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Updated Report on the Neko Application Use Case

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List of abbreviations

ACF	AutoCorrelation Function
AMR	Adaptive Mesh Refinement
CEEC	Centre of Excellence in Exascale CFD
CFD	Computational Fluid Dynamics
CoE	Centre of Excellence
CPU	Central Processing Unit
DMD	Dynamic Mode Decomposition
DNS	Direct Numerical Simulation
FEM	Finite Element Method
FWH	Ffowcs-Williams-Hawkings
GPU	Graphics Processing Unit
M	Month
MOS	Method of Snapshots
PIV	Particle Image Velocimetry
POD	Proper Orthogonal Decomposition
SEM	Spectral Element Method
SVD	Singular Value Decomposition
T	Task
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 since Month (M) 12 covering the second year of the EXCELLERAT P2 project. Based on the detailed roadmap of the workflow development defined in deliverable D2.1 “Use-Case Execution Roadmap” [14], 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 setup of UC-5 was finalised and tested by performing fully Adaptive Mesh Refinement (AMR) production runs using Nek5000. Moreover, the streaming algorithms task was finalised as well, and there was significant progress in aeroacoustics, uncertainty quantification and in-situ visualisation achieved. On the other hand, the initial Central Processing Unit (CPU) implementation of the AMR framework in Neko requires more effort than it was predicted, and this work will be continued in the third year of the project.

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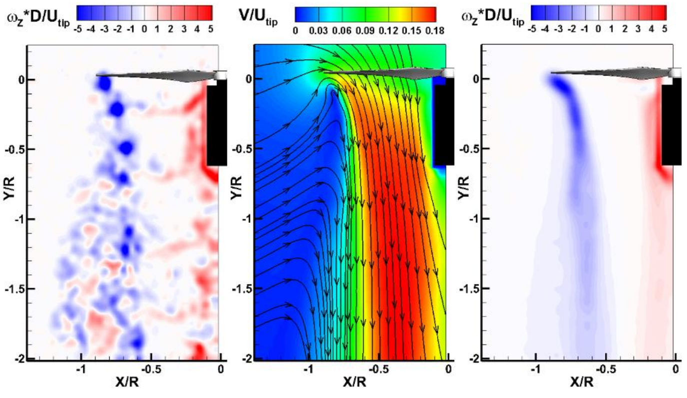
1 Use Case Introduction

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 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 Unmanned Aerial Vehicle (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 (Fig. 1). 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 extensive 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" Particle Image Velocimetry (PIV) measurement of the propeller in hover configuration [3]

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 Computational Fluid Dynamics (CFD) solver Neko using Graphics Processing Unit (GPU) accelerators. Neko is a Spectral Element Method (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 Uncertainty Quantification (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 Finite Element Method (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 Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (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 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 points 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 an 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 the velocity-pressure coupling, as in Nek5000 we used staggered grids (P_N-P_{N-2} formulation), and Neko only supports more modern, 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 is the CPU implementation, but the subsequent 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 implemented and utilised the integral method (Ffowcs-Williams-Hawkings (FWH) [9]) in-situ. This method has a low computational cost and has proven effective for predicting noise from rotating blades, particularly for free-field sound radiation in the acoustic far field [10]. However, integral methods cannot account for the reflection and refraction of acoustic waves. Therefore, for such cases 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 acoustic source term will be computed from the incompressible flow field computed by Neko. The accuracy of the sound predictions using different formulations will be verified against experimental data.

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 Method of Snapshots (MOS) [11], but for our implementation, we focus of methods based on Singular Value Decomposition (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 provides 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 transferred to Neko and corresponding GPU runtime, is based on modelled AutoCorrelation Function (ACF) [13]. The in-situ data transfer from Neko to UQit is achieved using ADIOS2. 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. According to the initial plan the SENSEI open-source interface library supposed to be used in the implementation. However, we found it beneficial to limit the number of the solver dependencies and instead use the novel PySEMTools package developed in collaboration with the EuroHPC Centre of Excellence in Exascale CFD (CEEC) Centre of Excellence (CoE). This software is based on the previous work done in ADMIRE EU project and allows to analyse data in-transit executing various tasks asynchronously.

4 Progress achieved since M12

In this paragraph, we describe the progress made during the second year of the project, while our first-year achievements can be found in D2.1 [14]. During this period, we continued our previous effort focusing 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 second year of the project, we continued the generation of a course, zero-level mesh using Gmsh Fortran interface. To keep a proper element aspect ratio at the blade blunt trailing edge we finalised implementation of a conforming refinement based on the modified 3-refinement [15] and 2-refinement [16] schemes. We combined it with a mesh smoothing appropriate for SEM solvers based on [17]. The resulting mesh at the rotor surface is presented in Fig. 2. An important aspect we had to improve was the blade model used to correct the blade surface while mesh refinement is performed. The blade model is based on stl file and in its original version extracted chord scaling and angle of attack as a function of the distance from the rotor centre were used. We found it insufficient, and the new blade model based on 2D-splines was developed. The last aspect was development of the refinement strategy, as for such a complex and deformed mesh approximation of the highly curved element located next to the nonconforming interface with a rectangular one (done in a pressure preconditioner step) could lead to instability. We developed an appropriate correction scheme for element refinement and were able to perform full AMR simulation using Nek5000. Result of a testing run with a Reynolds number Re=1500 is shown in Fig. 3. This setup was used to perform a simulation of a starting rotor with Re=15000. Visualisation produced from this simulation was selected as one of the finalists of ERCOFTAC Milton Van Dyke Flow Visualization Competition 2025 and can be seen in [18]. Parallel performance of the non-conforming solver in Nek5000 does not differ significantly from the conforming one. Testing runs were performed on CPU partitions of Dardel (PDC, Sweden) and LUMI (CSC, Finland) and the strong scaling plot is presented in Fig. 4.

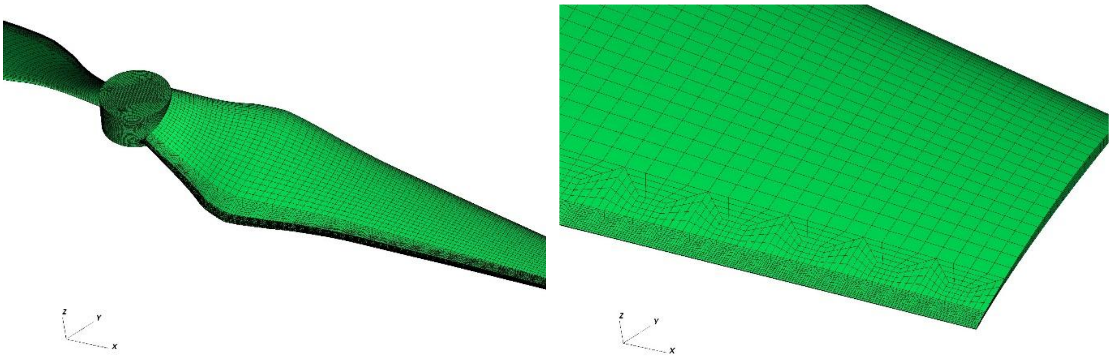


Figure 2: Mesh structure on the rotor surface. Element boundaries are mark with black lines. Right picture presents details of the conformal refinement at the blunt trailing edge

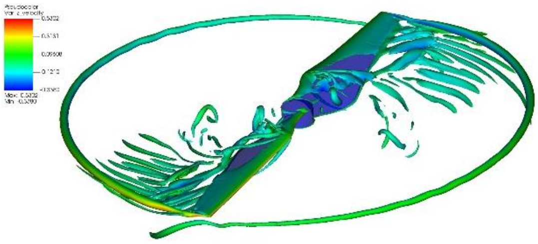


Figure 3: Vortical structures around a starting rotor. Result of a testing run with Re = 1500

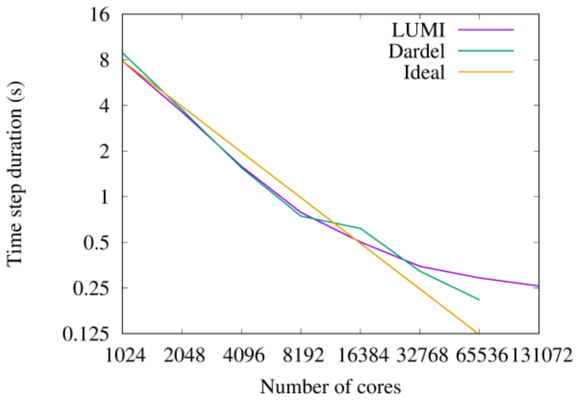


Figure 4 Strong scaling results for nonconforming Nek5000 solver performed on Dardel and Lumi using testing runs.

h-type AMR: During the second year of the project, we continued implementation of AMR framework in Neko. However, as our focus in the last year was finalisation of the rotor AMR setup and this was tested with Nek5000, the implementation of AMR in Neko did slow down. We introduced a new mesh description to the solver, but the non-conforming CPU version of the solver was not finalised. This work will be carried on in the third project year.

Aeroacoustics: Our initial implementation of the aeroacoustic solvers was done in Nek5000. In the second year of the project, we implemented our approach in Neko and we developed a Python package for computation, post-processing and visualization of sound propagation, i.e., *AcoNeko*. As the next step, we investigated the effect of various inflow conditions on the pressure field and the far-field sound radiation for the case of a spatially developing flat plate turbulent boundary layer. We then validated our approach by simulating the sound radiation for a forward-facing step, based on the descriptions in [19] and [20] against experiment. For the flow field, we performed a Direct Numerical Simulation (DNS) using Neko at Re_H=8000 based on the step height and Re_θ=761 based on the momentum thickness of the incoming turbulent boundary layer. Fig. 5 (left) shows isosurfaces of the λ_2 criterion and the corresponding dipole sources (right).

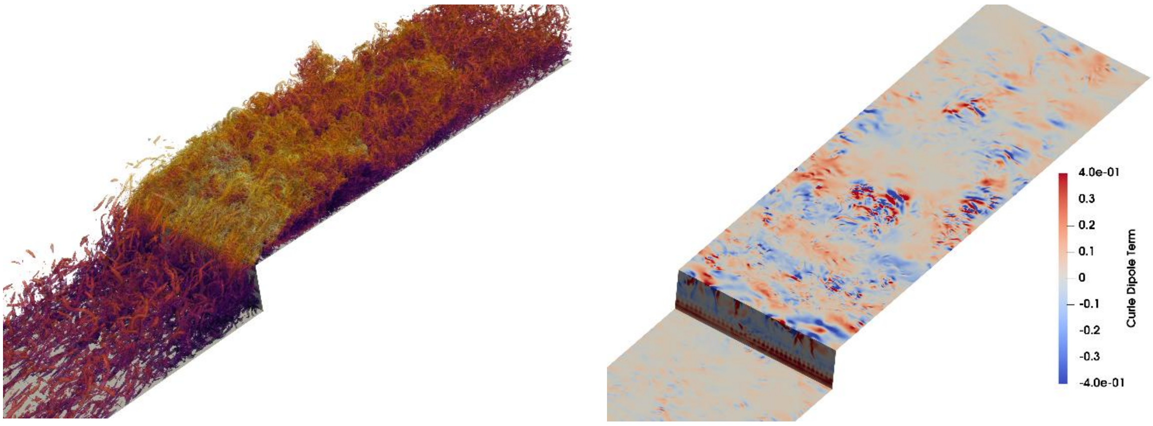


Figure 5: Isosurfaces of the criterion colored with velocity magnitude (left) and the corresponding dipole source term based on Curle's analogy

The dominant acoustic sources are found to be located near the downstream bubble which is in agreement with findings in [19] using beamforming. The sound radiation simulation was performed using Curle's analogy in AcoNeko. Fig. 6 shows the strong scaling of the Neko solver on NHR's CPU cluster Fritz with and without the Aeroacoustic solver. Furthermore, the roofline diagrams for 1152 CPUs (about 550 8th –order spectral elements per cpu) is shown in Fig. 7 and 8. When there are enough elements per cpu, both cases are near hardware's peak performance limit. Fig. 6, 7 and 8 show that the overhead from computing the acoustic sources and passing it to *AcoNeko* is negligible.

The result of the acoustic simulation, shown in Fig. 9, is in close agreement with the experiment which had not been achieved numerically before, as discussed in [20]. This work was presented at the 51st Annual Meeting on Acoustics in Copenhagen [21].

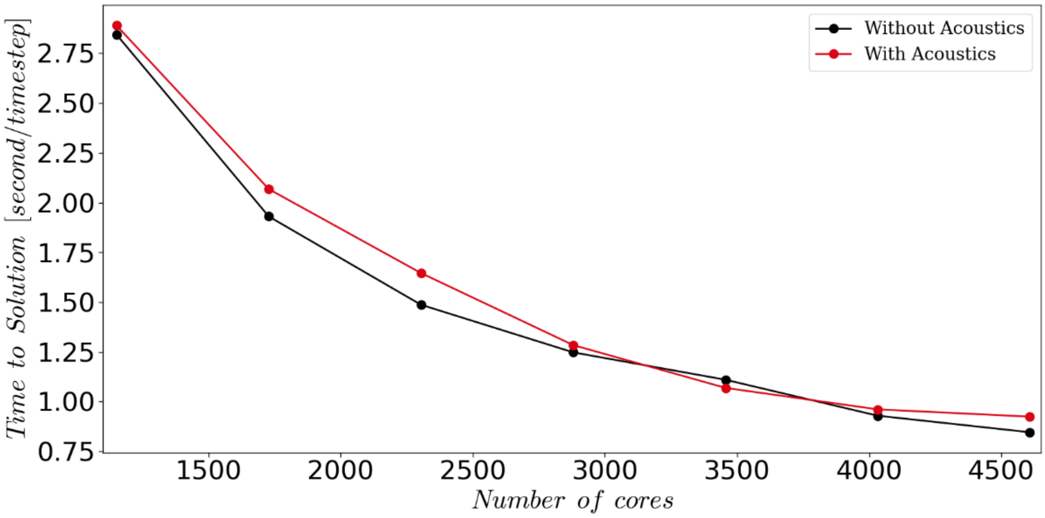


Figure 6 Strong scaling results for Neko performed on NHR Fritz cluster with and without the acoustic solver

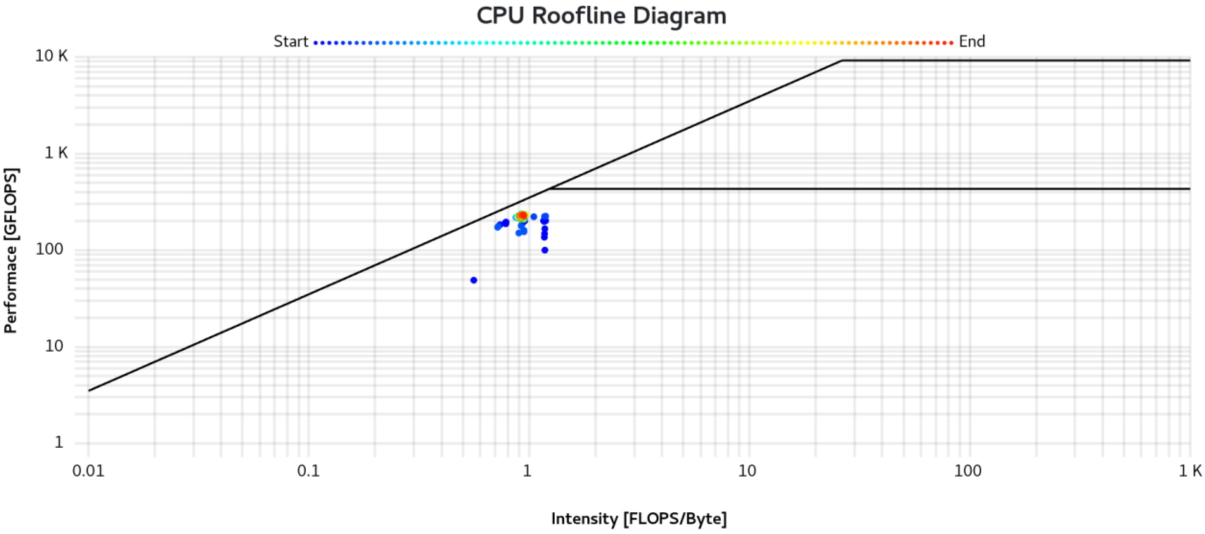


Figure 7 The roofline diagram for Neko on 1152 CPUs with the acoustic solver.

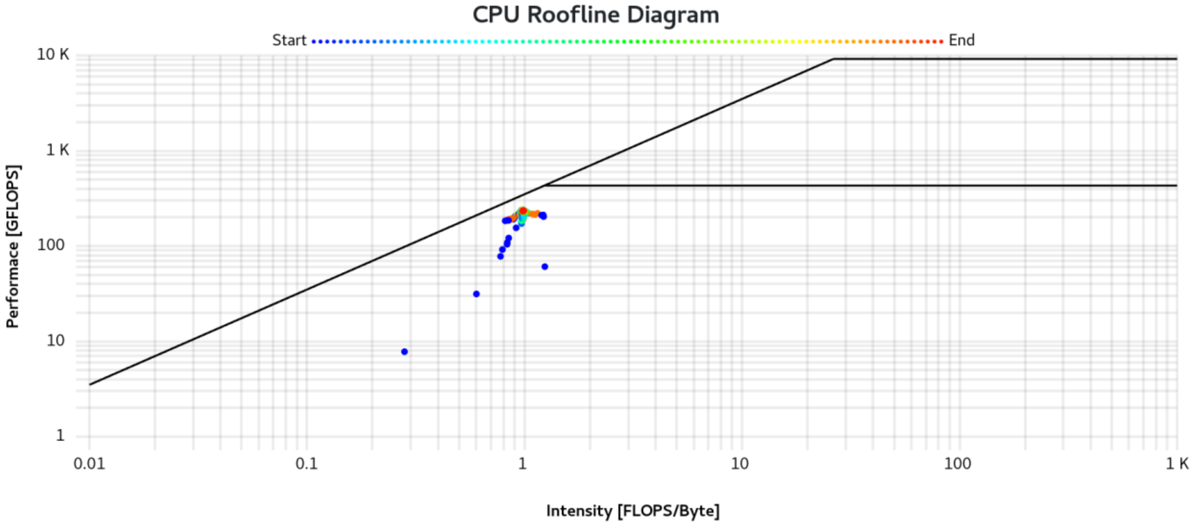


Figure 8 The roofline diagram for Neko on 1152 CPUs without the acoustic solver

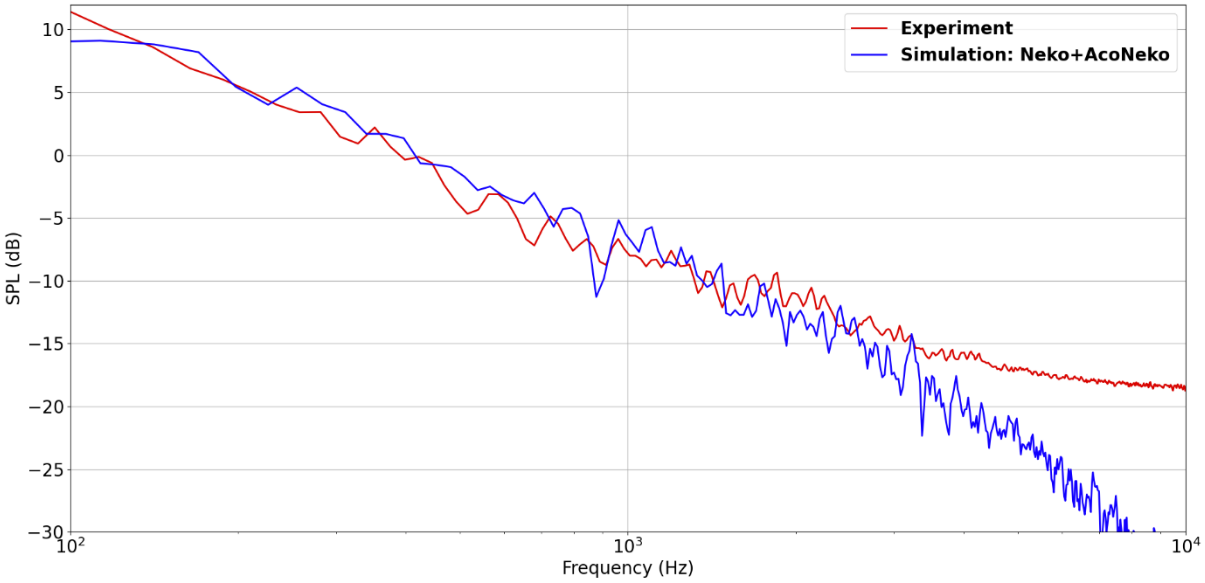


Figure 9 Comparison between the sound spectra obtained from experiment and simulation

Streaming algorithms: Our previous efforts were combined with the work done in CEEC CoE and resulted in development of PySEMTools package. This work was led by CEEC CoE. PySEMTools is a SEM specific python code allowing to perform various task both in pos-processing and in-situ mode. The library allows to perform streaming/parallel POD and, through exposing the data to the rich Python package environment, it opens the possibility to implement more functionalities based on existing developments by other groups.

Uncertainty quantification: We continued our work on the UQ framework based both on batch-based estimators, and sample-estimated autocorrelation functions. The framework is code-agnostic and allows the estimation of uncertainties in a robust way. Previously, we used Catalyst for our in-situ data transfer between Nek5000 and UQit. During the second year of the project, we extended our work by coupling our new solver *Neko* to *UQit* via an ADIOS2 interface. This work was performed in collaboration with WP4 and more detailed description of the workflow is given in deliverable D4.2 [22]. Currently, we are able to performed in-situ uncertainty quantification for first order statistics in *Neko*. Further development for higher order statistics is in progress.

In-situ visualisation: This work is done in collaboration with Work Package (WP) 4 and CEEC CoE. We found it beneficial to combine in-situ data analysis and visualisation tasks and preform them in a single step. For this purpose, we use PySEMTools package that allows to extract and analyse in-transit data from Neko using ADIOS2 library. Currently this tool supports simple visualisation based on standard packages available in Python. Examples of these are Matplotlib, which we use to create 2D plots of slices of data, and PyVista, a helper library for to interface with Visualization ToolKit (VTK) which can be used to perform more demanding tasks such as iso-surfaces, among others.

5 Next steps

During the second year of the project, we finalised work on the rotor meshing and AMR setup of the simulation. This setup was successfully tested with Nek5000. During the next year we are planning to finalise CPU version of the non-conforming Neko solver, and its GPU version should be implemented in the last year of the project.

Work on streaming algorithms was completed by combining Neko with PySEMTools. However, in the future we are going to collaborate with our partner FhG within WP4 task T4.2 and integrate Neko with the InSiDS tool as well.

Regarding aeroacoustics, we plan to perform hybrid aeroacoustic simulations of the drone rotor. We have so far validated our approach for the case of a forward-facing step both in *Nek5000* and *Neko* using integral methods, but the effect of moving surfaces and AMR remains to be studied and validated. We have seen spurious pressure fluctuations for the case of a rotating blade when AMR is used. To accurately simulate the emitted sound, we will investigate different methods to mitigate spurious pressure fluctuations at non-conformal interfaces. We will then validate the result of our simulation against available experimental data. The final step is to couple *Neko* to an external acoustic wave equation solver to allow in-situ hybrid Aeroacoustic simulations for both near-field and farfield. The acoustic source term will be calculated in *Neko* and will be passed via ADIOS2 to the python interface for interpolation on the acoustic grid. Once the data interpolated, it will be passed to the external solver to solve the wave equation. The result of these simulations will be validated against the experiment.

In case of in-situ visualisation the next steps involve extending visualisation capabilities of PySEMTools by exploring adding interface to CATALYST2.

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