XCompact3d: a powerful framework to study turbulent flows with turbulence-resolving simulations

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Our daily life is surrounded - and even sustained - by the physics of fluid motions. Blood moves through blood vessels in our bodies, air flows into our lungs, moving air disperses particulate air pollution in the urban and indoor environments, wind sets wind turbines in a rotating motion to produce electricity, vehicles move through air and water while powered by liquid fuel which mix and burn within the combustion chambers of engines. The list of fluid flow related applications seems to be never-ending as fluid flows play a crucial role in so many physical processes spanning from the biology of the human body to climate change. It can be argued that many of the remaining challenges we face today cannot possibly be tackled without a better understanding of fluid dynamics. From a practical point of view, fluid flows relevant to scientists and engineers are turbulent; as in nature turbulence is the rule, not the exception. The Navier-Stokes equations, a set of time-evolving, non-linear equations, used to describe fluid flow are extremely challenging to solve due to their admitting chaotic (turbulent) solutions. Further complicating the solution of turbulent flows is the inherently multi-scale nature of turbulence itself. Within turbulent flows, smaller scales impact larger scales while small changes to the boundary or initial conditions can have a dramatic impact on the final solution.

To this end, turbulence-resolving simulations of idealised isotropic, homogeneous turbulence have been crucial in our understanding of turbulence as they offer a possibility to simulate and display the time evolution of the full three-dimensional velocity field. Unfortunately, the computational cost of turbulence-resolving simulations, even for idealised turbulent flows, remains extremely high, especially with an increasing the Reynolds number (a measure of the range of scales to simulate). With the recent advances of computer technology, high performance computing (HPC) platforms are utilised in an effort to solve increasingly complex turbulence problems that were until very recently beyond our imagination. Computational fluid dynamics (CFD) is now a critical complement to experiments and theories in order to understand turbulent flows and how to manipulate them in various engineering applications.

In this work we present our open-source framework XCompact3d for performing high-fidelity simulations of turbulent flows using HPC. This powerful framework combines the versatility of industrial codes with the accuracy of the best academic codes (spectral accuracy). Thanks to a powerful 2D domain decomposition of the mesh and the use of the MPI library for communicating information across processors, it can scale up to one million computational processors for simulations using up to several billion mesh nodes. Sixth-order compact finite-difference schemes are used for the spatial discretisation while high-order schemes are used for the time advancement. If the flow is incompressible, a fractional step method requires solution of a Poisson equation, which is fully solved in spectral space via the use of relevant 3D Fast Fourier transforms. Combined with the concept of the modified wave number, this direct (i.e. non-iterative) technique allows the implementation of the divergence-free condition up to machine accuracy. A partially staggered mesh is used where the pressure mesh is shifted by a half-mesh from the velocity mesh in each direction. This type of mesh organisation leads to more physically realistic pressure fields with no spurious oscillations. The solvers within the framework can be combined with customised immersed boundary methods to model complex geometries such as wind turbines or a moving objects.

Various examples will be shown such as wind farms at full scale, gravity currents, plasma-controlled turbulent jet (PRACE project 2016163847) and wall-blowing control of boundary layers (PRACE project 2018184381). These examples will highlight how turbulence-resolving simulations can be use to optimize the power output of a wind farm, to enhance the mixing of a turbulent jet while reducing its acoustic signature and to generate net power saving by reducing the drag over a flat surface.