The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

Large-scale DNS of turbulence with efficient and accurate particle tracking

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Keywords: *Pseudo-spectral DNS, Particle Tracking, MPI/OpenMP, Modeling*

Over the past decades, a growing range of prototypical flows and particle models have been explored from the perspective of fundamental turbulence research. Supported by the increasing availability of HPC resources, nowadays direct numerical simulations routinely facilitate detailed investigations of both Eulerian and Lagrangian aspects of turbulence. Naturally, this raises the need for CFD tools that are flexible and accurate while minimizing the associated computational costs on available and future HPC architectures.

In this contribution, we present TurTLE ("Turbulence Tools: Lagrangian and Eulerian"), a hybrid MPI/OpenMP-parallel pseudospectral solver for particles and fields in turbulence research. TurTLE follows the object-oriented programming paradigm which eases code maintenance and extensions through C++ inheritance and virtualization, and facilitates development by an interdisciplinary team. In particular, our software design enables straightforward implementation of alternative methods or new algorithms to explore novel research directions. Specifically, we shall detail an accurate MPI/OpenMP particle tracking implementation [1] that can be coupled to arbitrary fluid models while scaling up to tens of thousands of processor cores on modern supercomputers. We will outline perspectives and challenges of heterogeneous (GPU accelerated) HPC platforms. We will also showcase recent works [2, 3, 4] that have been enabled by TurTLE.

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