscosity, velocity, and characteristic length, plays a critical role in describing this phenomenon. Computationally, turbulence is commonly addressed using different types of simulations, such as Direct Numerical Simulation (DNS), Reynolds-Averaged Navier-Stokes (RANS), and Large Eddy Simulation (LES). To study the fundamental physics of turbulence, DNS is frequently employed to solve the Navier-Stokes equations directly, capturing all turbulence scales. These algorithms are extremely computationally expensive, generally implemented in C/C++ or Fortran, and highly parallelized. This work aims to develop a Python-based method capable of generating high-resolution Direct Numerical Simulations (DNS) for high Reynolds numbers. Utilizing a Pseudo-spectral Galerkin method [1] and leveraging GPUs and/or MPI (via mpi4py), we create user-friendly code that operates efficiently on cloud platforms like Google Colab and Kaggle, and scales to supercomputers such as Santos Dumont. The focus is on producing 2D turbulence data from various colored noise initial conditions, which will be analyzed using Gradient Pattern Analysis (GPA) [2] and entropy measures [3] to investigate potential temporal phase transitions in turbulence.

MOTIVATION AND OBJECTIVES

The main idea is to build user-friendly scalable codes in Python to do Direct Numerical Simulations (DNS) of turbulence solving the Navier-Stokes equations:

$$\frac{\partial \vec{u}(\vec{x},t)}{\partial t} - \vec{u}(\vec{x},t)\times\vec{\omega} = \nu\nabla^2\vec{u} - \nabla P,$$

where $\vec{u}(\vec{x},t)$ is the velocity vector, $\vec{\omega} = \nabla\times\vec{u}$ is the vorticity vector, $P = p + \vec{u}\cdot\vec{u}/2$ is the modified pressure and $\nu = 1/Re$ is the viscosity coefficient, where Re is the Reynolds number.

Specific Objectives:

- *Implement scalable pseudo-spectral Garlekin DNS codes in Python;*
- *Create super-resolution surrogate models using neural networks algorithms;*
- *Analyse and characterize data from the simulations with entropy measurements and GPA.*

3D Turbulence from Taylor-Green ICs

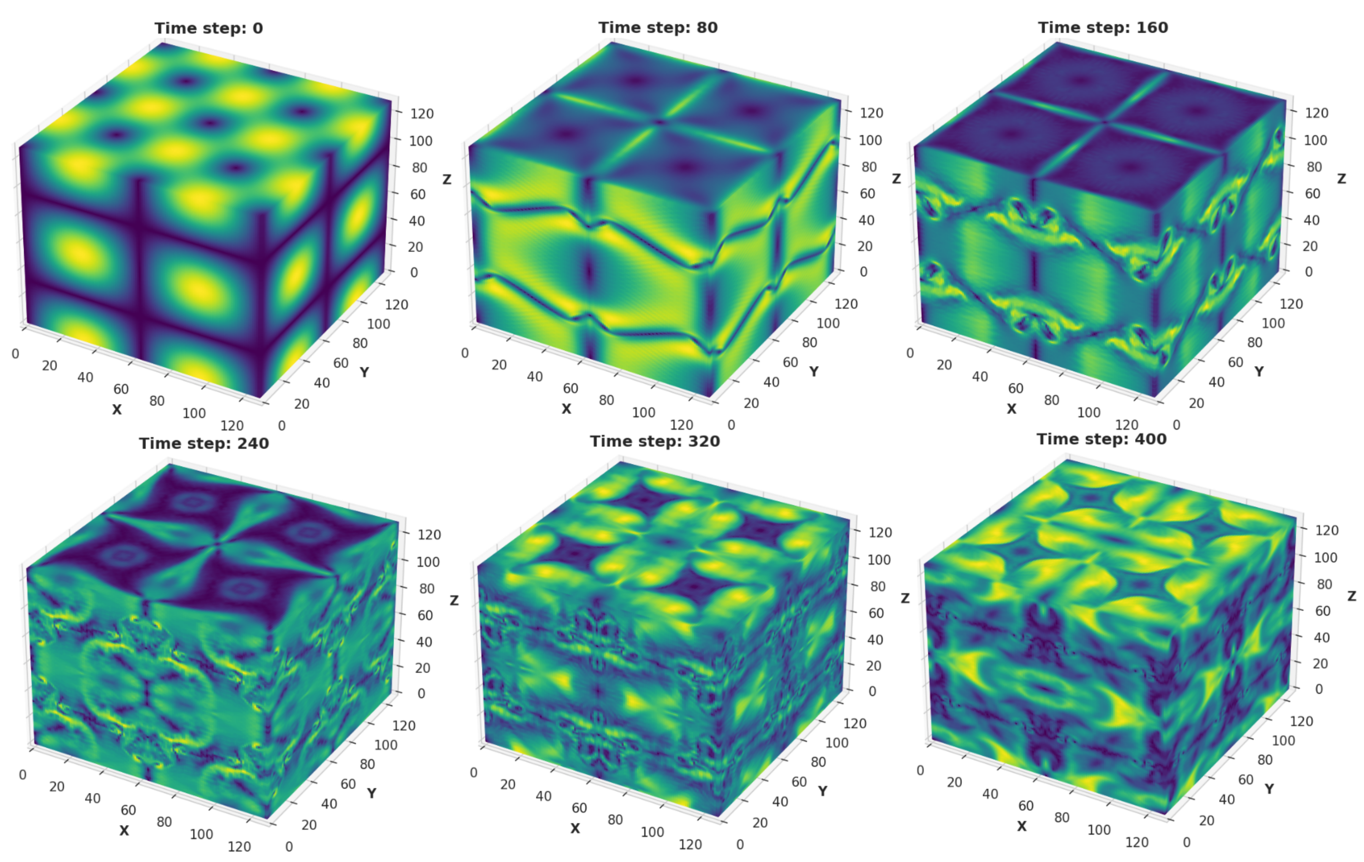


Figure 1: *3D Turbulence velocity fields.* $Re = 1600$, *time step size* $= 0.05$, *total physical time* $= 20$, *physical box* $= [0, 2\pi]$, *grid size of shape* $128\times128\times128$, *periodic BCs.*

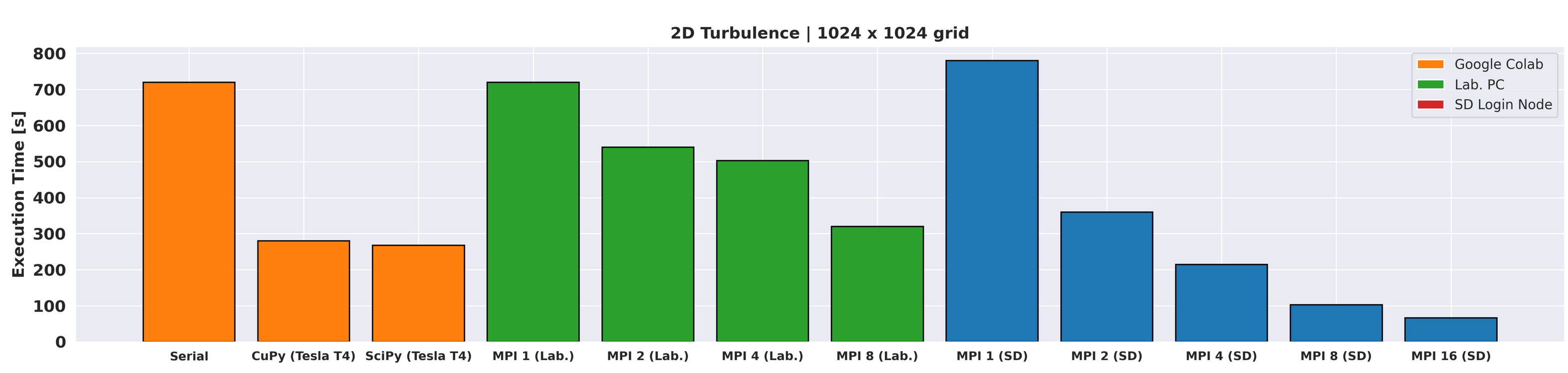


Figure 2: *Performance tests for the 2D turbulence simulator on Google Colab, a simple desktop machine (Intel Core i5, 8gb ram) and on the SDumont supercomputer.*

2D Turbulence from Colored Noise

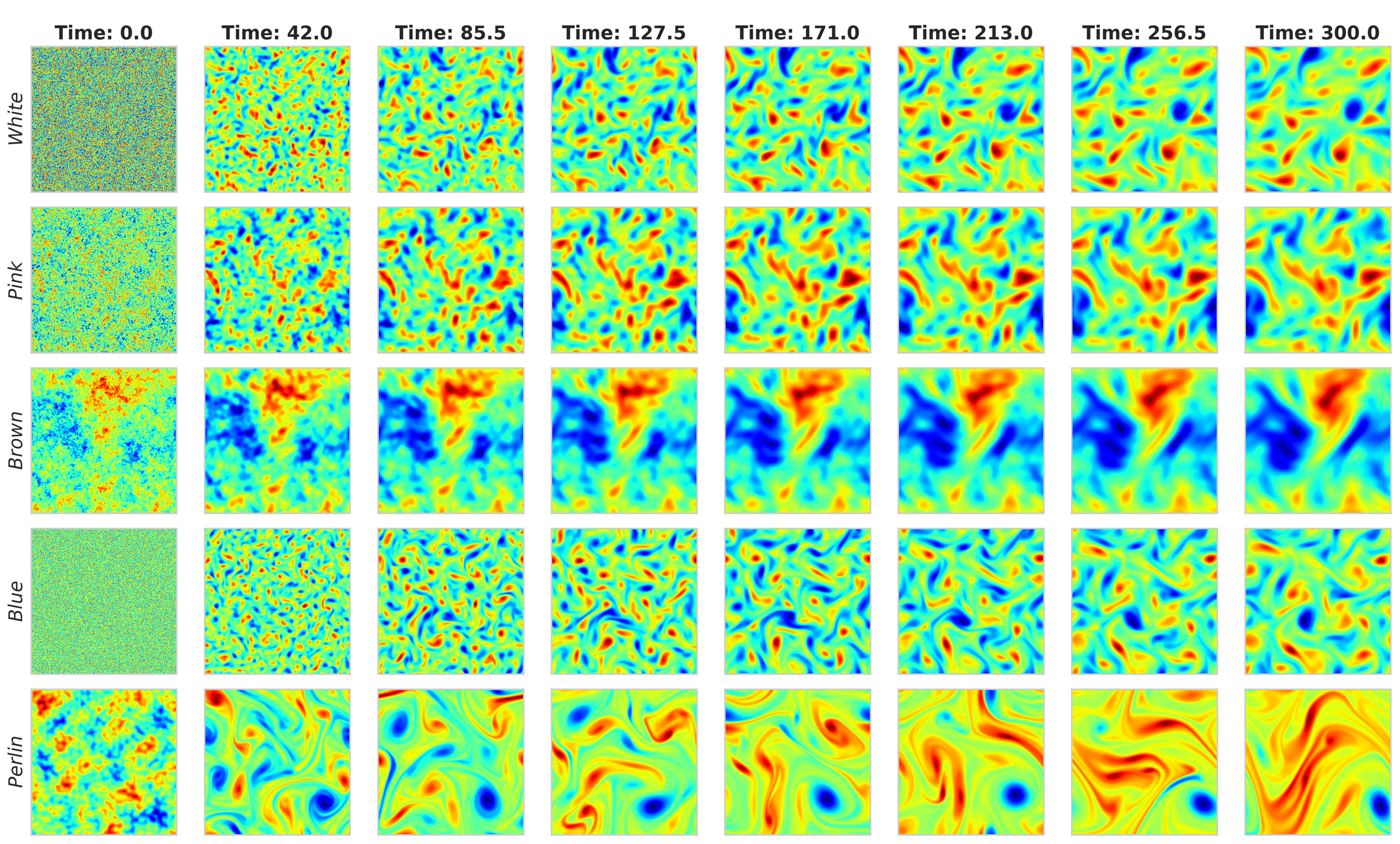
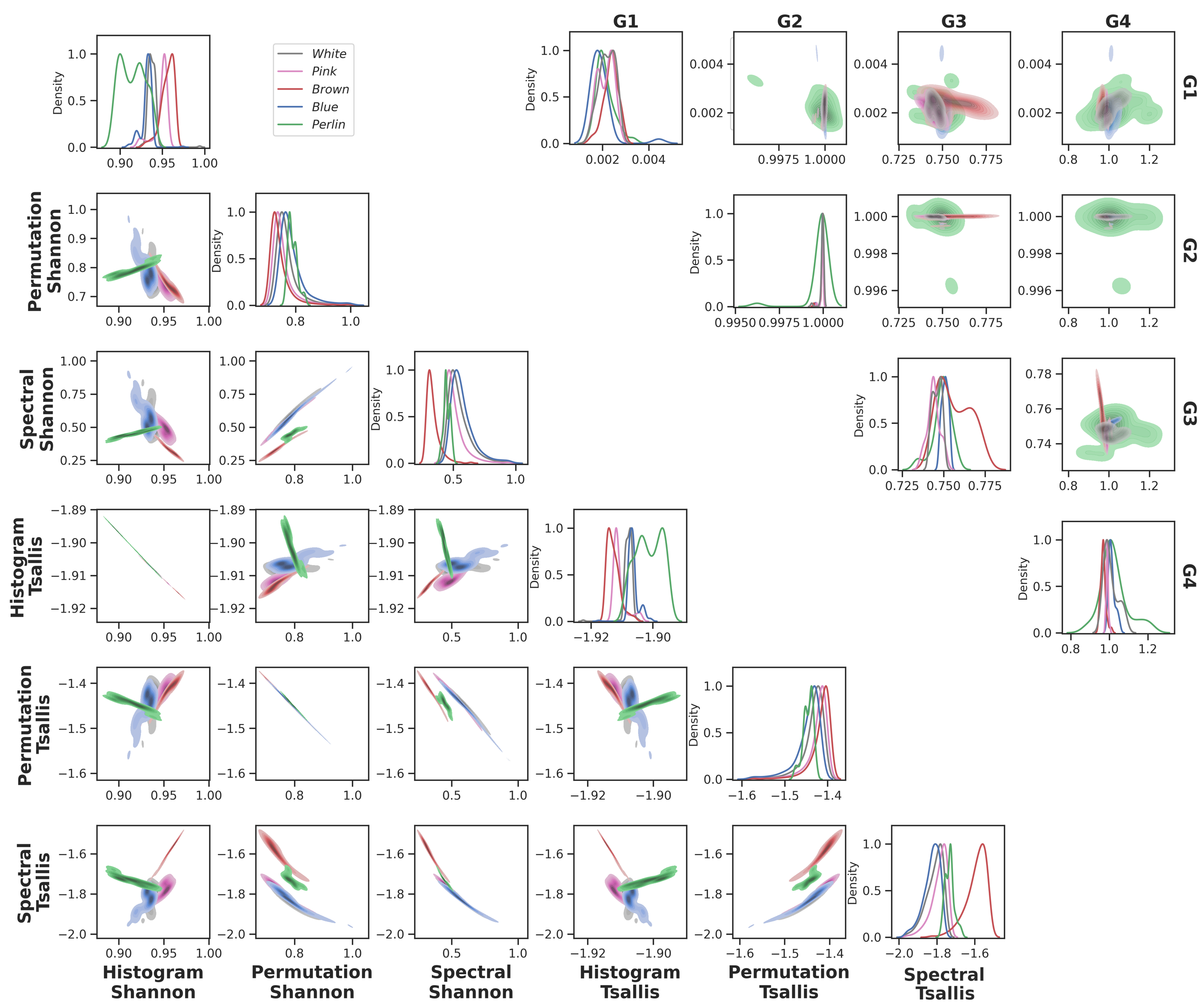


Figure 3: *2D Turbulence vorticity fields.* $Re = 16000$, *time step size* $= 0.005$, *total physical time* $= 200$, *physical box* $= [0, 2\pi]$, *grid size of shape* 512×512, *periodic BCs.*

RESULTS: Entropies and GPA Moments



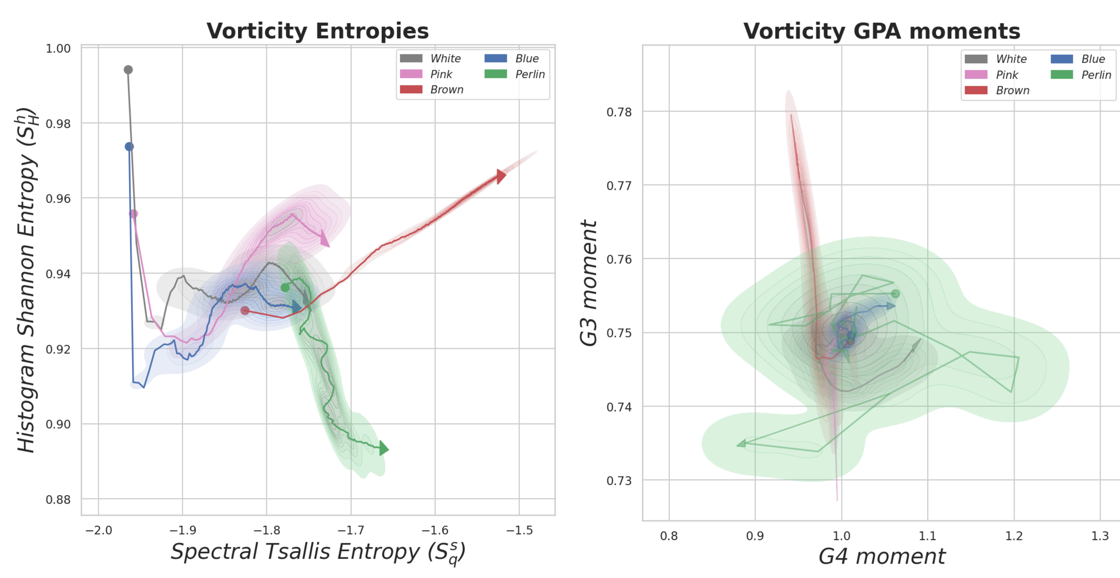


Figure 5: *Entropy and Gradient Pattern Analysis moments measurements from the colored noise ICs turbulence vorticity fields.*

FURTHER WORKS

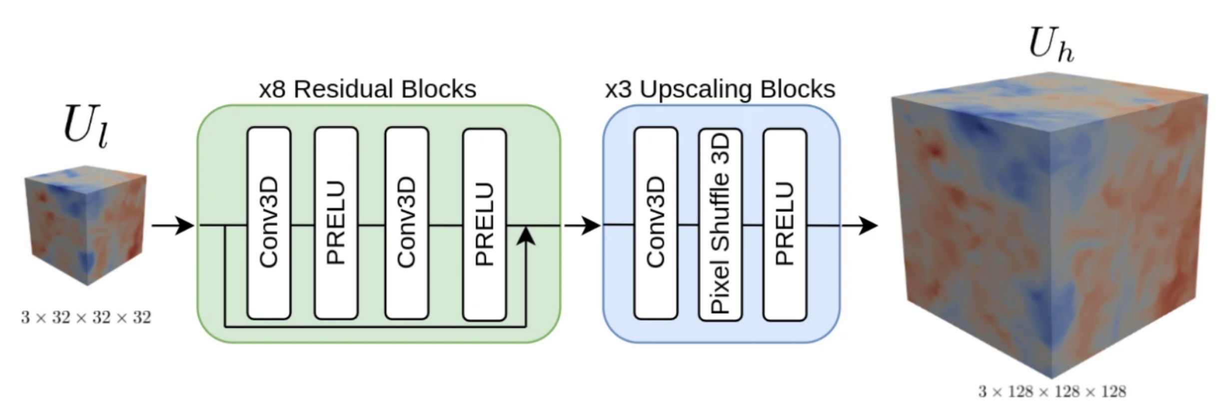


Figure 6: *Super resolution network trained for predicting high-resolution turbulent flow from a low-resolution input. Source: NVIDIA Modulus documentation.*

Acknowledgements

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LNCC Laboratório Nacional de Computação Científica

References

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[2] Rubens. rsautter/GPA, June 2024. original-date: 2016-09-13T21:19:43Z.

[3] Luan Orion Barauna, Rubens Andreas Sautter, Reinaldo Roberto Rosa, Erico Luiz Rempel, and Alejandro C. Frery. Characterizing Complex Spatiotemporal Patterns from Entropy Measures. *Entropy (Basel, Switzerland)*, 26(6):508, June 2024.