Towards Exascale CFD: Avoiding Big Data with Contour Tree based in-situ Vortex Extraction

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1 Background and motivation

Real world industrial problems, such as a design of "greener" aircraft, including aeroacoustic optimization of landing gear (Fig. 1), frequently involve unsteady high Reynolds number flows ($Re = 10^5$-10^8) in complex geometries. To accurately simulate such flows requires peta/exa scale computer resources. Moreover, recent development of engineering design tools, e.g., machine learning based methods and multi-objective design optimization exploration (MODE [1]), will also play a very important role for industrial problems, and require very large computational resources: for example, aeroacoustic design exploration of a flame deflector of a rocket launch pad [1] required 2,500 large-eddy simulations (LES) using 10% of the petascale supercomputer K (350 hours with 52,000 cores).

PyFR, a Python based CFD solver (`http://www.pyfr.org/`), is a good candidate technology to underpin the above such simulations. PyFR has already demonstrated excellent performance for 100Bn+ DOF high-order accurate unstructured grid simulations in terms of weak/strong scaling theoretical peak on leading petascale supercomputers including Piz Daint and Titan (peak performance of 13.7 DP-PFLOP/s [2]).

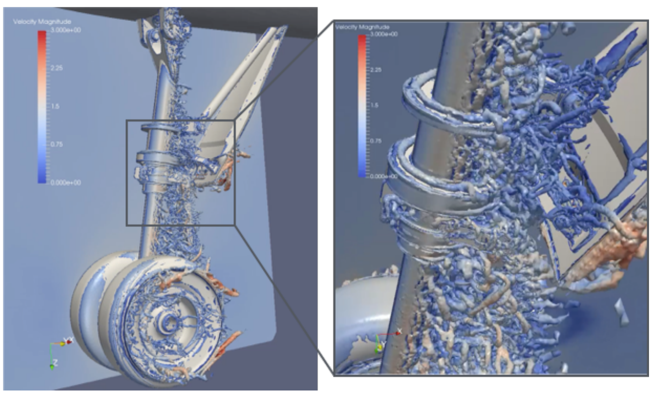

Figure 1: Instantaneous vortex structures around a Gulfstream G550 nose landing gear (computed by PyFR on Piz-Daint with 65 million cells.)

However, for such peta, and in the future exascale simulations, there still remain issues regarding extracting useful information from data that can be generated: 1) real-scale turbulent flows (at $Re \geq O(10^5)$) generally comprise unsteady turbulent vortices, which up until now have only been characterized statistically, without accounting for the behavior of individual vortices; 2) the data size of each temporal flow snapshot can be larger than 1 TB, and the disk I/O can be a bottleneck as well, hence conventional post processing methods are not feasible.

From a practical viewpoint in the simulation technology, the quality of a computational mesh can be locally improved on the basis of detecting turbulent vortex structures, e.g., the mesh adaptation in the turbulent wake simulation around a rotor ($Re = O(10^6)$) [3]. Furthermore, the importance of extracting individual vortex behavior has been pointed out in fundamental flow [4] ($Re_\lambda = O(10^2)$) to understand the turbulent flow physics, and it is recently more extensively studied towards effective modeling and control of industrial and geophysical processes [5]. However, the detection of these vortex structures from complicated industrial flows is mostly based on the visualization and qualitative analysis of Q-isosurfaces, afterwards, using spatiotemporal sampling, which will not be realizable on peta/exascale simulations in the near future.

2 Project objectives

This project aims to address the above challenges by developing a toolset with which the grid-scale vortex structures can be efficiently extracted even in peta/exascale LES/DNS simulations. For this purpose, we are planning to derive and use graphs representing flow structure and evolution based, for example, on Contour Trees (CT) [6]. The important milestones are the establishment of this new CT framework for quantitative vortex extraction and its implementation based on in-situ data processing suitable for peta/exascale computations. The objectives are as follows:

1. Extension of a CT vortex identification framework to **spatiotemporal wall-bounded flows with a periodic boundary condition**.
2. An in-situ implementation of the above tool in the PyFR framework, which is called the **in-situ vortex identification and tracking (IVIT) tool** hereinafter.
3. The application of the IVIT tool to demonstrate **construction of sparsified representation of wall-bounded flows**.

The CT is a graph-based representation to show how the topology of level sets for scalar values changes, where we focus on the Q-criteria to investigate turbulent vortices. The CT tool has been developed in Prof. Paul Kelly's group in the Department of Computing [6], which is capable of vortex tracking only in the spatial direction without accounting for a periodic boundary condition. The primary objective is to extend this tool to a spatiotemporal vortex tracking tool available for periodic wall-bounded flows. The in-situ data processing in the second objective has been partly established in the PyFR in-situ visualization framework using Paraview [2]. The present project attempts to extend this framework to be able to handle more generalized data sets with more sophisticated implementation. The third objective aims to demonstrate the IVIT tool, which is inspired from Nair and Taira [7] demonstrating a sparsified representation of turbulent flows using a network-theoretic approach.

3 Contour Tree (CT)

CT is a graph that describes the nesting relationship of isosurfaces of a scalar field. Figure 2(a) illustrates a schematic of CT, where the two-dimensional contours are mapped into simple graph representation. Figure 2(b) shows the example of vortex identification with visualization of colored isosurfaces. CT enables us to identify the individual vortex structures which are connected spatially, and also would provide the information how the vortex merges or splits temporally (Fig.2(c)).

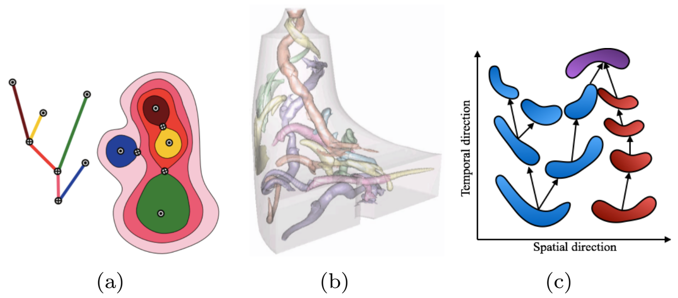

Figure 2: Schematic of CT: (a) shows a two-dimensional contour example [8]; (b) shows three-dimensional vortex identification by CT [9]; (c) shows spatiotemporal tracking of vortex deformation.

4 Work plan

I. Extension of the CT tool: 2 months

The CT tool developed in Prof. Paul Kelly's group will be extended to be able to handle spatiotemporal vortex tracking for the periodic wall-bounded flows. The algorithm for temporal vortex evolution will be based on the combination of existing frameworks for vortex tracking [10] and time-varying contour topology [11].

II. Development of the IVIT tool: 2 months

The extended CT tool is integrated into the PyFR framework to provide in-situ data processing. The original CT tool is written in C++, hence it should be converted to a library to be integrated to PyFR. Note that the code reads a flow field written in the VTK format so that the PyFR output can be directly used without implementing this section.

III. Demonstration of the IVIT tool: 2 months

A series of channel flow DNS will be carried out for variants of Reynolds number condition ($Re_\tau = 170$ to 5000). The turbulent vortex structures in the full DNS dataset are tagged and classified individually based on the CT information, which will be selectively removed to construct a sparsified representation keeping its bulk properties unchanged. The construction of the sparsified representation partly follows the procedure developed by Nair and Taira [7].

5 Impact

This project has strong impacts on both the fundamental and practical fields:

- To the best of our knowledge, there is no preceding work that employs a graph theory like CT framework to characterize the vortices in wall-bounded turbulent flows. The CT representation and vortex identification will provide a new insight to fundamental turbulent physics [4] as well as contribute to a construction of novel modeling of turbulent vortices [5].

- The application of the present IVIT tool to a real world industrial flows will realize an in-situ vortex characterization, which help users reduce a burden of big data processing (including a disk I/O). Reducing the "big data burden" will help enable use of peta/exascale high-fidelity CFD in the context of industrial design frameworks such as machine learning and MODE.

Other outcomes can also be expected: for example in the topics of fundamental fluid physics, it would be possible to track nonlinear growth of a disturbance in the turbulent transition regime, which is beyond a linear growth regime and difficult to be predicted so far; in a practical way, the in-situ vortex identification helps constructing more effective adaptation methods for the computational mesh, which avoids numerical instability as well as efficiently improving the resolution [3].

6 Alignment with PRISM strategy

The work plan is subdivided into three stages, and each section will be summarized in an individual report including conference presentation and journal articles.
Retention of key staff: Yoshiaki Abe is a member of Dr. Peter Vincent's group (PyFR developer) and has good experience of PyFR as well as good knowledge on turbulence theory.
Collaboration within PRISM: This project is highly interdisciplinary spanning across topics in mathematics, computer sciences, and fluid dynamics, as such it will require close collaboration with and between Dr. Peter Vincent in the Department of Aeronautics and Prof. Paul Kelly in the Department of Computing.
Long-term research: The project aims to establish the basis of a new quantitative vortex identification tool. The application of this tool to other engineering fields, e.g., construction of wall models for LES, and more fundamental topics in fluid physics such as nonlinear disturbance growth in turbulent transition will also likely lead to novel findings in the future.

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