HORIZON-EUROHPC-JU-2021-COE-01

EXCELLERAT P2

The European Centre of Excellence for Engineering Applications

Project Number: 101092621

D2.12

Report on the Neko Application Use Case

The EXCELLERAT P2 project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101092621. The JU receives support from the European Union's Horizon Europe research and innovation programme and Germany, Italy, Slovenia, Spain, Sweden and France.

Work Package:	2	Use-Case Execution
Author(s):	Jonathan Vincent	KTH
	Ronith Stanly	KTH
	Adam Peplinski	KTH
	Philipp Schlatter	KTH
Approved by	Executive Centre Management	15.11.2023
Reviewer	Arno Feiden	FHG
Reviewer	Andrea Palumbo	URMLS
Dissemination Level	Public	

Date	Author	Comments	Version	Status
2023-10-25	Adam Peplinski	Initial draft	V0.1	Draft
2023-10-31	Adam Peplinski	Updated draft	V0.2	Draft
2023-11-14	Adam Peplinski	Final version	V1.0	Final

List of abbreviations

ACF	Autocorrelation functions
AMR	Adaptive mesh refinement
CFD	Computational fluid dynamics
DMD	Dynamic mode decomposition
FEM	Finite element method
FWH	Ffowcs Williams-Hawkings
GPU	Graphics processing unit
LES	Large-eddy simulation
MOS	Method of snapshots
MPMD	Multiple program multiple data
PIV	Particle Image Velcocimetry
POD	Proper orthogonal decomposition
SEM	Spectral element method
SVD	Singular value decomposition
UAV	Unmanned aerial vehicle
UC	Use Case
UQ	Uncertainty quantification
VTK	Visualization toolkit
WP	Work Package

Executive Summary

This document presents the progress made in the Neko Application Use Case UC-5 within reporting period 1 covering the first year of the EXCELLERAT P2 project. Based on the detailed roadmap of the workflow development defined in deliverable D2.1, the workflow of the use case is summarised and the achieved progress with respect to the defined workflow, objectives and success criteria are presented.

In summary, the workflow development for UC-5 has progressed according to the schedule defined in deliverable D2.1. Work has been performed on the individual tasks planned for the first year of the project.

That is, progress has been made in all the topics defined in D2.1 including: high-order hex-based meshing, h-type AMR, aeroacoustics, streaming algorithms, uncertainty quantification and in-situ visualisation.

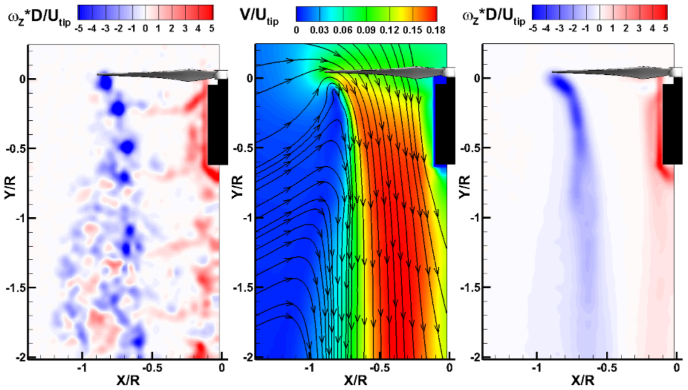
Table of Contents

Table of Figures

1 Introduction

The “High-fidelity simulations of rotating parts” Use Case (UC-5) is a continuation of a previous use case introduced in EXCELLERAT phase 1 by CINECA [1], aiming at studying the flow dynamics around the rotors. We have decided to continue with this use case as, despite of the significant development done during EXCELLERAT P1, it is still of scientific interest, challenging, and requires further code improvements. In addition, this class of flow cases is very industrially relevant, as rotors are used in many mechanical devices, where they allow the devices to exchange kinetic energy with the fluid. It is very important to better understand the dynamics of the flow around rotors, as by improving the energy efficiency, we can for example decrease the energy consumption of vehicles or increase the energy production of wind turbines. In EXCELLERAT P2 we will study rotors in context of aero mobility, looking closer at a drone rotor in hover configuration. This choice is motivated by the rapid expansion of the small UAV market, that is expected to reach USD 58.4 billion by 2026 [2]. Diverse use of drones, covering e.g., package delivery or law enforcement, makes them commonly found in daily life. A side effect of the frequent use of UAVs is noise pollution. This motivates detailed studies of the properties of the flow around the drone blade, both experimental and numerical.

We are going to investigate a two-bladed, twisted rotor studied by Ning [3] called “Iowa” rotor. This configuration was later investigated in several works including numerical ones e.g., Delorme et al. [4] or recently Nathanael et al. [5], but there is lack of results of high-fidelity simulations that do not rely on turbulence modelling. This flow case also constitutes an excellent platform to exploit high-order numerical methods using advanced meshing techniques (e.g., adaptive mesh refinement) in an industrially relevant case. The geometry of this case is relatively complex, but still affordable computationally for hex-based meshing. In addition, the complex flow dynamics are rich in a variety of flow features (e.g., tip vortices). This allows the testing of the whole simulation workflow starting with mesh generation, going through mesh adaptation strategies, in-situ data analysis, and ending with post-processing.



(a) Instantaneous vorticity (b) averaged velocity (c) averaged vorticity

Figure 1: “Free-run" PIV measurement of the propeller in hover configuration [2].

2 Objectives of the Use Case

The main goal of UC-5 is to perform high-fidelity simulation of an "Iowa" rotor in hover configuration focusing on the rotor thrust, the wake characteristics and noise generation. We will perform the runs using the high-order CFD solver Neko using GPU accelerators. Neko is a SEM [6] solver sharing multiple features with Nek5000 (which could be considered a predecessor of Neko). During EXCELLERAT P1 we worked successfully on the robust, fully three-dimensional h-type AMR framework for Nek5000, that was applied to two different use cases. In this approach the resolution is adjusted by splitting/merging the elements (elementary cells of the SEM grid) and this way changing the characteristic element size marked by “h”. The main limitation of this implementation came from the problems inherent in Fortran77 when using GPUs. These problems are solved in Neko using modern object-oriented Fortran 2008. Neko supports various hardware-backends by defining a device abstraction layer and then writing hardware specific kernels in CUDA, HIP or OpenCL. Although Neko provides very good support for GPUs, it lacks some of the features added to Nek5000 during EXCELLERAT P1 e.g., AMR or UQ. That is why our first aim is porting our previous AMR and UQ implementations to Neko. We will then further develop these methods. In case of AMR, we will focus on the performance of pressure preconditioner, work balance, collocated grid implementation (P_N-P_N formulation) and efficient GPU porting. For UQ further improvement of assessing the uncertainly of time-averaged quantities will be considered.

Moreover, we are going to implement in Neko acoustic solvers based on integral formulations as well as FEM/SEM solvers for the acoustic wave equation with different source term formulations [7]. The source term will be directly computed from the incompressible flow field solutions. The last aspect we are going to consider is an in-situ data analysis. A good example is that POD and DMD analysis are widely used in CFD community, but not affordable for exascale simulations due to large amount of required data. We are going to implement parallel streaming algorithms [8] for both POD and DMD in Neko and perform the whole analysis in-situ. We also plan to implement in Neko the data compression for SEM solvers developed as a part of the EU project ADMIRE.

3 Workflow Description

During EXCELLERAT P2 we are going to work on the whole simulation workflow covering pre-processing, running and post-processing stages. At the pre-processing step the main challenge is the generation of a proper hex-based, high-order, conforming mesh. This mesh is later evolved during the simulation through element splitting/coarsening according to the evaluated error indicator/estimator. This process is performed dynamically in a recurrent way, until a statistically converged mesh/solution is reached. Note, we assume here a statistically converged solution can be reached and we do not intend to track the time dependent features of the flow. After a statistically converged mesh/solution is reached, the refinement/coarsening process is stopped, the resulting nonconforming mesh gets frozen and is used for collecting and processing in-situ data. At this stage the incompressible fluid solver will be coupled with an acoustic solver, the streaming POD/DMD, the tool collecting statistics and UQ tool. At the post-processing step the statistics collected over several runs will be further analysed and the results of UQ will be used to quantify the error of the time-averaged quantities. In more detail, the workflow components are:

High-order hex-based meshing: Neko similarly to Nek5000 relies on a hex-based, high-order, conforming meshes. The generation of such meshes for complex geometries is a challenging problem that has not yet been fully solved. AMR and the resulting non-conforming meshes increase the meshing flexibility significantly, but even in those cases the starting point for the simulations are coarse conforming meshes. Most of the open source and proprietary mesh generators are very efficient in creating meshes with mixed-type elements, but building a hex-only mesh usually is a tedious and time-consuming exercise. The rotor geometry studied in UC-5 is relatively complex, but it is still possible to mesh it with most of the available software. As Neko is intended for both academia and industrial users, we are going to investigate both proprietary (e.g., pointwise) and the open source (Gmsh) mesh generators. During EXCELLERAT P1 we created a simplified "toy" rotor mesh using Gmsh and its scripting language and concluded that this scripting language is not flexible enough for more complex projects. That is why in EXCELLERAT P2 we test the Gmsh modern Fortran interface, where we benefit from the advantages of a more mature programming language.

h-type AMR: An important component of our simulation is AMR, which allows an optimal mesh to be built dynamically for a given flow case setup according to the estimated computational error. This feature becomes critical for large-scale simulation with limited a priori knowledge of flow dynamics. During EXCELLERAT P1 we developed a h-type AMR workflow in Nek5000 and now we will port it to Neko. In this approach we take advantage of a standard SEM mesh decomposition into a set of non-overlapping subdomains (elements) and perform recurrent split of existing subdomains into the smaller ones. As both codes are SEM solvers, most of the workflow will remain unchanged and we can directly use our experience from EXCELLERAT P1. The most significant difference is a velocity-pressure coupling, as in Nek5000 we used staggered grids (P_N-P_{N-2} formulation), and Neko only supports collocated grids (P_N-P_N formulation). In addition, Neko would require a few additional features like variable time step, or surface projection tool. The starting point will be a CPU implementation, but the next important task will be an efficient GPU implementation. Finally, we will assess the influence of the P_N-P_N AMR implementation on collected statistics.

Aeroacoustics: Aeroacoustic noise is an important factor that needs to be considered when designing a rotor for any application as it can affect its usability. For drones that operate in urban environments, it is essential to study their noise footprint, so they are less disruptive in its flying environment. Hence for the rotor that we simulate, we will investigate its noise emissions by using methods that can be coupled to our incompressible flow solver, Neko. As for most applications, the far-field acoustic pressure is of interest, we initially implement and utilize the integral method (FWH [9]) in-situ. This method has a low computation cost while proven to be effective for rotating blade noise prediction [10]. However, integral methods cannot account for the reflection and refraction of acoustic waves. Therefore, the acoustic wave propagation needs to be simulated using an acoustic wave equation. For this reason, we will solve the acoustic wave equation using FEM/SEM by considering different source term analogies. The source term will be computed from the incompressible flow field results in Neko. The acoustic source term and the predicted acoustic pressure will be analysed in combination with the analysis of the flow statistics in order to identify the noise sources.

Streaming algorithms: POD and DMD are among a widely used class of methods that aim to obtain a dimensionality reduction of the time dependent data sets. They are used with the aim to perform data compression, reduced order modelling and analysis of data by means of extracting meaningful flow structures from the field. An efficient way to perform POD is to use the so-called MOS [11], but for our implementation, we focus of methods based on SVD, a mathematical factorisation technique. We focus on combining certain aspects of parallel algorithms for the computation of SVD [12] and streaming algorithms [8] along with several optimisations to ensure that we can perform parallel and streaming SVD on many nodes, as is required by the large amount of data produced by large scale simulations. To be able to execute the in-situ task asynchronously while the main simulation runs, we implement the in-situ engines that ADIOS2 provide and that were initially implemented to allow data compression in Neko predecessor Nek5000.

Uncertainty quantification: Due to finite time averaging, computed statistics of turbulent flow simulations are always to some extent uncertain. The prediction of these error bounds is not a trivial task, in particular if the corresponding analysis should be done during the runtime, i.e., without writing out long time series. We will continue our work on a low-storage updating (streaming) algorithm for the online prediction during the run-time of a simulation. The proposed framework, partially implemented in Nek5000 and now being transferred to Neko and corresponding GPU runtime, is based on modelled ACF, through a VTK-Catalyst interface. Special focus will be placed on an extension of the previous framework, developed in collaboration with Fraunhofer SCAI and the University of Manchester, to higher-order general turbulence statistics such as the turbulent kinetic energy.

In-situ visualisation: In-situ visualisation is important because it allows the analysis of simulation results that would otherwise be impossible due to the size of the data sets that would be needed and the required post-processing execution time. During EXCELLERAT P1 in-situ visualisation was implemented for Nek5000 and will be it implemented for Neko in EXCELLERAT P2. The SENSEI open-source interface library will be used in the implementation. This interface allows the simulation to be coupled with a wide range of visualisation tools e.g., VISTLE, VisIt and ParaView.

4 Progress achieved

During the first year of the project, we worked on multiple aspect of the numerical modelling workflow, covering pre-processing, execution and post-processing stages. The achievements are summarised in the following points directly corresponding to the UC workflow defined in D2.1:

High-order hex-based meshing: During the first year of the project, we focused on generating a zero-level, coarse mesh of the “Iowa” rotor using the Gmsh Fortran interface. Producing a high-quality, high-order hex-only mesh is a challenging task and we had to change our approach, as we were not able to keep a proper element aspect ratio on the blunt trailing edge of the rotor. To solve it we implement conformal refinement strategies following 3-refinement [13] and 2-refinement [14] schemes. As a public Gmsh release does not support such operations, we had to restructure our software to have access to the multiple small mesh sections, that can be refined before the objects are created in Gmsh. This differs from our previous method, where the big sections of the mesh were created and meshed in Gmsh directly. We have to stress here that our goal is to increase meshing flexibility with Gmsh and not to write a stand-alone general mesher. The last aspect we work on is mesh smoothing appropriate for SEM solvers. In original workflow this was done directly in Nek5000 during the initialisation step using a method developed by Mittal and Fischer [15]. We currently work on implementing this method in our meshing software.

h-type AMR: Implementing AMR framework in a new solver requires development of multiple features needed by this framework. We started our work with integrating the mesh manager p4est with Neko so we would be able to import a dynamically changing mesh into the solver. While this work is mostly done, we found some limitations of the mesh representation inside Neko. That is why we are currently rewriting the mesh module in the solver to allow for various mesh configuration and to simplify coupling with an external mesh manager. The next aspect we will work on is refinement/coarsening of the flow variables according to the changing mesh. This is done using spectral interpolation and requires point-to-point communication to exchange each element’s parent/child data. Moreover, we are implementing a number of additional features i.e., a spectral error indicator, a surface projection and a variable time step. The development of the spectral error indicator is finalised, the work on the surface projection and variable time step is ongoing.

Aeroacoustics: As a starting point towards predicting aeroacoustic noise from the rotor mentioned above in Section 1, we implemented FWH acoustic analogy in Nek5000 and applied it to study the noise radiated from the simpler, 4 bladed (untwisted, constant cross-section bladed) rotor we simulated in EXCELLERAT I. The noise sources were examined, and sources of some spurious noise were identified. As a result, several strategies to reduce the spurious noise were determined and they are currently being investigated. In addition, acoustic pressure at some far-field observer points were also examined and their power spectral density was calculated. A sample snapshot of the filtered (i.e., with spurious noise removed) loading noise source term on one of the blades is shown in Figure 2.

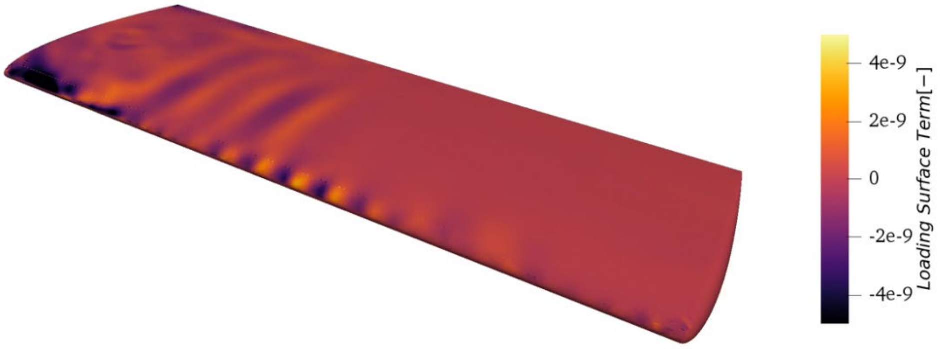


Figure 2: Filtered loading noise source term on a single blade of the 4-bladed rotor.

Streaming algorithms: The work related to streaming algorithms has been carried out as planned. The Neko communicator has been adapted to manage jobs that require Multiple Program – Multiple Data (MPMD) support and ADIOS2 adaptor functions have been added to the software together with Fortran modules that serve as an interface to ADIOS2. This work allows Neko to transfer data in-situ to data processors. An initial python implementation of the streaming algorithms has been completed and has been tested with data written from Nek5000 and in parallel execution in-situ with Nek5000 and Neko. More work remains however, in ensuring that proper restarts are implemented for the streaming algorithms and that the connection is robust enough to handle all use cases.

Uncertainty quantification: During the last period we have extended and finalised a journal paper based on the preparatory work in EXCELLERAT P1 on streaming algorithms for estimation of time-averaging uncertainties in turbulent flow simulations. During this period, we derived an updating formula for both batch-based estimators, and sample-estimated autocorrelation functions. The final workflow combines the simulator (assumed to be black box) with an in-situ data transfer using VTK, and finally the coupling of Catalyst to UQiT. The framework is code-agnostic and allows the estimation of uncertainties in a robust way.

In-situ visualisation: This work is done in collaboration with Work Package (WP) 4, task 4.1 in-situ techniques. Currently an initial port of the Nek5000 implementation of SENSEI and Visit into has been completed, however technical issues remain and a complete run connecting Neko to the visualisation tool has not yet been completed.

5 Conclusion

During the second year of the project, we will continue our work on meshing, testing proprietary meshing software and the dedicated for SEM open-source meshing software HOPR. We will proceed as well with an implementation of the h-type AMR framework in Neko focusing on the P_N-P_N formulation. The goal is to develop a fully functional AMR solver working on CPUs.

As noted earlier, work remains to be done on the streaming algorithms, particularly ensuring that proper restarts are implemented, and that the connection is robust enough to handle all use cases.

Regarding aeroacoustics, we plan to validate the FWH solver (which we already applied on the rotor case, as mentioned in Section 4) extensively by simulating a benchmark case (such as the flow and noise over a forward-facing step) where ample experimental data are available for comparison. This will first be performed in Nek5000 and then ported to Neko, were the influence of P_N-P_N formulation on the acoustic calculation will also be examined.

During the next year, we will explore the possibility to couple the codes using ADIOS2 rather than VTK/Catalyst. In this way, we can maintain the internal data structure better, however we may lose some of the VTK-based functionality. We will understand the limitations, and port the necessary in-situ framework into the Neko code (either VTK or ADIOS2). Eventually, we will extend the framework with in-situ modal decompositions as developed within the Admire project, as to provide a complete in-situ analysis framework.

In case of in-situ visualisation the next steps involve completing the port of the Nek5000 SENSEI interface in Neko. The port will be initially used to testing the visualisation initially with test data and following that production data.

6 References

[1] M. Sawyer, D. Scott, N. Jansson, Ch. Latini, A. Peplinski, G. Staffelbach, M. Wagner, D. Mira Martinez, A.-B. Bedouet, "D2.4 Report on Reference Applications Outcomes," Deliverable 2.4, EXCELLERAT P1 project, URL https://www.excellerat.eu/wp-content/uploads/2022/06/EXCELLERAT_WP2_D2.4-V2.0.pdf, 2022.

[2] A. Mehra, "CISION PR Newswire," MarketsandMarkets INC., 11 June 2021. [Online]. Available: https://www.prnewswire.com/news-releases/unmanned-aerial-vehicle-uav-market-worth-58-4-billion-by-2026--exclusive-report-by-marketsandmarkets-301310782.html. [Accessed 14 June 2023].

[3] Z. Z. Ning, Experimental investigations on the aerodynamic and aeroacoustic characteristics of small UAS propellers, Ph.D. thesis, Iowa State University, 2018.

[4] Y. Delorme, R. Stanly, S. Frankel and D. Greenblatt, "Application of actuator line model for large eddy simulation of rotor noise control," *Aerosp. Sci. Technol.,* vol. 108, pp. 1-12, 2021.

[5] J. Nathanael, C.-H. Wang and K. Low, "Numerical studies on modelling the near- and far-field wake vortex of a quadrotor in forward flight," *Proceedings of the Institution of Mechanical Engineers, Part G: Journal of Aerospace Engineering,* vol. 236, no. 6, p. 1166, 2022.

[6] M., Deville, P. Fischer and E. Mund, "High-Order Methods for Incompressible Fluid Flow" *Cambridge Monographs on Applied and Computational Mathematics*, Cambridge: Cambridge University Press. doi.org/10.1017/CBO9780511546792, 2002.

[7] A. Hüppe, J. Grabinger, M. Kaltenbacher, A. Reppenhagen, G. Dutzler and W. Kühnel, "A non-conforming finite element method for computational aeroacoustics in rotating systems," *20th AIAA/CEAS Aeroacoustics Conference,* 2014.

[8] F. Liang, R. Shi and Q. Mo, "A split-and-merge approach for singular value decomposition of large-scale matrices," *Statistics And Its Interface,* vol. 9, p. 453–459, 2016.

[9] J. Ffowcs Williams and D. Hawkings, "Sound generation by turbulence and surfaces in arbitrary motion," *Mathematical and Physical Sciences,* vol. 264, no. Philosophical Transactions of the Royal Society of London. Series A, pp. 321-342, 1969.

[10] F. Farassat, "Linear acoustic formulas for calculation of Rotating Blade Noise.," *AIAA Journal,* vol. 19, no. 9, p. 1122–1130, 1981.

[11] S. Lawrence, Turbulence and the dynamics of coherent structures. Parts I-III., Q Appl Math, 46(3), 561, 1987.

[12] Z. Wang, B. McBee and T. Iliescu, "Approximate partitioned method of snapshots for POD," *Journal of Computational and Applied Mathematics,* vol. 307, p. 374–384, 2016.

[13] R. Schneiders, "Refining quadrilateral and hexahedral element meshes". transition 2, 1, 1996.

[14] M. S. Ebeida, A. Patney, J. D. Owens and E. Mestreau, "Isotropic conforming refinement of quadrilateral and hexahedral meshes using two-refinement templates," *Internat. J. Numer. Methods Engrg.*, 88, 10, 974–985, 2011.

[15] K. Mittal and P. Fischer, "Mesh Smoothing for the Spectral Element Method," *J. Sci. Comput.* 78, 2, 1152–1173, 2019.