



## SHAPE Pilot Thesan srl: Design improvement of a rotary turbine supply chamber through CFD analysis

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### Abstract

*This work conducted in the field of the PRACE' SHAPE pilots deals with the optimization of a volumetric machine. The machine is under active development, and a prototype is already working and fully monitored in an experimental mock-loop setup. This prototype operates under controlled conditions on a workbench, giving as an output the efficiency of the machine itself. The main goal is to obtain an increased efficiency through the design and realization of the moving chambers in which fluid flows. In order to obtain such a task, an extensive CFD modelling and simulation is required to perform virtual tests on different design solutions to measure the physical quantities assessing the performance of a given geometry. The final goal is to design a better geometry of the different components, mainly the supply and exhaust chambers, cutting down time and resources needed to realize a physical prototype and to limit the physical realization only on a single geometry of choice. The CFD modelling should allow then, through scientific visualization paradigms and quantifications, to perform a detailed characterization of the fluid dynamics patterns present within the prototype and to identify the main geometrical parameters able to drive the optimal configuration. High Performance Computing facilities and Open-Source tools, such as OpenFOAM, are therefore of capital interest to handle the complex physical model under consideration and to perform a sufficient amount of design configuration analysis.*

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### 1. Introduction

Thesan, a spring-off of Savio, a 120-years old firm in the field of building sector, is a relatively young company in the renewable and green energy field, but its roots were laid early last decade, when the formation of an energy sustainability culture in Western countries concentrated around the first concrete technological applications. Thesan is committed in research project with Technical University of Turin, Padua and Naples and with the CNR, ENEL, CESI. His research and development team is composed of top notch scholars and key figures in the field of technological innovation both in industry and in the international centres of excellence. In order to get a more detailed insight about the fluid dynamics pattern present into a prototype turbine designed by Thesan the authors had to perform a well-defined set of activities:

- build a CFD rotating model using the OpenFOAM (OpenCFD Ltd.) toolbox [1] starting from the CAD of the prototype device;
- study 4 CFD rotating conditions fixing RPM and Mass Flow Rate at the inlet according to experimental measurements;

- visualize flow patterns to get a better understanding of the fluid dynamics;
- quantify meaningful fluid-dynamics indices.

In this section, therefore, we describe first of all the set-up concepts and the simulation protocols for the design and implementation of the adopted workflow to perform CFD study on CINECA High Performance Computing systems using the open-source computational tools.

Research activities have been carried out by means of several tools, which allowed for the implementation of an efficient workflow to perform CFD optimization study on High Performance Computing systems. All the tools are open-source so that the designed workflow can efficiently exploit distributed systems without any limitations due to licenses. Figure 1 reports the overall automated workflow and its components.

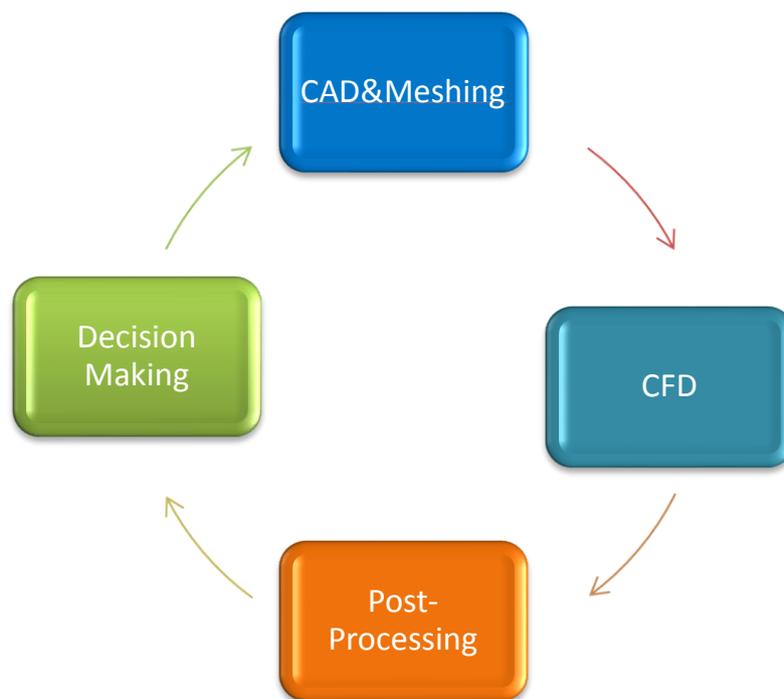


Figure 1. Automated workflow flowchart.

In few words the workflow designed and implemented in this SHAPE pilot project is an automated computational chain that, according the CAD geometry and input values ranges defined by Thesan [2], is able to iteratively repeat these tasks:

- generate a geometry discretization suitable for CFD analysis;
- setup the CFD model;
- solve the CFD model on a distributed set of computational cores;
- compute meaningful quantities by post-processing the CFD output;
- report and synthesize the obtained configuration.

This computational chain is therefore constituted by several bricks. Figure 2 shows in details the computational tools involved in the workflow:

- The Meshing brick (in blue) is constituted by snappyHexMesh (the OpenFOAM pre-processor tool for mesh generation);
- The CFD brick (light blue) is fulfilled by the OpenFOAM (OpenCFD Ltd.) library, version 2.3.0;
- The Post-processing brick (in orange) is constituted by ParaFOAM, a version of ParaView v3.98 (Kitware Inc.) able to read OpenFOAM datasets;

- the HPC infrastructure (in green) is provided by CINECA PLX machine [3] and is the underlying computational environment.

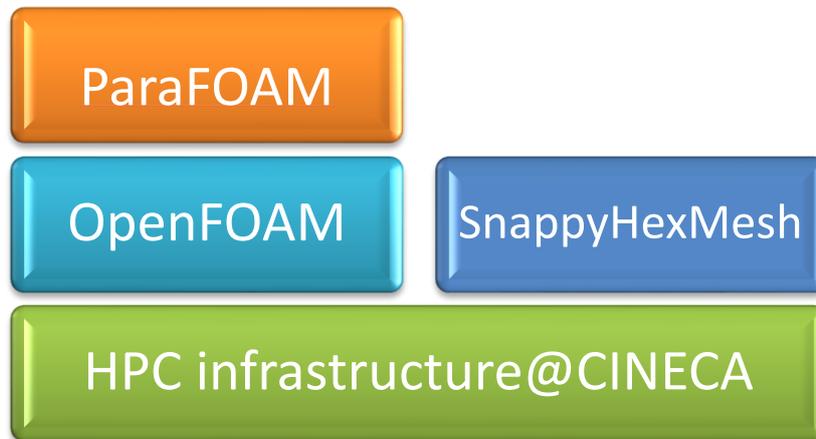


Figure 2. Computational bricks details.

As mentioned above, the overall work is focused on open-source applications in order to exploit distributed HPC resources without having limitations due to non-scalable and relevant licensing costs.

The designed workflow is very general and can be considered valid for a wide range of CFD applications; we applied it to the fluid dynamic problem specified by Thesan. The problem taken into account is a device for mini/micro hydraulic energy production prototyped by Thesan. The workflow main outcome is therefore designed to establish which fluid dynamic patterns are present within the prototype and determine possible adverse geometry characteristics in order to obtain concrete indication of future design pattern. For this reason in what follows if not explicitly mentioned all the information of the CFD settings, computing, post-processing and data analysis are referred to the study of the Thesan prototype and its fluid dynamics characterization.

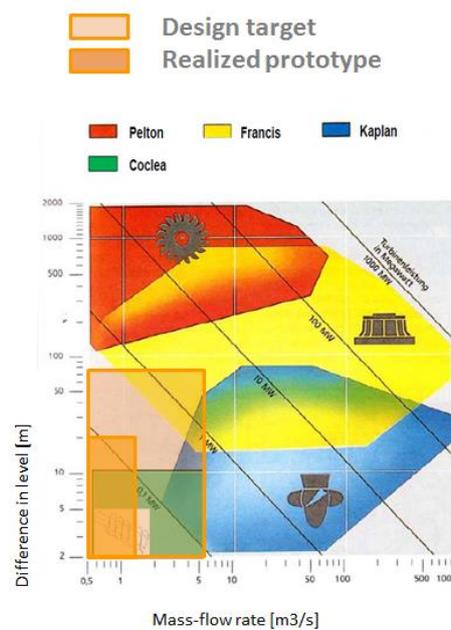


Figure 3. Design target and realized prototype efficiency compared to the market.

## 2. Material and methods

The first step of the CFD analysis is building the 3D geometries describing the volume occupied by the fluid as computational models. This 3D model need to be discretized (meshed) in order to solve the fluid dynamics problem involved.

The solid modeling was performed starting from CAD 3D provided by Thesan engineers. The geometry data were then imported in the OpenCFD toolkit through the stereo lithography file format (.stl).

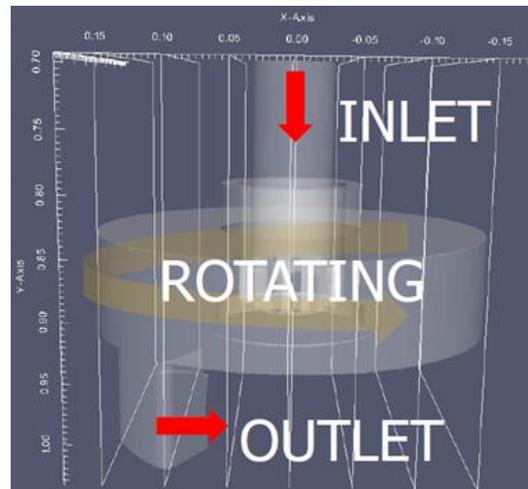


Figure 4. Views of the design and of the CAD prototype with parts description.

The previous figure displays a sketch of the resulting geometry for the prototype considered. Note that building 3D geometrical models for subsequent CFD analysis means modeling the volume occupied by the fluid; the volume occupied by solids is empty, or, more properly, doesn't exist at all in the model. The interface surfaces between solid and fluid domains do exist and may be visualized to check the model appropriateness.

The meshing process has been iterated using SnappyHexMesh functionality available from the OpenFOAM toolbox in order to get a satisfactory discretized representation of the fluid domain keeping the geometry characteristics in terms of reference quality descriptors of the mesh. The meshing procedure was carried out so that the inlet and outlet sections of the channel are made of very regular hexa-dominant grid while the fluid volume fulfilling the prototype geometry is meshed in a finer way. Thanks to this approach, we were able to have a reliable resolution of the fluid domain, and a higher number of cells where needed so that any relevant changes in the fluid dynamics pattern within the complex 3D geometry of the prototype can be efficiently caught. Each CFD model yielded meshes comprising less than 2 million cells each. The suitability of each mesh was tested by checking proper mesh parameters, such as cell skewness and aspect ratios, on a reference CFD model under different fluid dynamics conditions.

Simulation of fluid dynamics was carried out using a well-established open-source library, OpenFOAM. A model fluid is imposed to flow through the inlet lumen, inlet volume and outlet lumen. The simulation solves the fluid dynamic problem iteratively until convergence. Preliminary simulations were carried out, in order to determine the most proper simulation settings and/or resolve meshing size issues.

The simulation protocols (fluid properties, boundary conditions, simulation settings) valid for all the performed simulations are the following:

- *Fluid properties.* An incompressible Newtonian model fluid with constant kinematic viscosity and density has been used. The value adopted is those of Water (H<sub>2</sub>O) at 273 Kelvin. Using a Newtonian model for Water (H<sub>2</sub>O) can be considered a valid assumption for the cases treated.

*Boundary conditions.* The no-slip boundary condition was applied at all the boundaries of the fluid domain which are impermeable to the fluid itself (usually called walls). All walls were assumed as rigid so that a so-called no-slip condition can be applied.

Boundaries are of three kinds:

- 1) Boundary surfaces where pressure is applied. The end cross section of the outlet conduit is of this kind. A reference pressure  $p_r$  is applied as a boundary condition (typically  $p_r = 0$  [Pa]). Note that, in any case, the particular reference value used for  $p_r$  does not affect simulation results.
- 2) Boundary surfaces where fluid flow rate is applied. The initial cross section of the inlet conduit is of this kind. An inlet velocity, or equivalently an overall value of flow rate, is applied as a boundary condition in this case. The ranges studied were provided by Thesan.
- 3) Boundary volumes where the fluid is rotating with respect to other parts of the model. For this kind of boundary we used the well-established Multiple Reference Frame (MRF) modelling already available in OpenFOAM. The ranges studied were provided by Thesan.

Figure 5 schematizes the set of conditions applied at all the four selected configuration CFD model.

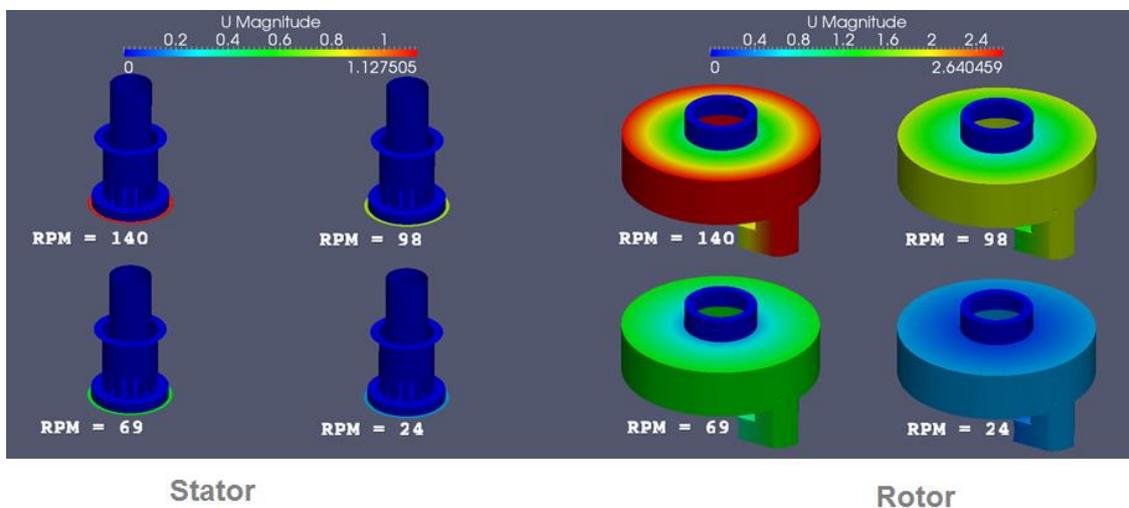


Figure 5. Conditions applied at the boundaries of the CFD model: stator (LEFT) and rotor (RIGHT). RPM values are also reported.

*Simulation settings.* All simulations were run with the so-called pimpleFOAM solver, which is the solver suitable for incompressible unsteady flows and RANS methods for turbulence. Energy equation is not solved, since the heat transfer is neglected in the problem. Due to the relatively low values of Reynolds number, the  $\kappa$ - $\omega$  model is used as turbulence modeling. The influence of the turbulence model is not relevant in the calculation of the pressure force, because the pressure force is essentially a pure normal force normalized by surface area, whereas the turbulence model is responsible for the shear stress (tangential forces normalized by surface area). Moreover, the wall boundary layer on the wall of the device is not resolved. RANS method for turbulent flows, solves the Navier-Stokes equations by accounting for the turbulence thanks to an appropriate heuristic representation of the turbulence effect in terms of energy dissipation and without considering the time variable. In this particular application, the boundary layer was not modeled since wall shear stress values were not the main output of the application. For this reason near wall grid refinement was neglected. Other simulation settings concern solution algorithms: all simulations were run with the 1st order upwind algorithm, which guarantees a sufficient accuracy to the numerical problem solution. In order to properly reach numerical convergence, relaxation factors were tuned for velocity and pressure update. Convergence was accepted when the residuals of continuity, momentum, velocity and turbulence quantities fell within each time iteration below  $10^{-7}$ . Time step size was adapted by the solver in order to grant a correct Courant number value along calculation.

*Post-processing.* The quantitative post processing of the resolved flow field into the device consisted mainly in the calculation of the total pressure drop of the device since this values has been considered by Thesan

engineers relevant to define the power loss related to fluid-dynamics adverse flow patterns. This quantity, computed for each BC configuration, has been used to define a percentage of pressure loss into the device first chamber (here studied using CFD). This value represents the main output of the CFD investigation presented herein. Computational results of fluid dynamics were then post-processed to extract and visualize also qualitative fluid dynamic patterns necessary to evaluate the device performances. All the fluid dynamics qualitative values were carried out using ParaFOAM.

### 3. Results

In the forthcoming, CFD results will be presented with selected visualization criterion to show if fluid dynamics adverse pattern are present and drive future geometrical changes.

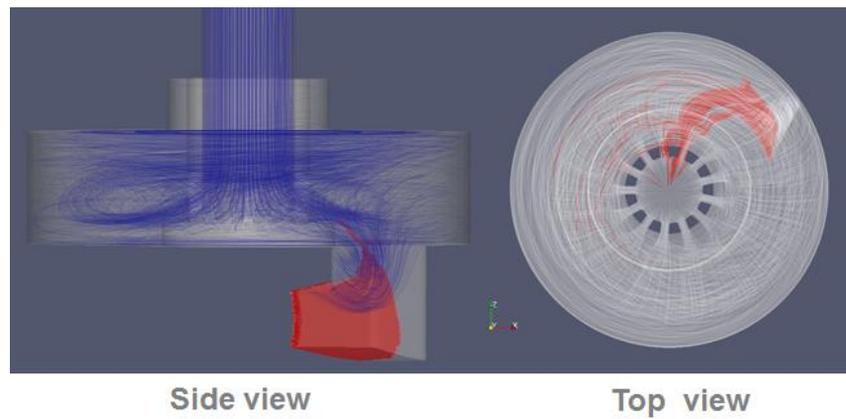


Figure 6. Fluid patterns present in the CFD model at higher RPM: side-view (LEFT) and top-view (RIGHT).

Flow patterns are coherent to measured integral quantities so that the most part of the outflow is taken by few slots (in front of the rotating outlet at a given instant) while the greater amount of fluid is experiencing a long resident time into the device. Moreover, flow patterns are coherent to measured integral quantities so that:

- Adverse velocity patterns are present at the outlet section (outlet detail);
- The adverse flow patterns at the outlet are related to a large stable vortex structure at the bending zone of the outlet duct.

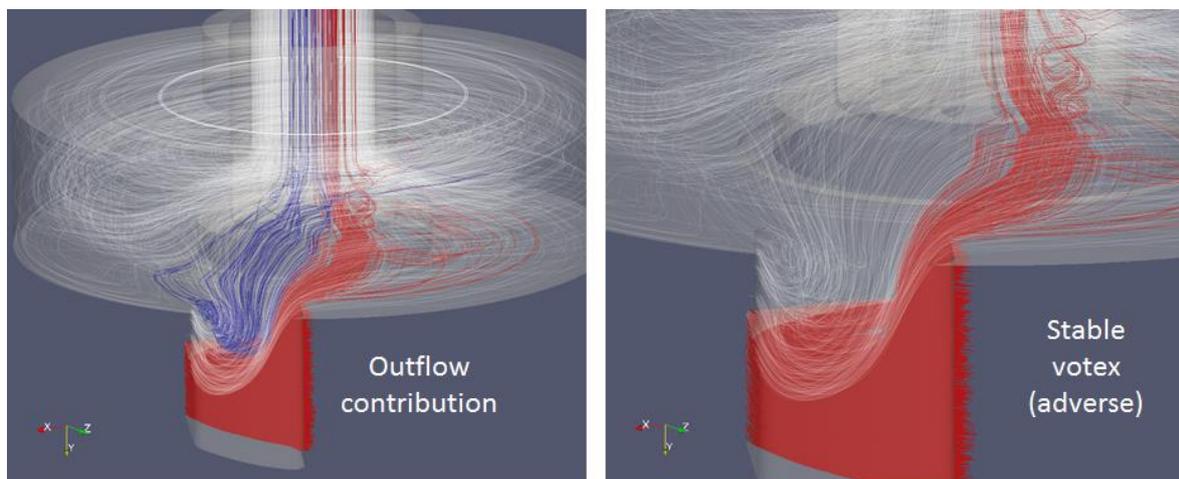


Figure 7. Fluid pattern present in the CFD model at higher RPM: emphasis on the limited inlet flow rate to the outflow mass flow rate (LEFT) and presence of stable vortex adverse (RIGHT).

Thanks to CFD analysis we were finally able to quantify some patterns meaningful to identify possible fluid dynamics inaccuracies. In table 1 the founded results are reported in a normalized way according to Thesan engineers.

CFD model #	Q	RPM	% dP_In_Out	% Eff_Area
1	1	1	8.03%	89.00%
2	0,75	0,7	3.96%	91.00%
3	0,6	0,5	1.81%	91.50%
4	0,3	0,17	0.36%	96.00%

Table 1. Fluid quantitative output.

In synthesis we found that:

- At higher RPM the device is experiencing an higher pressure loss and higher inefficiencies in total effective outlet area (area with forward flux).
- At lower RPM and flow-rate the device shows a more efficient behavior. Nonetheless similar trends are detectable.

In order to get a more useful evaluation of the gain obtainable with CFD tools when used into an HPC platform, we provided standard scalability test for a small mesh configuration (1.9 M cells) and highlighted meaningful quantities such as Averaged unitary computational cost: single loop starting from a stable result, Speed-up and Efficiency.

In our benchmark we found:

- an ‘optimal’ #mesh-cell/core that can be used for future larger mesh analysis keeping the best scalability (on similar HW)
- A possible cost per loop-device at a given number of cores (0.2 €/core-h) that is very convenient if compared to experimental costs.

In figure 8 the scalability results are shown.

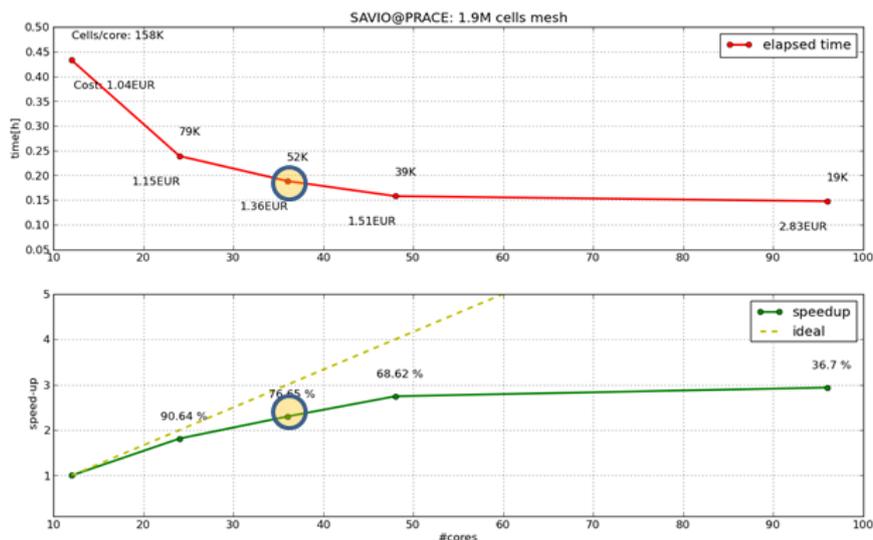


Figure 8. Scalability test details. Computational costs per single run (TOP) and related speedup compared to ideal (BOTTOM).

The HPC infrastructure provided by CINECA is an x86\_64 machine named PLX that is fully described within CINECA web site [3].

## 4. Discussion

### *Benefits of PRACE cooperation.*

In order to build the CFD models starting from the experimental prototype design and measurements, a strong interplay between technical teams of Thesan and CINECA has been necessary. Technical personnel at Thesan were able to describe the physical problem at hand, to define CAD design and fluid dynamics conditions while CINECA personnel dealt with the CFD modelling details (meshing, BC settings, results visualization, HPC servers usage).

### *Benefits for SME.*

According to the information provided the costs faced by Thesan to develop the first physical prototype and to perform the experimental measurement campaign were between 20 and 30 thousand of euros and involved Thesan qualified personnel for about 8 months. Building each new physical prototype to test new configurations is estimated to cost about 8 thousand euros and it will involve personnel activity for about 4 months. CFD-based prototyping using open-source tools on HPC systems allows a dramatic reduction in costs. A complete analysis of a new configuration requires about 15-20 thousand core hours and only 1 month for data achievement (here data interpretation and decision making is the main bottleneck).

## 5. Conclusion

We can state that CFD tools can be very useful in order to get a better understanding of industrial relevant problems when planning to define a new product prototype and especially when used together with experimental data.

Thanks to Thesan competences, the experimental setup was really effective and the hydraulic mock setup used to study the first prototype was able to characterize the prototype by measuring integral values at selected interfaces. This suggested the necessity of getting a better insight on the fluid dynamic pattern present in the device by highlighting discrepancies between designed performances and measures. Moreover, due to the high pressure at which the device is used, the possibility of build an alternative transparent version of the prototype and perform visual direct inspection of the fluid dynamics within the device is not physically feasible. At this point CFD, thanks to its ability of easily visualize in details and with a wide range of alternative methods the obtained results, showed up as a very strong candidate to support the design process at Thesan. But CFD competences, tools and a powerful enough computing infrastructure were not at hand of Thesan personnel. Even building a proof of concept CFD model just to understand if CFD would be effective to study the prototype fluid dynamics with rotating parts and high pressure boundary conditions and to get a reliable evaluation of the overall costs of the virtualized mock setup was not possible to them. Moreover, the cost of an external consultancy would probably have been of the same order of magnitude of second physical prototype.

The SHAPE pilot project was a key enabling possibility for Thesan to reach, in just five months, the competences and infrastructure necessary to build a virtualized model of the device and perform a deep evaluation of costs and benefits of the virtualization process within this specific case.

The outcome of the pilot is that CFD tools are cost effective with the respect to more traditional experimental tools, allowing for:

- dramatic time reduction in novel prototype design evaluation mainly thanks to the wide use of HPC platforms;
- relevant cost reduction mainly thanks to the use of open-source tools such as OpenFoam (OpenCFD Ltd.);
- easy and rich visualization of flow patterns;
- repeatable quantification of meaningful fluid-dynamics indices necessary to plan an improved prototype design of the proposed case study.

For all these reasons, in the future, the results obtained herein will be used by Thesan to design an improved version of the prototype device.

## 6. References

- [1] OpenFOAM: <http://www.openfoam.com/>
- [2] Thesan srl: <http://www.thesan.com/it/>
- [3] PLX: <http://www.hpc.cineca.it/hardware/ibm-plx>

## **Acknowledgements**

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