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Partnership for Advanced Computing in Europe

SHAPE Project Anemos SRL

SUNSTAR Simulation of UNSteady Turbulent flows for the AeRospace industry

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Abstract

The SUNSTAR project aims at improving the robustness and testing the predictive accuracy of an in-house CFD software for the simulation and the analysis of turbulent high-speed flows relevant for the aerospace industry, exploiting the HPC premises provided by PRACE. The software kernel is a compressible parallel flow solver, incorporating state-of-the-art numerical methods and advanced features for the direct numerical simulation of supersonic flows. The engineering of the code for industrial applications prompts efficient exploitation of modern computer architectures, which in turn requires optimization of vector and parallel efficiency, while conserving numerical accuracy. Numerical tests show that these results have been achieved.

1. The company's needs

Anemos SRL is a recently funded highly innovative start-up company established to leverage on the long-standing and internationally recognized competence of the CFD Group of the Department of Mechanical and Aerospace Engineering (DIMA) to set up services appealing to the Aerospace Industry. The applicant company is especially interested in the commercial exploitation of a novel CFD software developed at DIMA, which embodies advanced technologies for the simulation of three-dimensional high-speed flows, including state-of-the-art numerics and turbulence models, specifically designed to achieve accurate simulation of turbulent flows at high speed. This kernel allows the simulation of particularly challenging cases relevant for the aerospace industry, like the analysis of potentially damaging turbulence-induced vibrations around space launchers. Flows relevant to the aerospace industry typically involve a wide range of physical phenomena, with severe challenges for CFD practitioners, mainly related to unsteady phenomena as shock/boundary layer interactions, shock/shock interactions, recirculating flows, high-speed impinging jets, and more. In space launchers for instance, takes place a highly unsteady and three-dimensional process which can result in buffet excitation and side-loads, resulting in reduced aerodynamic efficiency, and potentially leading to aircraft damage. Improving aircraft efficiency and limiting chances of failure provides a compelling motivation for the development of novel CFD tools in the design of the next-generation aircraft, which should be able to accurately model the involved unsteady flow phenomena.

The CFD technology of current use in the aerospace industry heavily relies on Reynolds Averaged Navier Stokes models (RANS), which is relatively computationally affordable, but which is widely known to fail in the case of separated flows, and which is also of little or no use if information is needed regarding unsteady dynamic loads or noise. The CFD market in the Aerospace industry featured (US) \$180 million at the end of 2010, and is expected to reach (US) \$290.9 million by the end of the current year, with a 12.7 % growth, one of the key factors being the extensive use of CFD in aerodynamic design. This is a compelling enough motivation to develop new software

products which are capable to deliver improved performance over consolidated technologies. In this respect, the wider availability of highly powerful computers at affordable prices also for SME, makes higher-rank techniques (e.g. Direct Numerical Simulation, DNS) so far confined to the academic environment affordable, and possibly offering substantial competitive advantages for a range of industrial applications in which predictive accuracy is the key factor for success. The aerospace industry is certainly one of these fields, in which a few percent improvement may yields substantial savings. Referring for instance to aeronautics, it has been quoted that a bare 2-3% drag reduction on an Airbus A340 would result in fuel savings of about 100,000 Euros per aircraft per year. Such level of precision is well within the error bars of current predictive CFD techniques. Hence, the room for improvement is quite large.

The activities incurred in the present SHAPE project are aimed at improving the performance and the parallel scalability of an existing in-house solver which incorporates state-of-the-art numerical methods of academic derivation, and advanced features for the simulation of supersonic flows in complex configurations, including high-order shock- capturing capabilities. This code is the result of a long-standing research activity carried out by the CFD group of DIMA, as documented by a long record of scientific publications in major journals.

Concerning the numerical method, the key ingredient of the code is a dissipation-free, finite- difference discretization of the convective terms of the Navier–Stokes equations, capable of guaranteeing exact discrete kinetic energy preservation in the limit of inviscid incompressible flow. This property is a mandatory prerequisite for the accurate prediction of turbulent flows, and makes the computation of compressible (smooth and shocked) flows extremely robust, without reverting to typical expedients employed by commercial software packages (such as upwinding or filtering) which degrade the quality of the solution while yielding a significantly overhead in terms of the computing time. The other essential element of the solver, which makes it innovative in the industrial CFD context is the inclusion of an immersed boundary (IB) capability, i.e. the ability to deal with embedded geometries with arbitrary shape on a Cartesian mesh. The IB method implies substantial advantages with respect to standard body-fitted approaches, in that it entirely avoids the generation of complicated body-conforming meshes, which is probably the most time-consuming element in the CFD production chain. In our solver, the IB method is implemented following the direct-forcing approach originally developed at Sapienza for incompressible low-Re flows, and later adapted to compressible flows. High Reynolds-number flows, which are relevant for industrial applications, are handled thanks through simple and cost-effective wall models, which avoid the necessity to resolve the extremely thin near-wall turbulent layer in the attached flow regions, and large-scale turbulent structures are resolved according to the DES (Detached-Eddy Simulation) philosophy. Furthermore, one of the (many) advantages of the IB method consists in straightforward estimation of the global aerodynamic forces coefficients. The potential of the solver has been clearly shown during several national (ISCR) and EU (PRACE) HPC grants, for a total of 160 million core-hours on IBM BG/P and BG/Q architecture, carried out using CINECA HPC resources.

For the purposes of the present SHAPE project (i.e. optimization and improvement of parallel efficiency, and code validation) the kernel version of the solver has been considered (i.e. no complex immersed boundaries, no shocks) so as to focus on improving the key elements. The optimization activities have been carried out in close contact with CINECA, the Italian Partner in PRACE. In particular, specialistic assistance for code implementation and performance improvement was provided by Dr. Vittorio Ruggiero. A detailed list of activities and achievements follows.

2. Description of the activities

The baseline CFD solver considered in the SUNSTAR project solves the compressible unsteady Navier-Stokes equations on a Cartesian mesh using a finite-difference discretization. It has been previously used to perform direct numerical simulations (DNS) of wall bounded compressible flows, such as boundary layer and channel flow [1-2-3]. In the present project only smooth internal flows has been considered, in particular compressible channel flow. The nonlinear terms in the Navier-Stokes equations in Cartesian coordinates are discretized using locally conservative, energy-consistent formulas of arbitrary order of accuracy which guarantee that the total kinetic energy is discretely preserved from the convective terms in the limit case of inviscid flow [4]. This space discretization reveals to be very robust, since, for smooth flows, it allows numerical stability without the addition of numerical diffusion or filtering. Interestingly we have recently shown that the same approach can be used on unstructured meshes, thus allowing to threat complex geometries of industrial interest with a high-fidelity numerical algorithm [5]. The viscous fluxes are expanded to Laplacian form in order to benefit of a higher dissipation in the wavenumber space to avoid odd-even decoupling phenomena and approximated with the same order of accuracy of convective terms whereas time integration is performed using a third-order low storage Runge-Kutta scheme. The solver can also be used efficiently in the low-Mach number limit, through a semi-implicit time advancement scheme, which allows to relax the time step limitation. In order to evaluate central

spatial derivatives, nodes $j - 1$ and $j + 1$ are needed which clearly poses issues at the exterior boundaries, or at the block boundaries where nodes outside the domain are required. In present solver the ghost nodes approach is used for all boundaries and the number of ghost nodes n_g is proportional to the order of accuracy of the scheme. In the simulation of plane channel flow two directions (streamwise and spanwise) are periodic, thus their treatment is trivial, whereas the imposition of wall boundary conditions for compressible internal flows may be more critical. Most compressible flow solvers use co-located meshes and only few examples or staggered compressible solvers are available in literature [6]. The presence of the wall in co-located meshes, in which the wall coincides with a node, may lead to lack of total mass conservation in the case of internal flows. In order to solve this issue we stagger the first node off the wall in such a way that the latter coincides with an intermediate node, where the convective fluxes are identically zero, hence correct telescoping of the numerical fluxes is guaranteed, and no net mass variation can occur. A further benefit of this approach is that, for given distance of the first grid point from the wall, the maximum allowable time step associated with the vertical mesh spacing is doubled. In all simulations considered in this work the wall is isothermal, since this is the only realistic scenario in the case of internal flows. All simulations are performed in a convective frame of reference, in which the flow bulk velocity is zero, normally we set $u_{wall} = -u_b$, where u_b is the bulk velocity of the flow, which allows to increase the accuracy in the streamwise direction [7]. The flow field is initialized with the laminar velocity profile with superposed synthetic turbulent perturbations which allow transition to a fully turbulent state.

The code is implemented in the F77 language, and parallelization is based on a domain decomposition strategy, which is handled through Message Passing Interface (MPI). Contiguous blocks exchange planes at the interfaces which are needed to compute convective and viscous derivatives. Communication between neighboring blocks is handled by means of MPI Sendrecv directives by exploiting the Cartesian topological connectivity, which is directly implemented with MPI. Global transposition of the data is not required unless the semi-implicit time integration is used, thus the explicit version of the solver is expected to be highly scalable. The flow solver was successfully run on the BG/Q system Fermi at CINECA, where scalability tests were carried out, as shown in Fig. 1. The graph shows the parallel speed-up as a function of the number of cores (up to 65536 cores) obtained by keeping constant the problem size (number of mesh points) assigned to each core when increasing the number of CPUs (weak scaling), so as to mimic the run conditions encountered in the present project. In particular, the size assigned to each core is approximately 1.6 Millions of grid points, selected on the basis of a typical run for production. The tests have been performed running in the SMT mode, with 32 ranks per node. Since the minimum partition size has 64 nodes, this implies that the minimum number of cores (used as reference for normalization) is 2048. As seen in Fig. 1, the performance obtained from the solver in weak scaling is excellent, and the loss of efficiency with respect to the ideal behavior achieved with 65536 cores is very limited.

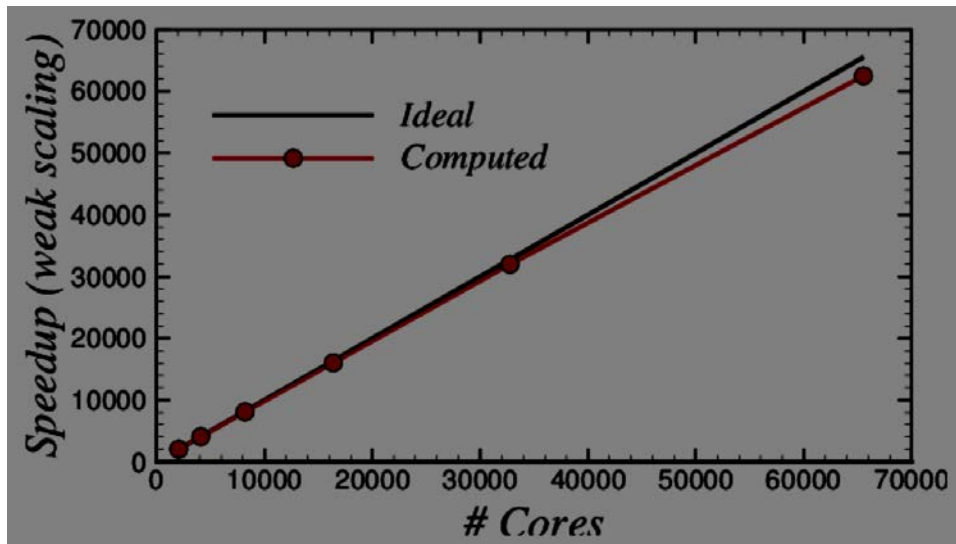


Figure 1: Speedup (weak scaling) performances of the baseline solver performed on the FERMI supercomputer at CINECA.

One the purposes of the project was to optimize the solver in order to enhance data vectorization, with the help of CINECA staff. Vector instructions are handled by an additional unit in the CPU core, called something like a vector arithmetic unit and if used to their potential, they allow to perform the same operation on multiple pieces of data in a single instruction. The main purpose of this process was to try to optimize as far as possible the solver for the

novel Intel architectures, in particular Broadwell and Knights Landing, used in the CINECA infrastructure MARCONI, and which are equipped with 256 (AVX) and 512 (MIC) bit registers respectively.

The optimization process has been performed on the MARCONI-Broadwell and GALILEO supercomputers, since MARCONI-KNL partition was not yet available at the time. As a first step the Intel Fortran compiler options “-qopt-report” and “-no-vec” have been used to access the whole compiling process and to figure out the total amount of loop vectorization of the solver. Through this preliminary study vectorization has been forced or interdict on each main loop depending where it was efficient or inefficient. [Tab. 1](#) shows the outcome of the optimization process on three of the main subroutines of the solvers, in which the convective fluxes of the Navier-Stokes equations are evaluated. Vectorization clearly allows to speed up the solver up to almost 60%.

<i>routine</i>	old	new	% gain
<i>euler_i</i>	268620.46	169546.83	26.9
<i>euler_j</i>	369708.88	170571.67	53.8
<i>euler_k</i>	446156.29	180130.26	59.6

Table 1: Elapsed time per visit (s) for the baseline version of the solver (old) and the vectorized version (new) with the respective gain. The data refers to serial runs.

The performances of the vectorized solver, compared to the non-vectorized one (-no-vec option), performed on Galileo are also reported in [Tab. 2](#) in terms of computational time per time step. The data show that vectorization allows to increase the overall performance of the solver of about 20-30%, depending on the size of the computational mesh.

grid size	novec	vec	% gain
64X64X64	3.80	2.76	27.4
128X64X64	7.78	5.49	29.4
128X128X64	15.4	10.9	29.2
128X128X128	30.8	27.3	11.4
256X128X128	64.6	54.3	16.0
256X256X128	141.3	111.6	21.1

Table 2: Elapsed mean time per time step (s) for the vectorized version of the solver and the non vectorized one (-no-vec option), with the respective gain. Different grid sizes are reported. The data refers to serial runs.

grid size	Speedup					
	4	8	16	32	64	128
64X64X64	3.6	6.7	11.5	18.4	25.1	25.1
128X64X64	3.9	7.0	12.8	20.3	28.9	36.6
128X128X64	4.0	7.7	12.4	18.9	33.0	40.4
128X128X128	4.1	8.2	13.9	22.2	39.6	58.1
256X128X128	4.0	8.1	16.1	30.2	46.4	66.2
256X256X128	4.1	8.3	16.5	32.4	51.4	72.9

Table 3: Speedup of the vectorized solver, obtained on Galileo for different grid sizes.

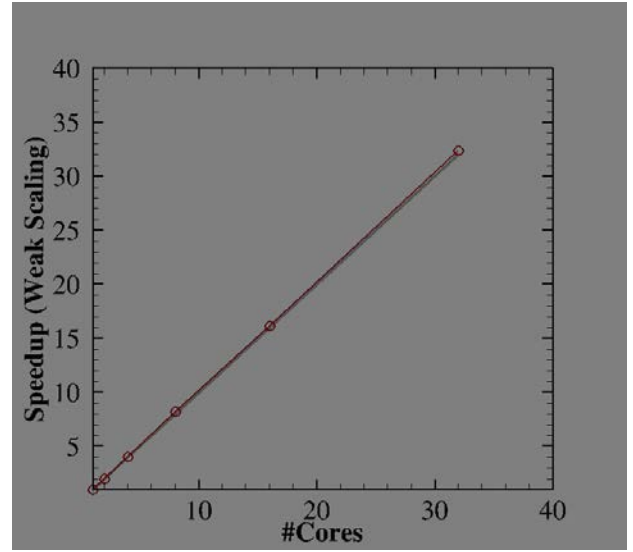
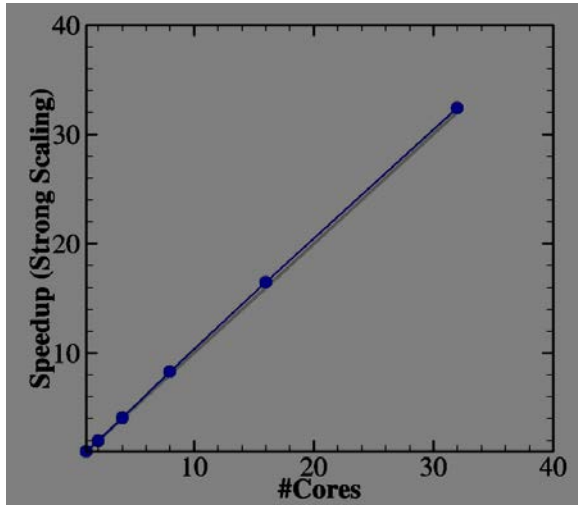


Figure 2: Speedup (left, strong scaling; right, weak scaling) of the optimized solver performed on the Galileo supercomputer at CINECA

Eventually the performance of the optimized solver are reported in terms of parallel speed-up in [Tab. 3](#) and in [Fig. 2](#), from which both weak and strong speed-up data can be gauged.

Code validation activities have been carried out to establish the predictive performance of the optimized solver. For that purpose, a series of DNS of compressible channel flow has been carried out on MARCONI-Broadwell at various Mach and Reynolds number, performed on the CINECA infrastructure is reported in [Tab. 4](#). The highest Reynolds number simulation here presented corresponds to friction Reynolds number $Re_\tau = 1000$, which is the highest achieved so far in the supersonic case [3].

Case	Re_b	M_b	Re_τ	$Re_{\tau H}$	$Re_{\tau B}$	N_x	N_y	N_z	Δx^+	Δz^+	M_τ	$-B_q$
CH01	5790	0.1	180	180	180	384	128	192	8.8	5.9	0.0063	9.7e-6
CH15A	6000	1.5	215	141	169	512	128	256	8.0	5.2	0.079	0.048
CH15B	15334	1.5	500	333	395	1024	256	512	9.2	6.1	0.072	0.042
CH15C	34000	1.5	1015	677	802	2048	512	1024	9.3	6.2	0.065	0.038
CH3	9760	3.	448	142	233	1024	256	512	8.2	5.5	0.11	0.14

Table 4: Setup of compressible channel DNS. The computational box size is $6\pi h \times 2h \times 2\pi h$ for all flow cases. N_i and Δx_i are the number of points and the mesh spacing in the i -th coordinate direction, respectively. Re_τ is the equivalent friction Reynolds number for Huang's transformation (H), and Brun's transformation (B).

Figure 3 shows a three dimensional visualization of the instantaneous velocity field in the streamwise direction through visualization of three slices of the channel, in the streamwise, spanwise and wall-normal planes (the latter taken at $y^+ = 15$). The figure highlights the complex organization of the flow field, featuring large-scale bulges in the channel core, and smaller near-wall streaks which are mainly responsible for friction drag.

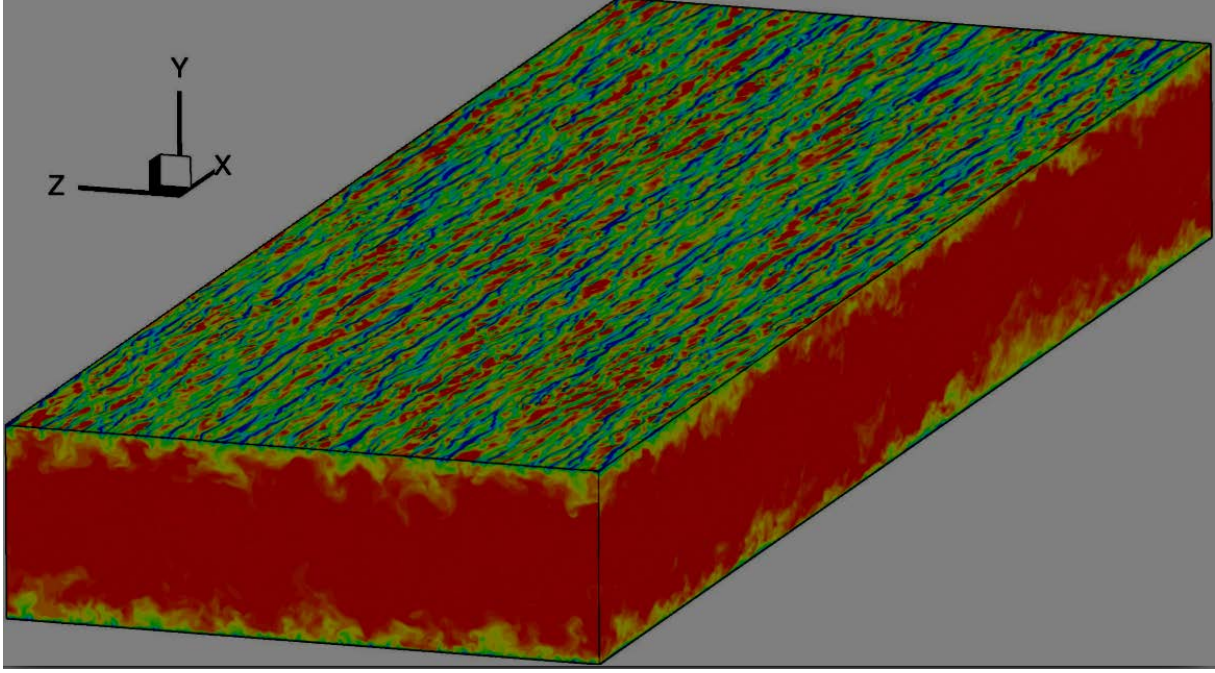


Figure 3: Instantaneous streamwise velocity field for the supersonic channel flow case CH15C. The XZ plane is taken at $y^+ = 15$.

A quantitative evaluation of the numerical results is reported in Fig. 4, where we show the mean velocity profiles across the channel associated with the various cases reported in Tab. 4, transformed according to Trettel and Larsson, highlighting that this transformation allows to fully take into account the effect of compressibility on the mean velocity. The comparison with the incompressible data is excellent in the whole range of Mach and Reynolds numbers herein considered.

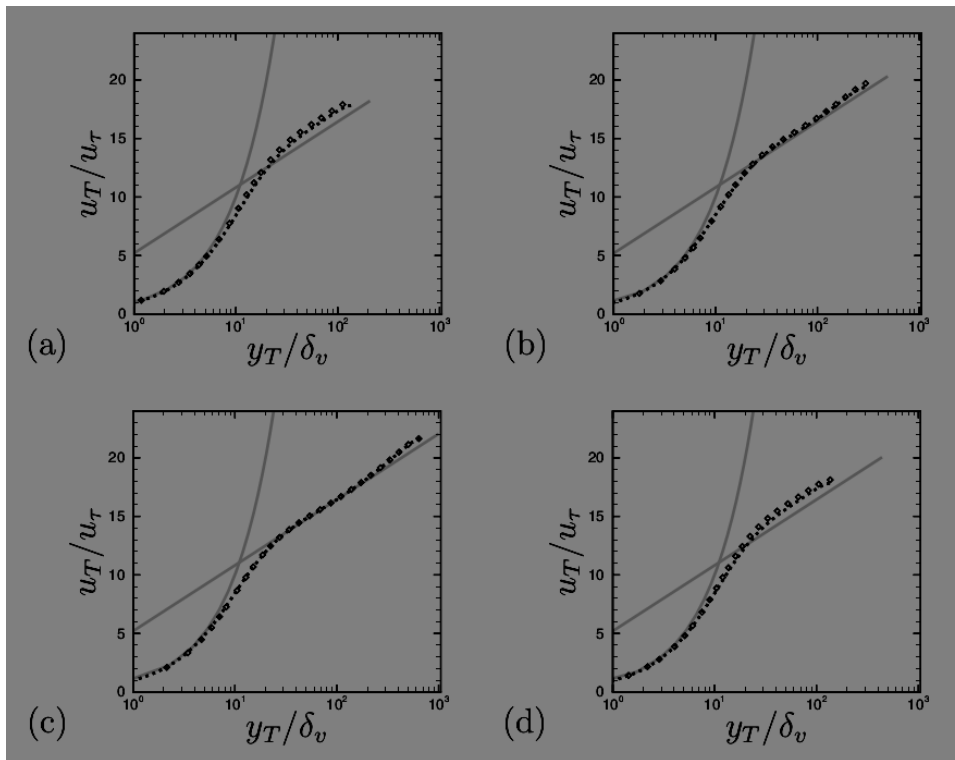


Figure 4: Mean velocity profiles transformed according to Trettel-Larsson in wall units for cases CH15A (a), CH15B (b), CH15C (c) and CH3 (d) compared with incompressible flow data at matching $Re_{\tau H}$.

3. Conclusions

The outcome of the project has been highly satisfactory for the applicant SME, having led to:

- i) successful implementation of the baseline software platform on modern parallel computer architectures, with special reference to the MARCONI-Broadwell and GALILEO machines;
- ii) improvement of the code vector performance;
- iii) improvement of the parallel scalability;
- iv) code validation on large-scale test cases.

To achieve those goals, close cooperation and feedback from the CINECA staff was essential.

The next step to be undertaken will be exploiting the implemented innovation to reach the market. The main idea for that purpose is to establish a cloud-based, pay-per-use CFD service for companies operating in the aerospace industry. The tool would provide high-precision CFD predictions together with ancillary pre-processing and post-processing web-based services. The present project will then help to fill the existing wide gap between academia and industry, by establishing an efficient HPC platform for the benefit of manufacturing European SMEs operating in the aerospace field, enabling them to get "one-stop-shop" access to novel simulation technologies, including expertise and tools for visualisation, customisation and integration, and dynamic, easy and affordable access to non-conventional HPC resources. The offered simulation services are likely to have a strong impact on the engineering and manufacturing aerospace market, bringing innovative solutions well different from those implemented in existing commercial CFD software of current use. The service will provide improved predictive capabilities giving easy access to non-conventional HPC resources, thus enabling European SMEs to be more competitive worldwide. In summary, the pay-per-use model to be implemented will also have the potential to create invaluable business benefits in terms of:

- substantial reduction of the simulation cost and time, allowed by smart integration of hardware, expertise, applications and visualization tools in a "one-stop-shop";
- greater efficiency in the advanced design stage thanks to the access to high-fidelity 3D, unsteady computations
- possibility to validate and improve simplified predictive tools, typically used for preliminary design .

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