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Partnership for Advanced Computing in Europe

SHAPE Pilot Lapcos: Virtual Test Bench for Centrifugal Pumps

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Abstract

The goal of this pilot project is the implementation on a HPC platform a software package we developed for the automation of an analysis workflow based on computational fluid dynamics (CFD) simulations of centrifugal water pumps. This software can compute the performance curve for pump head (meters) versus flow rate (liters/min). The tool features a rapid virtual test bench for the performances of new pump designs before manufacturing an actual prototype. CFD analysis was carried out using the open source application OpenFOAM. The exploitation of the HPC platform and the good scalability of the OpenFOAM software are a key factor in reducing the time to market of new designs.

1. Introduction

Lapcos was founded in 2005 with the scope to offer a highly professional support service in the engineering field using the latest technologies for virtual prototyping. Lapcos engineers are skilled in the use of software for numerical calculations and performance predictions such as structural analyses, computational fluid-dynamic simulations, multi-body analyses, fatigue behaviour predictions, thermal analyses, etc. Beside traditional engineering skills, software development for specific computer aided engineering (CAE) vertical solutions is becoming a trending activity in order to match the customer's needs in term to accelerate the time to market and the cost/efficiency of simulation.

The centrifugal pumps market in Europe is estimated to be around €10 billion. While in Italy it is expected to reach €2 billion in 2014 with a significant growth rate despite difficult economic conditions in the country. The power consumption of these pumps is estimated to be approximately 1.7TWh, which is a significant percentage of total electrical power consumption in the European Union [1]. The European Commission published several directives aimed at reducing the power consumption and at making more sustainable devices. In order to be more competitive and driven by strict regulations, centrifugal pumps manufacturers are investing in a continuous effort to optimize their designs [2].

For such a competitive and performance-driven market, computational fluid dynamics (CFD) methods improve the time-to-market by reducing the effort spent in prototyping and engineering which is a significant production cost for manufacturers. The actual validation of a prototype involves the measurement of the pump head versus the inflow velocity on a test bench prototype, producing a characteristic curve. Using a proper CFD model and given a particular geometrical design, it is possible to predict this characteristic curve by computer simulation. The use of high performance computing (HPC) resources holds the potential to further reduce computation time. In previous projects, Lapcos implemented a standalone solution for a centrifugal pump manufacturer that consists of a vertical graphical user interface (GUI) application and a specific CFD solver based on the open source software package OpenFOAM [3]. The GUI component automates the preparation of the input file for the

OpenFOAM solver and manages the multiple simulations necessary to compute the characteristic curve for a design.

This white paper describes the work of a SHAPE[a] pilot project where Lapcos and PRACE have collaborated to exploit the availability of HPC resources and the open nature of the OpenFOAM code, which can be deployed without any economical restrictions on supercomputers, in setting up a Software-as-a-Service (SaaS) platform for predicting the characteristic curves of centrifugal pump designs.

2. The proposed approach

The proposed HPC solution is based on a software for CFD analysis for centrifugal water pump originally developed by Lapcos. This software, namely OpenPump, is developed using the open source software package OpenFOAM that has been modified for better and faster convergence. The interface software is able to automate the job boundary condition, the multi-point analysis and extrapolation of the main output information in simple graph format. In particular the software can predict the performance curve pump head vs. flow rate, which is the goal of the virtual test bench. OpenPump is a both pre-processing and a quantitative post processing CFD software for the simulation of centrifugal pumps. The first version of OpenPump was developed with OpenFOAM-1.6-ext and it has been updated annually to accommodate many of the new features released by the OpenFOAM project community.

OpenPump has been conceived to perform several CFD calculations in parallel on the same geometry, aiming at providing the analyst with the pumping characteristic curve (pressure head drop versus volume flow rate) automatically starting from the mesh file and the pumping parameters (revolutions per minute or rpm, and volume flow rates). OpenPump was developed using Codeblocks IDE [4] and its graphical objects were developed using WxWidgets [5] to ensure cross platform compatibility. A new set of C++ routines was written to automatically create OpenFOAM dictionaries. The routines can be used to set up steady state or transient analysis and to manage meshes with arbitrary mesh interface (AMI). The software can also monitor residual, integral and mean flow data on specified patch surfaces and automatically plot the collected data using the Gnuplot [6] application.

Pre-processing stage

The initial stage of any engineering process is pre-processing, which often involves the “art” of transforming an input CAD file into a geometrical subdivision of the computational domain for successive analyses. The word “art” suggests that there is not a fully automated process to perform this kind of transformation for any computational problem and/or for any domain, but it is the operator’s background knowledge of the problem that enables him/her to drive the discretization process. This stage can be very time-consuming and it depends both on the quality of the initial CAD and on the type of analysis to be performed. For this project, we assumed the proper pre-processing steps had been carried out, i.e. a good quality mesh is available as input for CFD simulations. This should not be a limitation of the project as the implemented service prototype should target mainly:

- Companies that are already using CFD tools but are seeking faster solution times and reducing the time-to-market of their designs.
- Companies that are not using CFD directly but that are using CAE tools (such as finite element analysis) and thus have CAE expertise.

At this stage of the project, it may be premature to deliver CFD based results to companies where there is no an engineering team to handle the results, a common situation seen among Italian small and medium-sized enterprises. Even if a potential customer does not have a CAE pre-processor, this could be purchased for a few thousand euro. On the other hand, setting up a CAD-to-mesh translation service, even for a limited application domain, would have required effort beyond the scope of this endeavour.

Computation stage

Once the mesh is ready, the next step is to prepare the CFD analysis. In order to carry on the necessary simulations and to exploit the features of a HPC infrastructure we implemented a custom solver derived from OpenFOAM. The advantages in using an open source component are straightforward:

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[a] SHAPE, the SME HPC Adoption Programme in Europe is a pan-European, PRACE-based programme supporting HPC adoption by SMEs (http://www.prace-project.eu/shape?lang=en).

- No limitations on resources (i.e. number of CPUs or concurrent solutions) involved due to excessive licensing cost constraints.
- Possibility to customize the code

A study was carried out to improve robustness and stability of moving/multiple reference frame (MRF) solvers inside the OpenFOAM package. The fine-tuning of the solvers for a water pump application was carried out to optimize computation times with a significant reduction in early divergence during the start-up procedure.

The OpenFOAM toolbox provides a wide range of turbulence models. In the first version of OpenPump it used the K-ε model which is one of the most common turbulence models. Many benchmarks confirm the validity of the K-ε model and it showed preliminary good results. At the time of publication of this paper a new study on turbulence models is being carried out.

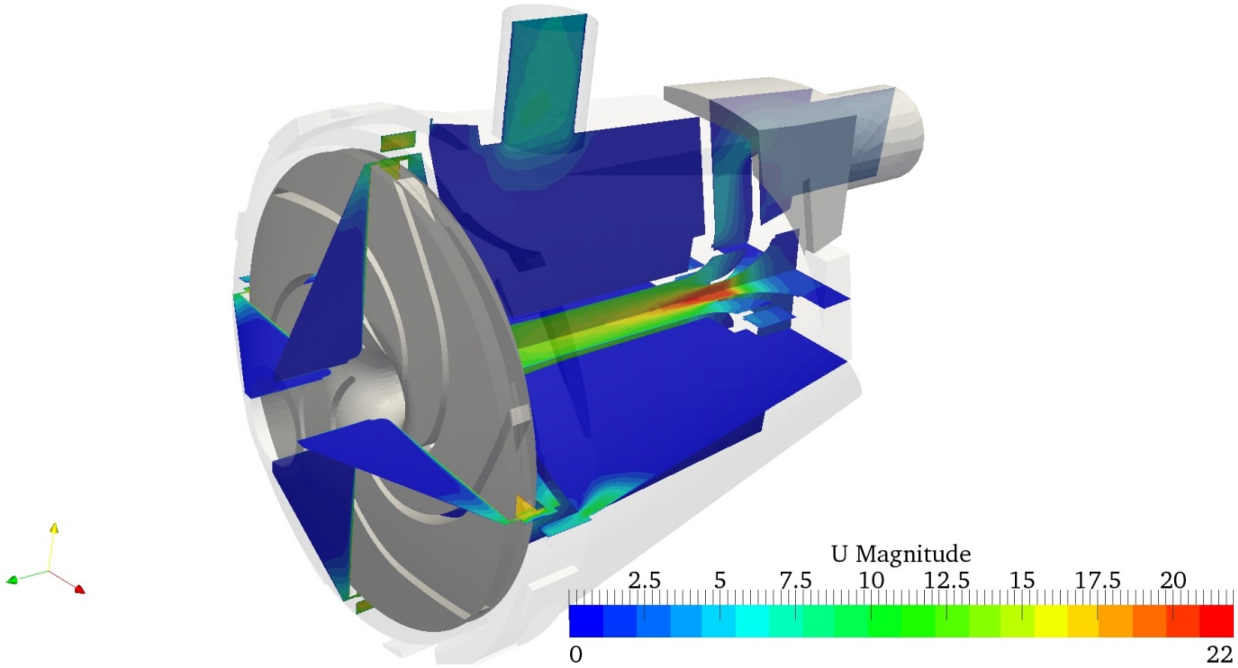

Figure 1 A schematic representation of a centrifugal pump mesh and CFD results.

Post-processing stage

In addition to the pump head/velocity response curve that is the key output from the virtual test bench, we have also generated a 3D representation of the flow domain (Figure 1) using the ParaView application (Kitware, Albany, USA), an open source post-processing tool that supports OpenFOAM output files.

ParaView is an open source data analysis and visualization application. The data exploration/visualization can be done interactively in 3D, but the software can be also scripted using the Python language. It is a versatile tool that can be installed on a range of hardware, from laptops to powerful supercomputers, to analyse extremely large datasets using distributed memory computing resources.

OpenPump, GUI

The value added feature of the virtual test bench is the graphical user interface, OpenPump. In fact, OpenFOAM does not provide a GUI and in order to release a specific piece of software for centrifugal pumps designers, Lapcos provides A GUI interface application to launch the simulations on a HPC cluster. A snapshot of the main interface, installed on the CINECA cluster is provided in Figure 2 below.

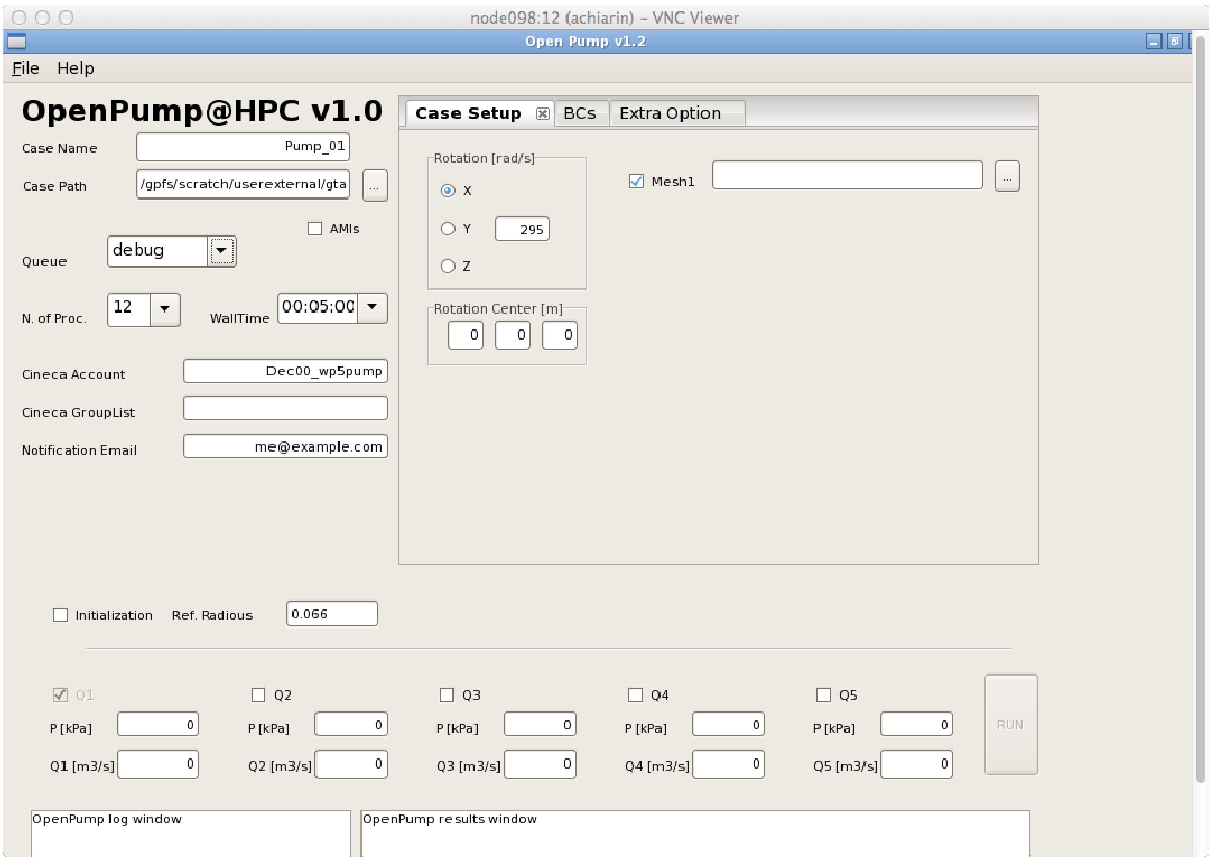

Figure 2 The OpenPump GUI on a Mac Os X client

OpenPump allows the user to carry out the pre-processing steps such as setting up the boundary conditions of the problem, to change some geometrical parameters that doesn't require a re-meshing step, to run and control the simulations' convergence and to display the characteristic curve as output.

The HPC version of the software developed within this project can be provided in a Software-as-a-Service fashion: a potential customer only needs to register on the CINECA *webcompute* portal [8] that enables the submission and management of remote jobs on the HPC cluster, including remote visualization and file management capabilities.

The authenticated user can request a remote visualization session (NICE Desktop Cloud Visualization, Italy [9]) from a list of available applications. When the scheduler assigns the resources, a remote visualization session file is generated and downloaded by the user. Then, from a proper multiplatform client, the user can start the virtual test bench application that is running on the cluster. When the analysis is set up for the specific mesh, the application creates the proper job scripts and sends them to the scheduler. An email is sent to the user to notify the end of computation, at this point the user logs in into the *webcompute* portal and he/she can retrieve the results or start an interactive 3D visualization sessions using ParaView, another service available on the *webcompute* portal.

In summary, this project involved the following activities:

- Compilation and porting of the source code on the CINECA system
- Integration with the HPC scheduler

- Testing and scalability analysis.

3. Results

The CINECA PLX supercomputer[b] was introduced in June 2011 it has been one of the fastest supercomputer available to Italian industrial and public researchers. It has been used to optimize and develop applications targeted at hybrid architectures, leveraging software applications in the fields of computational fluid dynamics, materials, life science and geophysics. The system is also available to European researchers as a Tier-1 system of the PRACE research infrastructure. PLX features 274 IBM iDataPlex M3 computing nodes, each with 2 hexa-core Intel E5645 processors, 48GB RAM and 2 nVidia Tesla M2070 GPU. The system has a total peak performance of about 0.3 petaflops. Node connectivity is supplied with Infiniband 4xQDR and storage is handled by the GPFS parallel file system. The operating system is Linux RHEL 5.6 and the resource manager is PBS Pro 10.6.

For the purposes of the project, access was provided to different queues on the system for different research activities (*debug*, *parallel*, *longpar*). These queues differ in the walltime and the maximum number of parallel processes available.

As stated above, the proposed solution is composed of two main components: a batch custom flow solver linked to the libraries of the OpenFOAM CFD software and the OpenPump GUI. Both were compiled and ported to the CINECA PLX cluster and tested. On the basis of the available solver and Lapcos' data, scalability tests were conducted in order to identify the best configuration for typical use cases.

OpenFOAM was compiled with GNU GCC 4.7.2 and linked against OpenMPI v1.7, while the OpenPump application required the graphical Codeblocks IDE.

Non-regression tests were performed in order to ensure that the performance of the parallel version of the software were the same reported on Lapcos workstations in terms of velocity of convergence and robustness. Figure 3 and 4 shows that convergence is reached within 2,000 iterations of the solver, which is a result comparable with other off-the-shelf commercial solutions.

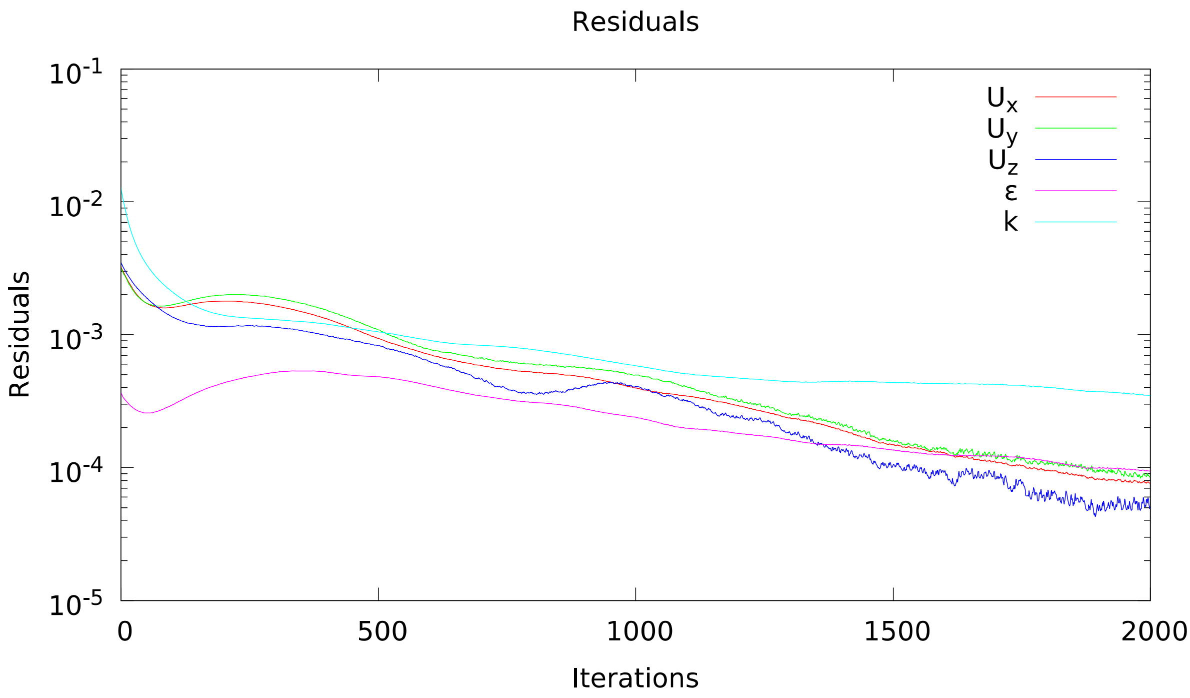

Figure 3 Solution convergence: plot of residuals

[b] http://www.top500.org/system/177417

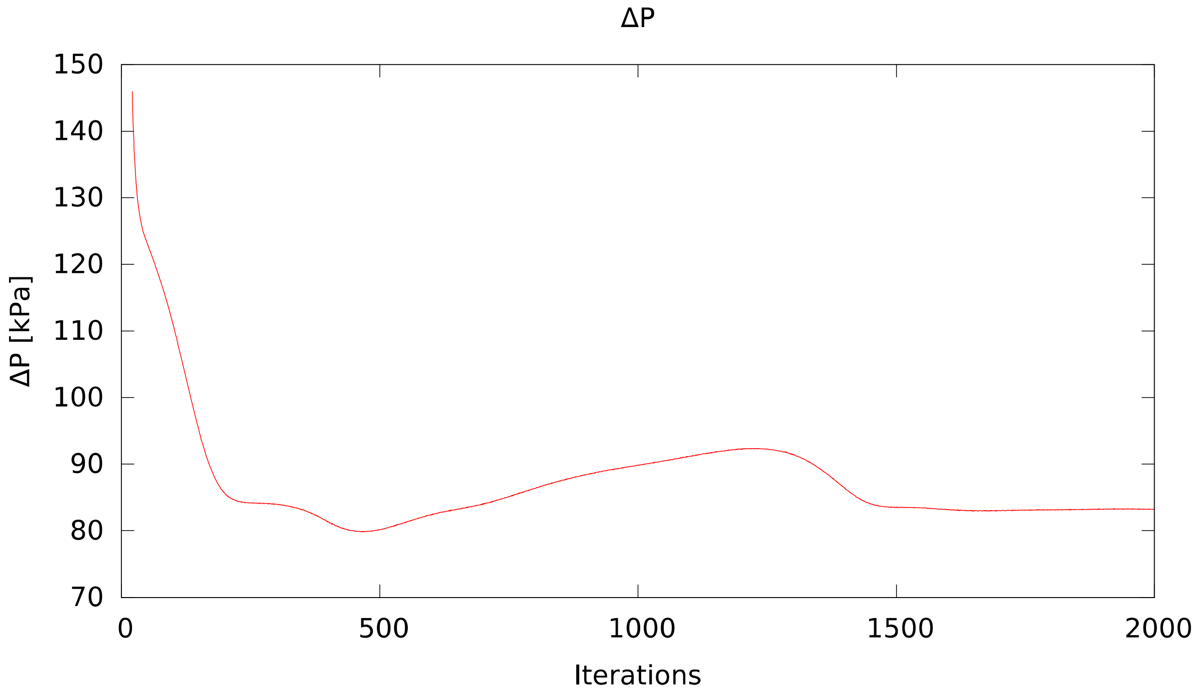

Figure 4 Quantitative monitor of pressure to check physical convergence

In order to reduce computation time, a primary goal of the project, a scalability analysis was performed using an exemplar dataset. The size of the test mesh was approximately 2.5 million elements. Performance analysis was carried out from serial execution up to 120 parallel processes.

A linear speed-up can be observed up to 100 processors, which gives a "computational density" for the OpenFOAM numerical engine of 25K elements/core, which is a value comparable with similar experiments [10][11][12].

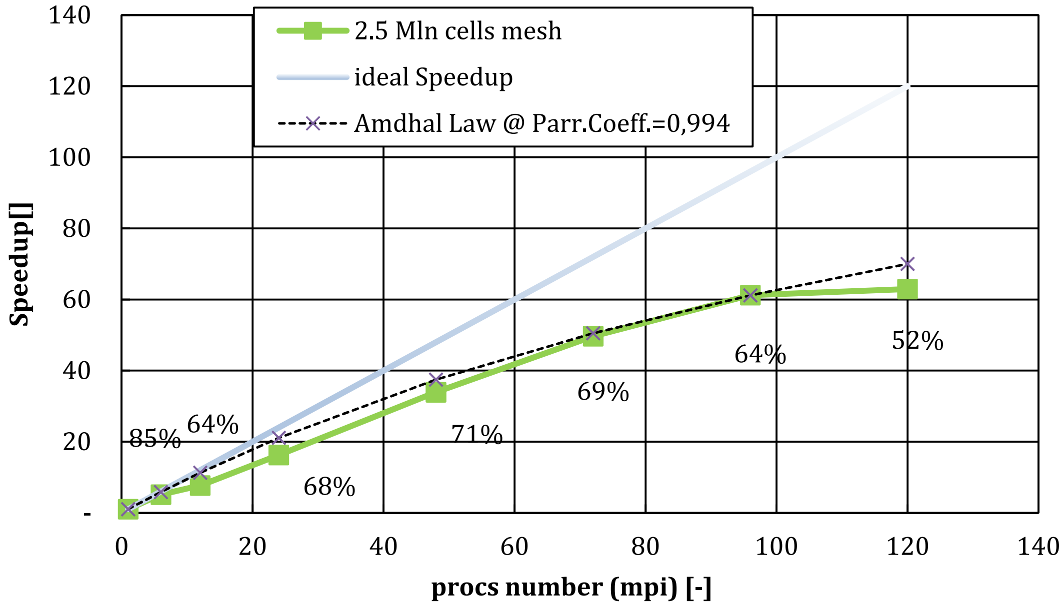

Figure 5 Scalability analysis for an exemplar simulation; the trait line indicates ideal Amdhal behaviour at 99.4%

4. PRACE cooperation

CINECA granted the use of the PLX cluster, a Tier-1 system with a pool of resources accessible by remote SSH sessions and a batch jobs scheduling system (PBS Pro, Altair Inc.). CINECA also supported the porting tasks by providing a C++ development environment, both for the batch component of the system (GNU gcc and Open MPI) and for the GUI component (Codeblocks, a C++ OSS IDE specific for the WxWidgets framework). The GUI is provided by a remote visualization service based on Nice DCV® protocol. CINECA staff, with expertise on HPC technical computing and in parallel architecture was involved to speed up the integration of the existing software with the CINECA platform, particularly in the integration with the resource scheduler.

5. Benefits for SME

Lapcos, along with CINECA as a technology partner, is looking to propose this new service to centrifugal pump manufacturers. On this activity, a pre-marketing email campaign/questionnaire was carried out (as a side activity) in order to obtain feedback from potential customers. Some potential users of this service were also identified and contacted for follow-up activities. The advantages for those customers are:

- Ease of access to sophisticated CAE tools thanks to the deployment of the platform on HPC services with a SaaS distribution model.

- The cost model better fits their needs as only the “consumption” of the service is being charged.

- They can smoothly scale up their problem on the HPC infrastructure, without worrying about fixed IT costs or additional licensing costs. Preliminary scalability analysis indicates that speed-ups by a factor of 20x are feasible in reducing the time-to-market.

6. Lessons learned

Porting and compilation of GUI components can be a tricky operation on a heterogeneous HPC cluster that have both computing and visualization nodes in the same environment. The use of GUI based components is, however, necessary when you “replicate” a typical CAE workflow on a remote HPC cluster.

Simulation response times as a key performance index for an industrial usage is vital and should be carefully taken in consideration when you set up your queues in a shared resources scenario. Guaranteeing short waiting times is essential in a production scenario.

A massively parallel large cluster, rather than medium-sized industry systems, can improve time-to-market for the design of a product; it has the potential to increase the quality and the return of investment of final users.

7. Summary

The goal of this SHAPE pilot project was to adapt an existing software solution for a specific engineering problem to run on a HPC facility and made accessible with a remote interface for end users as a SaaS platform. It has succeeded in (a) optimized the computational time and (b) to simplify for the end user the set-up and installation of such tool. The OpenPump application, developed by Lapcos was successfully compiled and installed on a CINECA supercomputer and integrated with the platform. The application was made accessible from the *webcompute* portal available at CINECA. A scalability analysis was conducted in order to correctly size the simulations. With current software and hardware architecture, a speed-up of 20x (that is yielded by a 4x number of parallel processes than the average and the parallel execution of the simulations to get curve points, typically 5) can be achieved in compute-intensive simulations with the potential to significant reduce the time-to-market for centrifugal pump manufacturers.

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