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FORTISSIMO

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Open Call 2 Application Experiments Public Report

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Executive Summary

Fortissimo Marketplace is a web-based portal, accessed at www.fortissimo-marketplace.com that provisions a one-stop-shop of simulation services and tools running on a cloud infrastructure. It will greatly simplify access to advanced simulation, particularly to SMEs and will make hardware, expertise, applications, visualization and tools easily available and affordable on a pay-per-use basis.

There were 11 experiments in the second open call of Fortissimo, the outcomes of which are reported in this document. A typical experiment consisted of an end-user, a technology provider (for example an Independent Software Vendor (ISV)) and an HPC expert.

These application experiments had the objective of showcasing technologies for cloud-based HPC-enabled modelling and simulation. Additionally, these experiments provided further requirements to the Fortissimo cloud-based HPC marketplace and provide further validation of the approach taken and the business processes developed.

Collectively these experiments show that the Fortissimo approach of providing cloud-based HPC is one that allows business benefits of modeling and simulation to be enjoyed by SMEs, with value for all stakeholders. Typical benefits, all of which lead ultimately to financial gains for the companies involved include reduced times to market, lower production costs, improved quality of manufactured products and the opportunity to expand customer base. Many of the experiments have concrete plans for placing services in the Fortissimo Marketplace.

The experiments also contributed to a number of project's dissemination activities (in addition to their own dissemination activities). The experiments have created success stories concentrating on the business impact of the results generated from the work carried out. These will be available from the Fortissimo web pages.

Table of Contents

1 Objectives of the Experiments

1.1 Overview

The application experiments from the second open call had the objectives of showcasing technologies for cloud-based HPC-enabled modelling and simulation. The experiments showcase how end users get a "one-stop-shop" access to simulation technologies novel for them, including expertise and tools for visualisation, analytics, customisation and integration; and dynamic, easy and affordable access to computing resources. These experiments provided further validation of the implementation of the Fortissimo HPC Cloud.

The 11 experiments and the role of each partner are listed in Table 1 (the numbers in the brackets indicate the partner number as listed in Fortissimo Description of Work (DoW). The motivation, relevance to Fortissimo, impact and business benefits are covered in more detail for each experiment in Section 0. There were over 20 partners taking part in the experiments (in addition to the core Fortissimo partners). A typical experiment consists of an end-user, a technology provider (which may be, for example an Independent Software Vendor (ISV)) and an HPC expert.

Experiment Title	Partners
Experiment 601: HPC-based Simulation-as-a-Service tool for motorcycle helmets design and development.	End User: Nolan (97) Application Experts: Nolan (97) HPC Expert: CINECA (7) ISV: Moxoff (96) HPC Provider: CINECA (7) Host Centre: CINECA (7)
Experiment 602: Integrated Design Workflow for the Manufacturing and Product Simulation of high performance composite structures.	End User: Formtech Composites Ltd (99) Application Expert: KIT FAST (98) HPC Expert: Fraunhofer SCAI (25) HPC Provider: GOMPUTE (12) Host Centre: GOMPUTE (12)
Experiment 603: Improved ICP estimations using cloud based simulations of the cerebral blood flow.	End User: Vittamed (100) Application Expert: Simula (101) HPC Expert: Simula (101) HPC Provider: CINECA (7) Host Centre: CINECA (7)
Experiment 604: High-Fidelity Virtual Rheometer for Complex Fluids	End User: Ioniqa (103) Application Expert: Ioniqa (103), EAL (102) ISV: EAL (102) HPC Expert: EAL (102), SURFSara (8) HPC Provider: SURFSara (8) Host Centre: SURFSara (8)
Experiment 605: HPC-enabled System for enHanced sEeakeeping and stAtion-Keeping design (HPC-SHEAKS)	End User: WAVEC (106), VICUSDT (105) Application Expert: COMPASSIS (104), ISV: COMPASSIS (104) HPC Expert: CESGA (11) HPC Provider: CESGA (11) Host Centre: CESGA (11)

Experiment Title	Partners
Experiment 606: Enabling Fatigue Life Assessment in HPC-Cloud to SMEs (FLASH)	End User: ISONAVAL (108) Application Experts: COMPASSIS (104), FNB-UPC (107) ISVs: COMPASSIS (104) HPC Expert: CESGA (11) HPC Provider: CESGA (11) Host Centre: CESGA (11
Experiment 607: SOUTH Clouds Shape Optimization under Uncertainty through HPC Clouds.	End User: Automobili Lamborghini SPA (111) Application Expert: University of Strathclyde (110) ISV: Optimad engineering (109) HPC Expert: CINECA (7) HPC Provider:CINECA (7) Host Centre: CINECA (7)
Experiment 608: Microscopy in the cloud (VIRTUM)	End User: University of Zurich (113), OpTecBB (114) Application Expert: MicroscopeIT (112) ISV: MicroscopeIT (112) HPC Expert: ARCTUR (10) HPC Provider: ARCTUR (10) Host Centre: ARCTUR (10)
Experiment 609: Marine CFD Online Platform	End User: HydrOcean (117), VPLP (118) Application Expert: NEXTFLOW (115) ISV: NEXTFLOW (115), DIST (116) HPC Expert: BULL (3) HPC Provider: BULL (3) Host Centre: BULL (3)
Experiment 610: Delft3D as a Service (DaaS)	End User: HKV (120) Application Expert: Deltares (119) ISV: Deltares (119) HPC Expert: SURFSara (8) HPC Provider: SURFSara (8) Host Centre: SURFSara (8)
Experiment 611: Improved releasable buoy design with CFD on an HPC platform	End User: Alseamar (122) Application Expert: K-Epsilon (121) ISV: K-Epsilon (121) HPC Expert: BULL (3) HPC Provider: BULL (3) Host Centre: BULL (3)

Table 1: List of experiments from the second open call

2 The Experiments

This section contains a brief description of each experiment in terms of the motivation, relevance to Fortissimo, impact and business benefits.

2.1 Experiment 601: HPC based simulation-as-a-service tool for motorcycle helmets design and development

2.1.1 Motivation

Moxoff is an Italian SME whose business consists in applying mathematical modelling to solve complex industrial problems. Its expertise is the development of cutting edge software solutions to meet its industrial customer's challenges. The company's projects cover a wide range of applications, from multiphysics modelling, numerical simulations, statistics and big data analytics, as well as a wide range of industrial market segments.

NolanGroup is a MID-CAP Italian manufacturing company of motorcycle helmets (approx. 350 employees, 42M euro sales volume) who owns the commercial helmet brands Nolan, X-Lite and Grex. Nolan produces helmets for professional, leisure and racing activities, participating in the main international motorcycle competitions. Production facilities are located in Italy and the market reach is worldwide with 80% of the sales generated in Europe (35% Germany, 20% Italy, 15% France). In the rest of the document NolanGroup is referred as "Nolan".

Moxoff has already established a partnership with Nolan, on going since 2010. A dedicated multiphysics platform, named CASCo (Computer Aided Simulation COde) was developed by Moxoff to simulate motorcycle helmets with respect to comfort and safety issues and to support Nolan innovation process including the introduction of numerical modelling and simulations in their design process. Traditionally, Nolan helmet design was experiment-based as stylistic and functional features were developed through helmet prototypes. Only recently they have introduced the simulation based approach, thanks to the simulation platform developed by Moxoff. Nolan engineers can easily perform simulations, even if they are usually not experts in simulations, through multiphysics coupled workflows: aerodynamics for external flow, thermo-fluid dynamics for heat exchange in the internal ventilation channels, wave propagation for helmet acoustics and noise evaluation, and non-linear structural dynamics to simulate impacts. This represents a brand new approach in helmet design, as no evidence of such a multiphysics simulation driven design is currently available in the motorcycle helmet manufacturing industry's process, giving Nolan a powerful tool and a significant head start to compete on the market.

Two key aspects need to be considered simultaneously when dealing with such simulation based approaches, not only for helmet design but in general in a CAE or simulation-based approach: the ease of performing accurate simulations and the computational effort required. For the first point, the development of customized workflows in the simulation platform is required, for the second point, the choice of the computational platform is critical as simulation computing time can run in minutes, hours, days or weeks depending on the computing platform used. In this experiment, access to an HPC infrastructure has reduced the computing time by a factor of 100.

For helmet design, the extensive use of simulations along the whole design process increases drastically the computational cost, in a framework where multiphysics effects must be calculated at each step to track and define the design patterns. Due to the complexity of CAD models and the need to capture details effects, numerical meshes contain millions of cells; this significantly increases the required computational effort. For vibroacoustics simulation, the helmet layer thicknesses combined with wave propagation speed lead to very small time steps (10e-7 s). Considering that the simulation should cover at least 2s to capture the frequency range of interest, the number of time steps increases to the order of 10e7 to get the measure of a Sound Pressure Level (SPL) frequency graph, and so does the computational time. With a 16 processors machine, 4 computing days are required to obtain the expected result. For crash simulations, 12 hours are required for a single impact run, on 4 processors. This run reproduces the test required by European regulation ECE 22-05 for motorcycle helmet safety, and must be performed in several configurations to validate the compliance, varying the impact position, the environment temperature and other parameters. This corresponds to tens of runs for an exhaustive validation of one helmet.

In this experiment, Moxoff intends establish a new Simulation as a Service (SaaS) paradigm based on a HPC infrastructure accessible via web. More specifically, Moxoff aims at porting its current multiphysics platform (CASCo) to a cloud infrastructure coupled with HPC resources provided by CINECA, creating a new platform (namely HPCASCo, High Performance CASCo). This will allow Moxoff to optimize and exploit the platform performance, provide dynamic, easy and affordable access to computing resources, not only for Nolan, but also for any other Moxoff customers needing HPC facilities. This solution is configured as a “one-stop shop” where users can prepare and launch these simulations on demand through a user-friendly interface.

For Moxoff, this new “on demand” service is ready to be used by Nolan and represents a strategic asset to expand its customer base, accelerate its market penetration towards new customers and in new industry segments.

For Nolan, its simulation platform has a dual characteristics: smaller simulation can be run in house, whereas larger simulation or time critical ones can be scaled out to the significantly larger computation facility, available at CINECA. This opens a new paradigm in term of compute, design process and economic model. Practically one helmet simulation could be done in 18K hours using the in house system and in only 17 hours using the Cineca services. A 90% time reduction!

2.1.2 Relevance to Fortissimo

Fortissimo offers the possibility to industrial applications to participate in an experiment in order to access HPC resources and evaluate the economic benefits of this new model. This perfectly suites Moxoff interest to provide access to major HPC resources to tap new markets and Nolan’s needs for steep performance improvements.

The experiment approach taken is to exploit a cloud-based HPC architecture by porting the existing simulation platform to access and compute on a remote HPC infrastructure. Moxoff has developed new software tools, new procedures and new workflow to integrate the HPC framework in its existing set of software tools. These new competencies lead to new services which can be deployed by Moxoff through the Fortissimo Marketplace, to existing, new and future customers. This marketplace is a major asset in terms of dissemination and communication: Nolan can benefit from a dynamic and modern brand image through its indirect integration in the platform. Moxoff can use this success story to enhance its marketing and business development activities, with customer testimonials and press releases. This platform is also a networking tool to develop new partnerships with the platform members.

Nolan is already benefitting from cost reduction and faster time to market in its helmet development and has avoided a significant IT investment through the access to remote HPC resources.

CINECA, the HPC centre, is the ideal partner to support the project as HPC experts, to port the cloud base application to HPC resources, to run experiments and finally to amortise its own investments by developing its user base. CINECA made available part of its Tier-1 cluster, Galileo**Error! Reference source not found.**, for this Fortissimo experiment.

2.1.3 Impact and Business Benefits

The creation of a new “Simulation as a Service” offering based on the HPC resources, is the main objective of the experiment.

The business impact for each of the participants can be summarized as follows: For Moxoff, Nolan is one of its most important customer since 2010 with a 10% contribution to Moxoff annual turnover. In this experiment, the SaaS development and the HPCasco platform are designed and tailored made for Nolan. The porting to an HPC infrastructure is a game changer and a strategic asset for both Moxoff and Nolan as it brought down by up to 90% the computational time required to simulate helmets. This consolidates the relationship between Nolan and Moxoff, as the platform developer and technology expert, and Moxoff role as a strategic partner. Additional services are likely to be provided when the simulation platform will be in full production mode such as maintenance, further modelling and software improvements. Moxoff collaboration with Nolan expands to projects undertaken with other departments, and this HPC approach can be replicated with them. All these new opportunities are expected to increase Nolan share of Moxoff business up to 15% in the coming 3 years.

Through this collaboration, Moxoff has developed a platform which can easily be reused in similar industry challenges requiring huge computational efforts. Thanks to this investment, Moxoff current and future customers can directly gain the same benefits experienced by Nolan, boosting their growth and their revenues. In addition, marketing activities outlining this new business model for growth and enhanced competitiveness should generate a turnover increase of 30% while maintaining current profitability rates. Finally, project costs should be positively impacted by the reuse of the platform’s building blocks, generating a cost saving estimated to 10% of the overall project costs.

In conclusion, Moxoff has been able to establish through this project and its collaboration with Nolan a versatile simulation platform, capable of accessing massive HPC resources which is a critical asset for its growth, for its customer base and for its long term financial stability. Moxoff estimates that its exploitation of the SaaS and the platform will increase its turnover by 10% and will significantly contribute to its planned growth for the coming 3 years. Furthermore, through the wider development of this platform, Moxoff will reduce its software development costs by €50K per year.

NolanGroup estimates that, for each new helmet developed, the intensive usage of HPC simulations will save 50% of the costs of the physical prototypes, of their testing and of the final product tuning. This new approach will provide a net saving of €52K per helmet once the cost of compute cycles and software licences are deducted. Furthermore, advanced simulations will lead to a 3-month reduction in the current 15-month development cycle which can have important implications for Nolan’s market impact.

Globally, factoring the cost of the simulation and of the software licenses, the net saving is estimated at 6.5% of total development budget. In addition, the time to market is reduced by 20%, delivering the final product in just 12 months (a 3 month reduction).

This experiment offers a success story for CINECA which should attract at least two new SME customers per year, with an estimated 5% increase in commercial services revenues.

2.2 Experiment 602: Integrated Design Workflow for the Manufacturing and Product Simulation of high-performance Composite Structures

The industrialization of CFRP (Carbon fibre reinforced plastic) is being driven by the increase in use of composites for light weighting in the automotive industry where cost and performance are driving factors. Legislation around the world increases the requirement for lightweight vehicles and composites are seen as one of the best ways to drive this requirement. With tooling budgets running well into the 100's of millions of Euro, the prediction of processes and manufacturing times is of utmost importance to deliver quality products with confidence. **Figure 1** shows the major steps from design over simulation to real manufacturing.

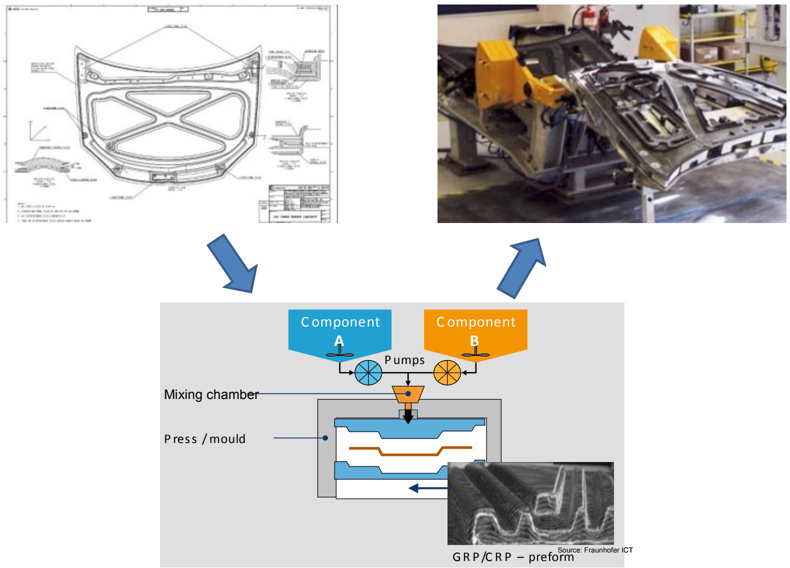

Figure 1: Design, process and product simulation, and production of a CFRP part

2.2.1 Motivation

For the development of high-performance composite structures like CFRPs there is still no integrated virtual engineering workflow available, which could be used to combine design, manufacturing and virtual validation. This simulation gap causes cost-intensive development loops including numbers of real hardware prototypes, which still make the potentially high-performance CFRP material economically unprofitable.

The aim of the experiment therefore is the development of a virtual manufacturing process chain for composite structures running on a cloud-HPC system. This new solution will has closed the simulation gap for SME's that cannot bear the costs for such expensive simulation environments but would prefer a pay-per-use-model fitting much better to their needs and financial capabilities.

Formtech Composites (UK) is a small manufacturer of composite components using carbon, glass, aramid and other high performance fibres. As a concrete example Formtech produces inner bonnets for automotive vehicles. A realistic prediction of manufacturing times and costs would allow Formtech to deliver CFRP components with reduced development costs and much faster than they can do now.

2.2.2 Relevance to Fortissimo

The virtual process chain in this experiment consists of multiple simulation domains: one to three steps for the different manufacturing processes (draping, moulding, curing) and a final step for the structural simulation of the product. The simulation steps are connected by information flows, which comprise the transfer of important composite data. If simulation results show a change of the geometric design (e.g. due to bad feasibility or due to bad structural performance) is required, the process chain starts again. This loop as well as each possible sub-loop may build the basis for an iterative optimization of the product itself and also the manufacturing processes.

In order to make efficient use of the HPC system, the decision points between each simulation steps need to be evaluated quickly using all generated information during the simulation step. Therefore the four decision points (shown in Figure 2), are implemented directly with scripts in Python or Perl able to communicate immediately with the simulation pre and post processing modules.

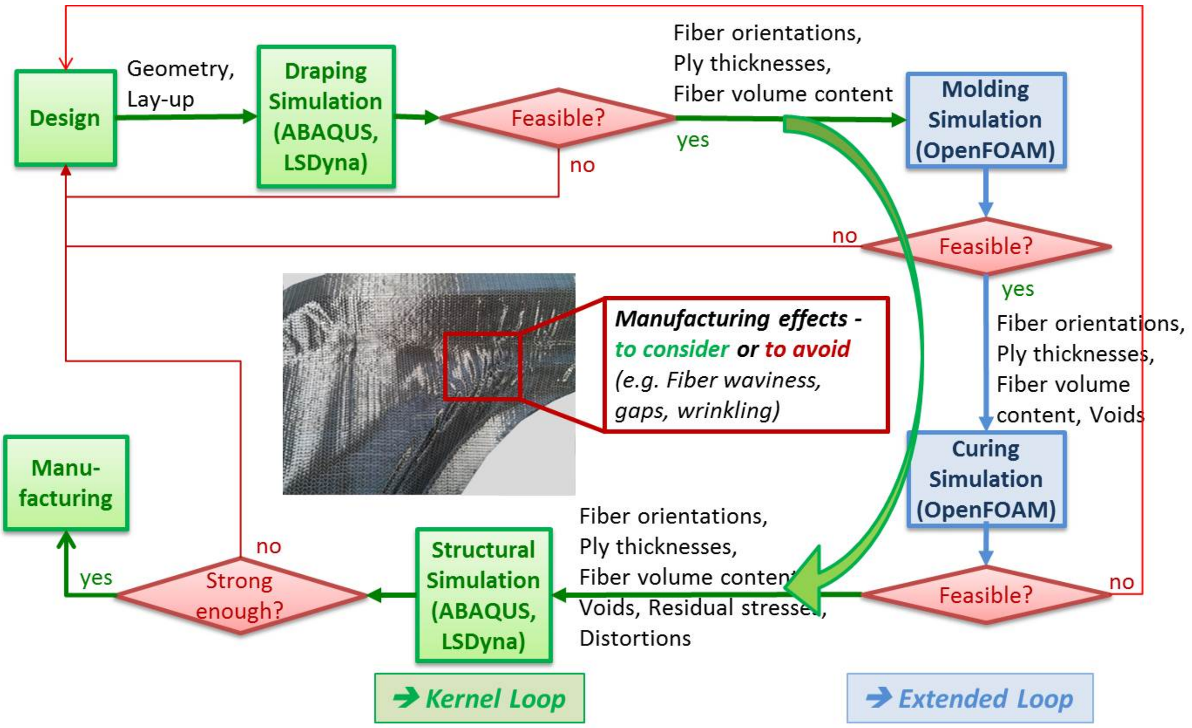

Figure 2: Detailed CAE Workflow on the HPC Cluster

The user can define many design parameters such as the fibre orientation of each ply, the laminate layup, the parameters for holders during the draping simulation and the material parameters for the given fabric. Each simulation step needs a suitable decision criterion. Since fabric material has been predefined for the draping simulation, the maximum shear angle (and macroscopic wrinkling) needs to be minimized to achieve the best results for the draping process. The structural simulation concentrates on the maximum stresses and the maximum force bearing. The overall decision criterion for the workflow is satisfied when the structure can be manufactured and is capable of bearing the applied load.

The overall optimisation workflow and its performance was analysed for a typical door reinforcement beam. At first Formtech has prepared meshed forming tools from the existing CAD data as well as the required structural load case model of the RTM component (Resin Transfer Moulding). These models have then been executed on the Gompute's HPC environment. Formtech, in corporation with KIT and SCAI, has further defined a set of parameters for two reference configurations which were used to control the automated model setup and the ongoing optimisation workflow. Below the performance and resource consumption (defined in CCH – Compute Core Hours) for the door reinforcement beam example are shown:

Configuration 1 (early stage):

- optimization setup with 4 layers
  - 5 generations of draping layouts, each with a population size of 10
- 16 CPU draping simulation / 16 CPU structural simulation
- Complete job ~ 5,000 CCHs / 4-5 variations ~ 20,000-25,000 CCHs

Configuration 2 (final development stage):

- optimization setup with 10 layers
  - 10 generations of draping layouts, each with a population size of 15
- 48 CPU draping simulation / 48 CPU structural simulation
- Complete job ~ 50,000 CCHs / 2-3 variations ~ 100,000-150,000 CCHs

2.2.3 Impact and Business Benefits

The platform developed increases the quality of designs. It adds functionality while reducing the work load on the engineer's side. It shortens simulation times from days to hours whilst offering more detailed simulations. Such simulations lead to less material usage and the need for fewer mechanical tests. Formtech has already exploited the HPC capacity of Gompute to meet a project deadline where a 50% reduction in compute time was imperative. Clearly advanced simulation enables Formtech to maintain a competitive edge over other companies world-wide. As a result of using advanced simulation, Formtech anticipates an increase in revenue per annum of ~€100K.

KIT estimates that, due to time saving through using HPC systems, it will increase its annual revenues by around €30K. Additionally, annual personnel costs will be reduced by €10K.

Fraunhofer SCAI expects a strongly growing demand for customised and integrated CAE development. Fraunhofer SCAI estimates that, during the next 2 to 3 years, it can increase its regular annual licence revenues for such developments by ~€60K.

The outcome of this experiment has given valuable feedback to Gompute. The success of this CAE chain implementation has already brought new business with annual turnovers of over €2K for the sale of compute cycles.

KIT and Fraunhofer SCAI plan to offer a CFRP simulation service via the Fortissimo Marketplace starting in Q3 2017.

2.3 Experiment 603: Improved IntraCranial Pressure (ICP) estimations using cloud based simulations of the cerebral blood flow (iBrainSafeCLOUD)

2.3.1 Motivation

A non-invasive accurate and quick measurement of the intracranial pressure (ICP) is of paramount importance for the diagnosis and treatment of neurological diseases, brain injuries and other neuro-pathologies. The world's first accurate non-invasive ICP absolute value measurement device, based on two-depth ultrasound Doppler technology, was developed by a Lithuanian SME, Vittamed, within the EU FP7-funded project BrainSafe. Despite the technological achievements and success of measuring ICP non-invasively, Vittamed faces technological challenges seeking to increase accuracy and precision of the device, its user-friendliness and cost effectiveness to reinforce the company's leadership and open access to new markets.

Driven by this business need, our ambition is by performing high resolution 3D simulations of the blood flow in specific cerebral arteries under external conditions to generate new or deeper understanding that allows further improvement of the non-invasive technology. These simulations will help to shed light on several problems related to the errors and artifacts in Doppler measurements.

The synergy is achieved by exploring the leading-edge blood flow models developed at Simula Research Laboratory and their adaptation to the HPC cloud resources, provided by CINECA, as well as the advanced remote visualization technique at CINECA.

2.3.2 Relevance to Fortissimo

Mathematical modelling and simulations are key instruments for Vittamed's technology improvements because of impossibility to obtain this information in other ways (e.g. experiments with humans). Computational fluid dynamics (CFD) analysis enables velocity and pressure calculations in high spatial and temporal resolution. The disadvantage is that the computations are demanding and that an accurate description of the anatomy is required. In addition, the complex, possibly transitional blood flow is very difficult to compute.

Previous experience has shown that a typical simulation of an intracranial aneurysm, for instance, with time resolution of fifty thousand steps per heartbeat and spatial mesh with five million cells, takes over 168 CPU hours for 5 heartbeats.

In the iBrainSafeCloud experiment we have performed simulations on a large scale. The simulation software scales well and a large simulation of 15 million cells takes about 500 CPU hours per cardiac cycle. We remark that 10.000 timesteps per second are used because we aim to catch high frequency fluctuations that potentially cause cluttering. Indeed, Doppler signal assessed by ultrasound is generated by flows inside the body and tissue motion. The latter is called cluttering and it is a noise signal that needs to be filtered out. The simulation software is an open source, state-of-the-art solver that may be used within the Fortissimo project for transitional flow investigations.

Within iBrainSafeCloud experiment we have successfully created initial mathematical model and developed necessary software tools required to study the flow in the Internal Carotid Artery/Ophtalmic Artery (ICA/OA) system which enables simulations of any system involving the interaction between a fluid and a thin-walled structure. Using the results of the project Vittamed will be able to perform follow up simulations on the Cineca HPC infrastructure to refine its product.

The outcome of the experiment on cloud computing modelling is that cluttering is an unlikely consequence of the hemodynamics according to the computational models. Furthermore, computational tools based on a fluid-structure interaction (FSI) solver has been developed and can be used to determine the relationships between blood flow dynamics in the ophthalmic artery depending on dynamic modulation of blood flow parameters and characteristics by external applied pressure. Reactions of the ophthalmic artery blood flow to step function type partial and temporal compression of the External Opthalmic Artery (EOA) will be defined. Also, complex transfer function from periodic EOA diameter changes to OA blood flow envelope will be investigated depending on the anatomical and physiological characteristics of the blood vessels.

2.3.3 Impact and Business Benefits

This experiment demonstrates the feasibility and benefits of such simulations to Vittamed and how the necessary computational experiments can be performed via a pay-per-use Cloud-based-HPC solution. These simulations will shed a light on several problems related to the errors and artefacts in Doppler measurements appearing from inter-patient variability, arterial wall vibration, eyeball movement and other individual patient dependent influential factors. This experiment will lead not only to a better-quality device but also enable manufacturing leadership of Vittamed on a world market by reducing production costs and exploiting know-how.

Using the obtained productive knowledge Vittamed will start internal project for development of the next generation cost effective device offering much faster and more reliable non-invasive ICP measurement. This technological breakthrough would open up new markets for Vittamed, which currently are inaccessible due to limitations of the technology. In particular, the innovative device would enable to reach markets outside standard ICU setting - i.e. move towards outpatient settings in neurology, ophthalmology and primary care units.

The impact of this technology will be highly significant across a wide spectrum of levels. The clinical impact will mean earlier, faster and more accurate diagnosis of intracranial pressure. A much greater number of patients will benefit from screening by this technology because it will not be necessary to have highly specialized personnel operating the device. Patients will be treated earlier and, thus, fewer patients will suffer secondary complications as a result of their raised ICP; the Traumatic Brain Injuries (TBI) patient outcome will improve and therefore more patients and their families will have a normal life. Healthcare providers in all countries will benefit due to significant cost savings from reducing the incidence of TBI.

Vittamed can gain a significant commercial benefit resulting from the global expansion of the market for ICP diagnostic devices in ophthalmology. The global market for ophthalmic diagnostic equipment is estimated to reach $947M in 2017. The new market niche for SME in ophthalmology will create a commercial opportunity with an estimated potential of more than €100M per year.

Additionally, the impacts of the experiment are expected to range across the industrial, clinical, and scientific communities across Europe and abroad. Simula Research Laboratory, a Norwegian research institute, will exploit the results in developing research projects and in valorizing their results to industry and health care community, keeping Norway at the front line of innovative simulation and modelling research in the physiological field. The results of the experiment will enable the HPC cloud provider, CINECA, to offer its services in a more user-friendly way to the biomedical market, enabling SMEs to benefit from HPC capabilities within a simple to use and complete package. This experiment offers a success story for CINECA, in the application field of biomedical devices simulation, which is estimated to bring at least two new customer SMEs per year, with an approximate 5% increase in commercial services revenues.

2.4 Experiment 604: RheoCube – A Virtual Rheometer for Complex Fluids in the HPC Cloud

2.4.1 Motivation

A broad range of industries deal with complex fluids or manufacture them under the term “smart materials”. These materials very often have extreme flow and transport properties that either pose serious challenges for their processing or can be exploited in an innovative product. All these effects originate from the interactions and structure of the material's constituents. The possibilities to study these properties experimentally, for instance using rheology, are very limited. Material design is often a process of trial and error making it very cost intensive. A dead end is quickly reached when it comes to trying to understand and improve the performance of complex fluids. Computational modelling provides a very promising alternative to fill this gap. Computational Fluid Dynamics (CFD) is a common tool in research and engineering. However, currently available commercial software implements only macroscopic approaches in which rheological properties are required as an input (as opposed to being a result from it). Traditional CFD software provides no real insight and predictive power in the material design process. Quantitative modelling of multiphase materials on the small scale is inherently elaborate and the complexity of bottom-up numerical material models poses various challenges.

Electric Ant Lab (EAL) has developed methods for detailed simulations of complex fluids that provide a solution to many of these difficulties. These state-of-the-art scientific simulation models bring material research and engineering to a new level of detail and accuracy. However, the high-fidelity simulation of the internal dynamics of a material sample of 1mm^3 over 1s would take in the order of 10 years on a single CPU-core. State-of-the-art HPC resources with dedicated compute nodes, high-end GPGPU accelerators, and fast interconnect are prerequisites to bring the total runtime down to an acceptable timescale of 1 or 2 days.

A complete virtual rheometry solution is needed that combines access to these novel models, HPC resources, large-scale storage, and pre- and post-processing into a single service that can be utilized just like a real material synthesis and rheometry lab. We are convinced that, in order to exploit the full potential of HPC beyond a small expert community, we need to bridge the full technological gap from HPC and simulations to end-users such as experimental material scientists that do not know anything about models, simulations, computing, storage, and data analysis environments at all. The goal of this experiment was to successfully demonstrate the feasibility of this ambitious and far-reaching vision. Such a service, without the need for middlemen, will provide a much more efficient way to design new materials and would result in a considerable reduction of both, time-to-market and development costs of new products or processes. The service also needs to provide maximum data security by implementing dedicated hosting solutions in order to take away the understandable fear of exposing business-critical intellectual property (IP) which (still) is associated with the term “cloud”.

EAL was interested in this experiment because it allowed the thorough exploration of the technological and commercial feasibility of such a service. If successfully developed further, RheoCube will not only enhance EAL’s simulation-based consulting workflow but will create an important revenue stream based on a super-linear business model when operating as a SaaS provider.

Ioniqa was interested in exploring the potential of high-fidelity material simulations in their product development. The reduction of time-to-market and of the costs associated with running a wet lab is essential to improve the profitability of their business.

2.4.2 Relevance to Fortissimo

HPC and simulations are rarely used in complex-fluids markets and current use is limited to macroscopic flow simulations. Models with sufficient predictive power have not been available until now and the necessity of maintaining HPC infrastructure and expertise to run these models have been a too large barrier for many industries, and in particular for SMEs. RheoCube is an ambitious and visionary service that combines novel simulation techniques developed by EAL allowing such virtual material prototyping, with making the required HPC resources available to an end-user that has no simulation expertise whatsoever. By that, it addresses the need for HPC simulations in the complex-fluids markets directly. This vision, bridging such a large gap, comes with high technological and commercial risk of failure. Fortissimo facilitated the study of technological and commercial feasibility of such a service through this experiment in which EAL as service provider and SURFsara, the HPC center in this experiment and possible future resource provider, also had the chance to closely collaborate with Ioniqa, an SME manufacturer of smart magneto-rheological fluids (MRF). This use case, in which MRF formulations have been virtually tested successfully, helped shaping the service and demonstrated the considerable reduction in time, costs, and the increased insight HPC simulations can offer directly to innovative SMEs.

2.4.3 Impact and Business Benefits

During this experiment EAL has developed a working prototype of RheoCube as a complete virtual complex-fluids rheometry environment including a scalable integration of HPC, storage, and pre- and post-processing resources. At this stage, it has all the basic features needed for virtual prototyping and research on MRFs. This capability has been successfully tested in collaboration with Ioniqa, a manufacturer of MRFs without any simulation or HPC expertise. A pricing model has been developed that not only results in large time (~30 to 80%) and cost reduction (~30 to 90%) for the user. It also provides sufficient revenue for EAL in the order of 2k to 11k EUR per material characterization based on which a potentially sustainable SaaS business can be developed over the next 5 years when combined with consulting activities. Over such 5 years, EAL will need to further invest in the order of 300k EUR into extending the models and features in RheoCube, and extensive and specific marketing to be able to address more sections of the total 2-Billion-EUR rheometry market beyond MRF. Based on the results of this experiment which include an analysis and projection of the business, EAL is convinced that RheoCube can be developed into the leading virtual material prototyping service and a very important revenue stream of more than 1Million EUR per year over the next 5 years.

Using RheoCube, Ioniqa has gained much insight into their MRF products during the experiment and is convinced that HPC simulations have a large potential to speed up their future product development in general. Although, during the experiment but not related to it, Ioniqa decided to pivot their focus onto a different market (circular PVC recycling based on magnetic particles), Ioniqa plans to continue to use EAL's HPC simulation services (consulting and RheoCube) for predictions of transport and processing of PVC and magnetic particles in their future recycling plant. Using HPC, costly trial-and-error based engineering can be efficiently replaced by cost and time efficient high-fidelity virtual prototyping, also for the new development focus of Ioniqa.

2.5 Experiment 605: HPC-enabled system for enhanced seakeeping and station-keeping design (HPC-SHEAKS)

Seakeeping is the study of the response of a ship or marine structure to waves under different sea conditions whereas the station-keeping can be defined as the study to determine how to maintain a ship or marine structure in a fixed position in relation to a fixed object under different sea conditions. In its broadest sense, seakeeping of a marine structure includes activities related to; determination of the probability of damage of the structure, cargo and equipment; evaluation of comfort and seaworthiness; station-keeping design; evaluation of motions in ships and floating platforms; assessment of wave energy converters, etc.

The main goal of the experiment is to perform the simulation of an industrial process example for seakeeping and station-keeping design. This process requires large amounts of computing power that result in viable calculation times when using the available computing resources offered by a remote HPC provider. In this framework two different seakeeping software were adapted to run in HPC resources and their performances were studied:

- SeaFEM -**Error! Reference source not found.** a commercial seakeeping software developed by COMPASSIS
- XFire - an advanced seakeeping solver, in pre-commercial state, based on the semi-Lagrangian particle finite element method developed by CIMNE.

2.5.1 Motivation

Computational numerical methods such as Computational Fluid Dynamics (CFD), have become an essential contributor in design and technology development in every field that involves fluids. In this context and from a broad perspective, CFD have been applied in a wide variety of problems, from supplementing experiments and testing of systems (which are typically extremely expensive) to performance evaluation, safety, structural and reliability assessment, etc. Engineers across a wide range of industries, such as the automotive, defense, aerospace, life science and turbomachinery, need to make use of CFD in almost every design aspect that involves fluid dynamics. This applies as well to the ship-building and offshore industry where both, generic CFD tools and more specialized seakeeping solvers are being applied to the entire design and production processes. Nevertheless, despite the usefulness of all these tools related to the aid in obtaining better insights into product performance, this type of numerical tools entails some problems. In particular, they tend to be extremely compute-intensive and time demanding. This drawback has kept away potential users since they do not have computational resources to exploit these numerical tools and turn to less reliable and simplified numerical alternatives (as for instance frequency domain solvers for seakeeping applications).

The evaluation of the seakeeping ability of a ship or floating structure along the different design phases is of paramount importance to fulfil the different operational requirements. Experimental tests are considered, today, as the most accurate tool for seakeeping performance evaluation despite the known limitations to extrapolate the ascertained results from model to real scale. The main drawback of the experimental results is not the aforementioned limitation or the costs of these tests, but the incapability of creating an efficient feedback loop with the design process does not provide room for improvement. Therefore, to solve this lack of design improvement the study of the seakeeping ability of ships and marine structures ends up depending on low accuracy numerical models such as the strip theory or in complex CFD which, as described before, result in prohibitively expensive computation times.

2.5.2 Relevance to Fortissimo.

Analyzing the industries that eventually depend on computational services reveals that shipbuilding, offshore oil & gas and deep-water wind-turbines sectors are characterized by a large number of SMEs and a few large companies. In fact, most of these companies have a small technical department and when computational services are needed these companies subcontract specialized SMEs. The practical limitation to access the HPC infrastructures and the huge computational resources required by the most advanced computational tools prove to be a problem for these last specialized SMEs. These two limitations represent the main barriers to an industry that could widely use computational seakeeping analysis in the design stage. Overcoming these barriers is of major importance as it represents a relevant reduction in the overall design cycle and production time, a reduction in fuel consumption and maintenance costs, determinant increase in safety, unlocking the potential for the emerging deep-water wind-turbines, etc.

The opportunity given by the Fortissimo Project allowed this SME to establish a collaborative partnership to evaluate the benefits of pay-per-use HPC infrastructure applied to seakeeping analysis for ships or floating structures and to check that these barriers can be eliminated to achieve the potential benefits. Also, the Fortissimo Project initiative has helped this SME collaborative partnership to provide cloud-based seakeeping analysis adapted in an early-stage design using the HPC infrastructure to ship owners and shipyards.

Fortissimo Marketplace provides synergies with other potential end-users from the shipbuilding, offshore oil & gas, bottom fixed and floating offshore wind energy and wave energy industries, involved in other experiments.

2.5.3 Impact and Business Benefits

The main objective of the Fortissimo project was to provide new tools to SMEs that are looking to expand their activities to services based on high-performance computing resources. Within this context, the main benefits of the project were:

- The development of an execution manager. The new management tool simplifies the use of the HPC infrastructure as the end user has no need to worry about performing tasks directly with the HPC infrastructure since most of the post-processing tasks are automated. Therefore, the user can only focus on preparing the model locally while all communications with the HPC infrastructure is handled by the management tool.
- The adaptation and deployment of the seakeeping software SeaFEM into the CESGA HPC infrastructures, where the execution time was reduced by a factor of 45 (with respect to a local implementation).
- The adaptation and deployment of XFire code into the CESGA HPC infrastructure. The corresponding scalability analysis demonstrated an improvement by a factor of 40 with respect to sequential execution.
- Over the next four years, from 2017 to 2020, WAVEC expects an increase in its total profit of ~€550K, based on a revenue of €1.8M, due to an increase in its consultancy activities. Over the same four-year period, VICUSDT expects an increase in its total profit of €480K, based on a revenue of €1.4M, due to an increase in its consultancy activities. Over the same four year period, COMPASSIS expects an increase in profit of €2M based on an increase in its license sales of €4.5M.
- The demonstration of commercial readiness and viability of cloud-based HPC services. From the perspective of WAVEC, Fortissimo outcomes will contribute to

speed up technology innovations, aiming at improving performance and cost-effectiveness of offshore renewable technologies. In the offshore renewable sector, capital intensive areas comprise turbines/PTO equipment, foundations, mooring systems, structural materials, installation and maintenance. Optimizing design, transport, installation and sea-keeping equipment requires using a wide-range of numerical tools that are extremely time demanding and computing-intensive and so requires the extensive use of cloud-based HPC in a simple and effective way. Technology innovations in these areas are nowadays a drawback and a big challenge to leverage economies of scale and to reduce the cost of energy of offshore renewable sources in the coming years.

- The experiment solutions based on SeaFEM are planned to be present in the Fortissimo HPC-Cloud through the Fortissimo Marketplace by offering a set of business containers, offering both a pay-per-use solution and a turnkey consultancy service.
- Results obtained for XFire have demonstrated the capabilities of XFire in HPC environment, leading towards a commercialization plan in a mid-term.

2.6 Experiment 606: Enabling fatigue life assessment in HPC-Cloud to SMEs (FLASH)

With the successful development of FLASH experiment, the efficiency of the design, engineering and building processes of a marine structure was increased, by offering to the market added-value tools that permitted drastic computational time reductions. The experiment also demonstrated the technical and commercial viability of cloud services for HPC simulation.

2.6.1 Motivation

The FLASH experiment was motivated by the need for an effective solution for the integration of the fatigue life assessment and other complex structural direct calculations into the design cycle. HPC can enable this by reducing the computing times up to the point of making the simulations feasible within the time requirements set by the design process itself. Furthermore, the experiment was focused on marine structures, but it could be easily adapted for its application in other engineering disciplines involving intensive computational activities in their design processes.

The evaluation of the fatigue life of a marine structure is far from being a trivial task. The main difficulty is that the assessment of the fatigue life requires calculating the accumulated damage of the structure during its lifetime. This implies to identify the different operation conditions that the structure will find in its service life and evaluate the effects that the corresponding operating loads generate in the structure. The statistical nature of the fatigue life assessment increases the CPU-time requirements, having to perform numerous non-linear dynamics structural analyses. A typical fatigue or structural assessment analysis representing real life scenarios requires long physical times. It implies that the corresponding computing times could reach thousands of hours. In practice, the resulting CPU time requirements for these studies, clearly exceeds the capabilities offered by modern workstations, and makes impossible to integrate these structural life predictions in the design loop.

The numerical tools resulting from the FLASH experiment should allow end users to provide services to optimize the fatigue life design. Such services consequently reduce the inspection programs requirements, and therefore significantly improve the OPEX of the product while facilitating the economic viability of the project, since OPEX can represent about 50% of the total investment effort.

2.6.2 Relevance to Fortissimo

The computing capabilities provided by the Fortissimo project are essential to make RamSeries software an efficient and competitive solution to undertake structural assessment analysis. This kind of analysis requires extremely large simulation times in order to successfully represent the long physical times associated to the process under consideration.

Hence, within the framework of the Fortissimo project, the opportunity arose to develop an efficient software solution to be run on available HPC infrastructures. To this aim, RamSeries code was adapted and optimized to be run on the Linux environment provided by the HPC infrastructures. A tailor-made execution manager was developed to provide an easy-to-use integration of RamSeries into the HPC environment, making the end-user experience much more comfortable.

The Fortissimo Marketplace will provide the opportunity to establish synergies with other potential end-users from the shipbuilding, offshore oil & gas, bottom fixed and floating offshore wind energy and wave energy industries, involved in other experiments.

2.6.3 Impact and Business Benefits

The exploitation of the FLASH experiment aimed to increase the efficiency of the engineering design of a marine structure, by offering new added-value services to the market that could be used throughout the design phase. In particular, the main objective of the FLASH experiment was to develop an easy-to-use HPC-Cloud service for fatigue life calculation and to validate and demonstrate its usage. However, during the experiment tasks, it has become evident that structural fatigue assessment is extremely time consuming, even when HPC infrastructures are employed. This makes a complete full vessel fatigue assessment calculation still unaffordable and avoids the possibility to provide a commercial solution to the market. In view of this, other structural applications in the naval field were addressed to determine the actual potential of the new developed solution. In this sense, standard strength assessment of container ships and tankers has been identified as a good alternative case study. Its direct calculation via Finite Element Method is becoming mandatory for most Classification Societies Rules, and represents a type of analysis that implies the simulation of a large number of static analysis (more than 200 independent cases). The integration of the RamSeries structural solver into the Fortissimo HPC infrastructures permits to run simultaneously this large amount of simulations, thus reducing the total computational time from days to hours. Potential end-users for all these applications are shipyards and other design offices that need to complement their structural design capacities with these kind of structural assessments.

Furthermore, with the successful development of FLASH experiment, we intend to increase the commercial penetration of the RamSeries software in the offshore and ship design industry by integrating the leading-edge fatigue life and structural analysis software (RamSeries) with the Fortissimo High Performance Computing (HPC) infrastructures and to develop an efficient and easy-to use execution manager, integrating a middleware front-end for the resulting tool.

The experiment solutions can be offered in the Fortissimo HPC-Cloud through the Fortissimo Marketplace, providing a set of business containers with both, a pay-per-use solution and a turnkey consultancy service defined with a closed price based on the well-known requirements of the analysis and depending on the geometrical dimensions of the vessel/structure.

COMPASSIS will increase its market by introducing the use of the RamSeries software for the direct strength assessment of a complete ship structure. This assessment requires large computational and data storage resources. COMPASSIS estimates an additional annual revenue of €24K in 2017 growing to €120K in 2020, due to the sale of direct strength assessment of complete ship structures using RamSeries integrated with a Fortissimo HPC infrastructure.

ISONAVAL estimates an additional annual revenue of €15K in 2017 growing to €60K in 2020, also due to the sale of direct strength assessment of complete ship structures.

CESGA will offer new HPC added-value services for SMEs such as benchmarking to analyse performance of HPC applications, including multi-core scalability and its dependency on different parameters such as size of the problem and processor frequency. It expects a consequent increase in its HPC services and customers. New alliances with ISV and application experts have been formed during this experiment. Revenues based on 3 benchmarking studies and an annual fee for hosting the ISV software and for infrastructure maintenance will be around €35K over a 4-year period.

2.7 Experiment 607: SOUTH cloud

2.7.1 Motivation

Over the last two decades numerical simulation has become a key enabler for product innovation in the manufacturing industry. The capability of virtually analysing the performance of a new product, without the need to build a real prototype, has lowered cost and time to market allowing the definition of better products.

A further step is using numerical simulation to automatically optimize a product, rather than analysing only the performance of a solution candidate. Only few industrial players have taken this step towards automatic shape optimization (ASO), since significant changes in the current design practice should be introduced, and the associated costs may not be amortized.

The goal of the SOUTH (Shape Optimization under Uncertainty through HPC clouds) experiment is to demonstrate that by combining High-Performance Computing (HPC) and ad-hoc software, the difficulties due to changes in the design practice may be significantly mitigated and ASO might be brought to a wider audience of small and medium enterprises.

All the members of the consortium are stakeholders in simulation based design optimization of mechanical systems. The successful implementation of the SOUTH platform will permit:

i. the end-user (Automobili Lamborghini) to design at a more competitive cost better products

ii. the independent software vendor (Optimad) to differentiate its customer portfolio

iii. the application expert (University of Strathclyde) to disseminate and valorise its research towards industry

iv. the HPC provider (CINECA) to increase its commercial revenues and underline its commitment towards industrial problems.

2.7.2 Relevance to Fortissimo

The issues associated with the practical use of automatic shape optimization are manifold:

i. it takes significant computational power since many simulations need to be evaluated
ii. only specialized engineers which have an in-depth knowledge of the product can set up a sustainable ASO procedure
iii. several different software packages need to be interfaced/integrated within a single platform

HPC resources are one of the focal points of the solution which has been envisaged: in fact, they are used not only to allow the end-user to out-scale with respect to his on-premise resources, but also to generate the data needed to train a decision making module, which replaces the specialized engineer.

Fortissimo gave the opportunity to complementary players to put together their expertise to develop and interface the software needed to produce an integrated solution for non-expert users.

This cloud based provisioning allows an affordable one-stop-shop solution with an intuitive interface to end-users that are in need of ASO only occasionally.

2.7.3 Impact and Business Benefits

The platform created by the SOUTH experiment (hereafter "SOUTH platform") will have a long lasting impact on all players involved within the experiment:

End-user: Automobili Lamborghini (ALA). Regarding the aerodynamics department of ALA, the SOUTH platform allows a reduction of the development time up to 75% for a typical aerodynamic surface (like air intakes, spoilers or diffusors) with an associated cost saving of 40%. As an integrated Software-as-a-Service (SaaS) solution, the SOUTH platform allows ALA to scale out during productivity peaks to avoid bottlenecks due to limited in-house capacity. This possibility to deal with simulation peaks with a reliable outsourcing infrastructure allows also for a better investment strategy regarding the internal HPC resources.

Independent Software Vendor: Optimad (OPT). For many potential customers of OPT the total cost of ownership (TCO) of a ASO platform cannot be amortized since shape optimization is only a cyclic task. By distributing SOUTH as a cloud based Software-as-a-Service platform, the TCO is drastically reduced making it an attractive solution to a large basin of manufacturing industries.

Furthermore, OPT will exploit the platform in order to offer competitive consultancy services, which will benefit of reduced time-to-market thanks to HPC.

Application Expert: University of Strathclyde (STU). The research group at STU extensively works on design optimisation techniques for a multitude of applications: naval, aerospace and oil and gas industries to name a few. The implementation of a cloud-based environment will increase the research, consultancy and technology transfer activities by reducing the time for menial tasks like system administration that managing local resources require. Moreover the use of a cloud based solution can also be attractive for undergraduate and post-graduate research projects and can be the platform for publicly funded research projects on a European scale.

HPC Provider: CINECA (CIN). This experiment offers a success story for CINECA, in the application field of automatic shape optimization, that is estimated to bring at least two new customer SMEs per year, with an approximate 5% increase in commercial services revenues.

2.8 Experiment 608: Microscopy in the cloud (VIRTUM)

2.8.1 Motivation & Relevance to Fortissimo

MicroscopeIT is a technological company, founded in 2012, which introduced a prototype of an internet service called VIRTUM. The purpose of VIRTUM prototype was to provide computations in a Software-as-a-Service (SaaS) model, initially in the context of microscopy. At the beginning of the Experiment, VIRTUM worked in a client-server architecture and was using *in house* HPC hardware.

Principal aim of our Experiment was to adapt VIRTUM to work with *external* HPC hardware, including one of the HPC clusters within the Fortissimo framework. For Fortissimo HPC providers adapting VIRTUM to external HPC provides an *additional gateway* to SaaS market. The SaaS market continues to grow quickly: in 2016 it was estimated as $111 billion, and is predicted to increase to $216 billion in 2020 ["Market Insight: Cloud Shift — The Transition of IT Spending from Traditional Systems to Cloud" Gartner, 2016]. From MicroscopeIT's perspective adapting VIRTUM to external HPC would extend SaaS model benefits by adding i) scalability (hardware resources can be rented as a function of need allowing to cope with virtually any-size of computation) ii) cost optimization (at SME scale, renting HPC resources is cheaper for MicroscopeIT than running its own HPC infrastructure).

To achieve principal aim we searched for real-life Use Cases, related to our domain which is Microscopy Image Processing. Our Experiment assumed 4 different, completely separated Use Cases, conveyed with different partners. All Use Cases had one thing in common: they all could *potentially* benefit from converting into SaaS model, and HPC computations in particular. These cases were:

- Use Case 1: Analysis of the images from remotely controlled fluorescence microscopy
- Use Case 2: Processing of the data provided by super-resolution microscopy
- Use Case 3: Management and visualization of the data from spectroscopy
- Use Case 4: Whole Slide Imaging & Analysis (WSI&A) in Digital Pathology and High Throughput Screening (Biotechnology: drug discovery and biomedical research)

Our partners were interested in gaining understanding of benefits, pitfalls and innovation which can be generated by implementing Use Cases in SaaS model, enabling HPC as a side effect.

Finally, our goals were to i) adapt VIRTUM to *external* HPC infrastructure (Goal I) ii) test if VIRTUM can be applied in each Use Case, leading to significant benefits (Goal II) iii) identify the commercial potential of Use Cases (Goal III) iii) if the commercial potential is high enough, create and initialize a plan of commercialization in the domain of Use Case 4 (Goal IV).

In the first phase of the Experiment, we adapted VIRTUM prototype to work with external HPC infrastructure and we prepared the scaffold for implementing User Cases 1-4. In this phase we benefited from the close collaboration with our partner ARCTUR.

In the second phase of the Experiment, together with our Experiment's partners, for each Use Case, we successfully established a prototype of a system using VIRTUM (Goal II).

During phases I and II of Experiment, we were constantly adapting VIRTUM to match requirements imposed by Use Cases. We identified common parts shared by all Use Cases in dedicated VIRTUM service prototypes. Working further on VIRTUM service prototypes we realized that we have developed a generic technology, which can be applied to many various computational tasks, that could be used for both scientific and business praxis exploration in such areas as: medicine, biotechnology, material engineering, optical inspection, etc. (side-effect of Goal I&II).

We quickly realized that VIRTUM technology brings most of the benefits in a situation when one deals with relatively Big Data and complex computations. In such cases, one perfectly exploits two signature properties of VIRTUM: practically unlimited storage and scalable computations.

In this context we analyzed all Use Cases and we found Use Case 4 ("Whole Slide Imaging & Analysis (WSI&A) in Digital Pathology and High Throughput Screening") was exceptional: it required both, dealing with big data and complex computations. After analyzing business opportunities, we decided to build up on a VIRTUM service prototype developed during duration of Fortissimo project to develop a commercially available service for Digital Pathology. Currently it is running under the codename VIRTUM-DP (Goal III-IV).

VIRTUM-DP is addressing an important problem, but also targets the growing market of Digital Pathology, we therefore expect to observe more benefits with passing time. In brief, according to WHO, there's 14 million new cases of cancer each year, expected to grow by 50% in the next 2 decades [Report "Digital Pathology Market: Global Industry Analysis, Size, Growth Trends, Share, Opportunities and Forecast 2012 – 2020", Allied Market Research, 2012]. The only way to conclusively establish a diagnosis is a histopathological exam, which is performed by a pathologist. However, the number of pathologists around the world is dwindling (10.4% decline in active physicians 2008-2013, 60.7% active physicians are age 55 or older), and that is a bottleneck for cancer diagnosis [Report "Testing Times To Come? An Evaluation Of Pathology Capacity Across The UK", Cancer Research UK, 2016].

VIRTUM-DP is based on the observation that managing histopathology scans is very cumbersome for pathologists. The files are huge (usually several gigabytes each), so storage and backups are costly and easy to get wrong. Scanner manufacturers use incompatible image formats. It's hard to keep files and metadata in sync. Software to view and manipulate the scans must be installed on every computer a pathologist wishes to use. Sharing scans with a colleague usually means handling them a hard drive or optical disk.

VIRTUM-DP is a software for doctors to manage their slide collections and provide it in SaaS model. Most of the shortcoming resulting from large data sizes can be addressed thanks to HPC.

Goals I-IV were finished during the duration of Fortissimo project. Prototype of VIRTUM-DP will be available in Fortissimo Marketplace by the end of Q2 2017. Execution of the plan proposed in Goal IV is larger project which MIT executes starting from Q1 2017 financing it from its own R&D resources.

2.8.2 Impact and Business Benefits

VIRTUM-DP has the potential to remove obstacles and bottlenecks in current oncological diagnostics. Its main benefits are a significant improvement in clinical diagnosis due to an increased speed of diagnosis, an increased quality of diagnosis, an increased throughput of diagnoses and more accessible storage of samples. VIRTUM-DP can result in a reduction in staff costs by 50% through increased efficiency. Extrapolating this to the USA alone results in an overall saving per annum of $1.7 billion.

Furthermore, there is a significant cost saving in IT infrastructure through the use of Cloud-based processing. In most cases, computer resources available via the Cloud are more cost-effective. As a result of the development of VIRTUM-DP, ARCTUR will see an increase in its sales of cycles of approximately €20K per annum.

2.9 Experiment 609: Marine CFD Online Platform

2.9.1 Motivation

The use of CFD is a key asset for the maritime industry, because it enables the prediction and optimisation of ship's and offshore structure's performances. Numerical simulation is used more and more as a complement and even a replacement of experiments performed in towing tanks that are expensive and require long time schedule. Nevertheless, CFD is not easily accessible due to the following main aspects:

- CFD is expensive due to licence costs, CPU costs and also engineering costs required to use complex CFD software
- Access to CPU resources is complex for non-experimented engineers, and requires complex installations, licence managements, FTP transfers …
- CFD is complex to use, due to the large number of parameters (numerical and physical parameters), and can produce low quality results is not applied with guidelines and methodologies
- CFD requires much more pre-processing than most other simulation fields, because of the complexity of the geometries involved coupled to high requirements of solvers in terms of mesh quality. This represents a bottleneck in terms of human processing required, which can only be addressed through a very high level of automation in mesh generation.
- CFD licences are provided on local clusters and on a yearly base, without the ability to be flexible and adapt the number of licenses / CPU during project periods

The objective is to enable the maritime industry to have access to CFD software, through an innovative approach developed in this project. The key concept is to provide an integrated environment so that the End User can easily access and use CFD tools without having to focus on complex numerical parameters, meshing and remeshing, software licence installation and CPU resource access and management.

2.9.2 Relevance to Fortissimo

Nowadays, numerical simulations in the maritime field are achieved through two main ways:

1. **Out-sourced solution**

The services are provided by specialized companies. The simulations are performed by experienced engineers, who have developed high levels of experience by performing numerous and various projects. The simulations provide results to a specified problem, and client gets in return a report or simulation files that they can analyze. Depending on clients, this service can have drawbacks with regards to reactivity, autonomy, or financial cost if a large set of computations is required.

2. **In-house solution**

When companies want to provide this simulation service in-house, they currently buy licenses and local cluster. The deployment of CFD solvers is not always straightforward. The main obstacles are:

a. Need for internal CPU resources with complex maintenance, upgrade, server administration, …), or external with specific skills in complex HPC environments.

b. Installation of the software and associated license keys,

c. Need for specific skills for the selection of adapted numerical schemes, generation of volume meshes, model setup, computation monitoring (job scheduler, submission scripts), analysis of numerical results.

A second major drawback is related to the simulation load that is not constant, whereas the license and CPU local cluster is yearly defined. The following chart present an example of required CPU/License during the year, compared with available power based on a yearly license. The mean power over the year is exactly the same (64 x 12 cores / licenses seats). We can observe that this offer is not adapted to production phases that require a lot of resources during short time periods.

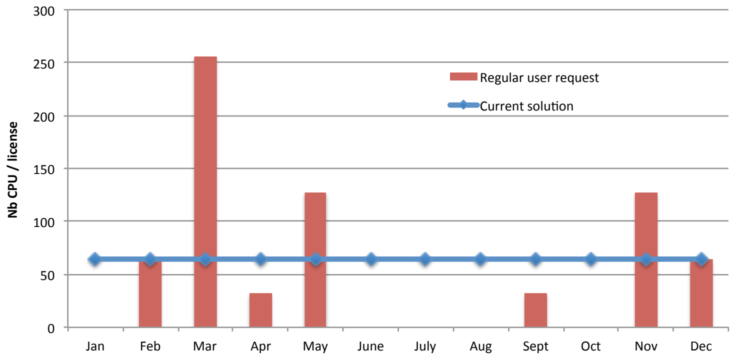

Figure 3: Example of simulation load during one year

These two ways for accessing CFD constrains the potential users to be only major companies with sufficient financial and human resources. Thus the majority of shipyards and naval architects cannot benefit from using simulation, and must rely on empirical methods or results from similar projects limiting innovation.

The present experiment concept aims at exploring a third intermediate way, proposing a global and complete and flexible Marine CFD platform with a pay-per-use model, including a simplified user interface and an automatic use of adapted CPU clusters.

The main objectives were:

- Make available in an easy way the accuracy of advanced CFD solutions for end-users, with a user interface fitted to each kind of problem of naval hydrodynamics (ship resistance, wave added ship resistance, ship manoeuvrability, open water characteristics for propellers) presented in the specific language of naval architects.

- Possibility to easily access a large number of CPU cores for a short duration, and avoid constraints related to installation, maintenance of software for end users,

- Add the expertise of NEXTFLOW and HydrOcean, with a pre-selection of adapted numerical schemes and solvers (accuracy, robustness, elapsed time) for each kind of hydrodynamic problem,

- Add automatic re-meshing capabilities with Distène, allowing the evaluation of several operational conditions (change of displacement, trim angle …) without human interventions.

2.9.3 Impact and Business Benefits

NEXTFLOW Software develops with the support of the Ecole Centrale Nantes' Fluid Dynamic Laboratory the most advanced CFD solutions for marine industries. Most of the solvers are nowadays mature, and can be proposed to clients. However the costs can still be high. The strategic positioning of NEXTFLOW is thus to develop cloud access of its marine software, with a new economic model (pay-per-use against annual license with cost per core and without CPU power for traditional model). NEXTFLOW has already developed and distributes marine software in the case of the earlier generation of solvers, based on the potential theory: integration of the hull form directly in the Naval Architect format, automatic meshing of the hull, and of the fluid domain, set-up of the numerical and physical parameters, post-processing of the results.

This experiment has enabled the same kind of deployment for the next generation of CFD solvers. The full package from CAD to mesh generation and solver computation and eventually the post-processing has been addressed, through an automatic workflow. NEXTFLOW has gained experience in the deployment of cloud-based end-user oriented solutions, validated by VPLP and HydrOcean.

In the short term, new scenarios will be added to the Marine CFD solution, in order to cover the main hydrodynamic problems encountered by the market. In the long term, NEXTFLOW expects a significant part of its revenues from cloud solutions, with an estimated licence revenue from 500k€ to 900k€ each year.

With customers including Dassault Systemes, PTC, Autodesk, Siemens PLM, Altair, MSC Corp etc., The MeshGems suite is today a reference product in the market of numerical simulation technology providers. As the CAE market evolves and matures, more and more specific needs and requirements emerge. This is typically the case in this experiment, where automated meshing technology for the specific needs of the naval industry is required. Furthermore, the growing usage of cloud computing stresses even further the need for foolproof automated tools, which require as little as possible user interaction, if only to preserve network bandwidth usage, in order to perform their tasks.

The business benefits for Distene are multiple: the first is to gain expertise and make the MeshGems product evolve to address the naval CFD field, and more generally speaking, the CFD market, better. A second benefit is to prove its adequacy for addressing the requirements of cloud-based simulation.

In the short term, it is expected to conclude a business partnership with the partners of this experiment once completed to enable them to exploit commercially the extensions of the MeshGems suite, inducing additional software revenues for Distene. In the longer term, Distene expects a significant growth thanks to a specific CFD offering in MeshGems to which this experiment contributes, increasing licence revenue from 300k€ to 750k€ annually.

2.10 Experiment 610: Delft3D as a Service (DaaS)

2.10.1 Motivation

Forecasting of flooding, morphology, and water quality in coastal and estuarine areas, rivers, and lakes is of great importance for society. For this purpose, the modelling suite software Delft3D was developed by Deltares. It is used worldwide, users range from consultants and engineers or contractors, to regulators and government officials, and is open source since 2011. Delft3D consists of modules for hydrodynamics, waves, morphology, waterquality, and ecology. One of the several SMEs that use Delft3D is HKV Consultants. They provide consultancy services and implement research in the field of safety, drought and flood risk analyses for rivers, coasts, estuaries and urban water systems. Their clients include private businesses, governments, research institutes and regional water authorities worldwide. To improve the quality of their work and opening new opportunities (increasing their competitiveness) HKV needs easy access to an environment with a pre-installed and validated Delft3D version that can scale the hardware resources in a flexible way depending on the application. This may include many computational cores for running large ensemble simulations for risk analysis or parallel computing over many cores for high resolution modelling for the design of structures in a river. For precisely this type of SMEs and applications, Delft3D as a Service (DaaS) is intended. In this experiment the aim is to have a pilot version of DaaS running for remote use by HKV. With this pilot version, HKV should be able to perform production work with a certified Delft3D version on (HPC, Cloud) hardware.

DaaS opens new possibilities for SMEs: they don't have to install Delft3D themselves and/or buy separate hardware resources, they have quick, efficient, and flexible access to hardware resources for modelling and simulation with Delft3D. In this way they can focus on their core business. DaaS will allow an SME to adapt more quickly to the needs of their clients and to improve the quality of modelled results. Here, added value of DaaS is in new opportunities like running large ensemble simulations and high resolution modelling with Delft3D. This is an immense added value to existing work methods (running Delft3D on local desktops/clusters) and will help increase the competitiveness of an SME. Therefore, focus in this Fortissimo experiment is on large scale HPC and less on Cloud Computing.

2.10.2 Relevance to Fortissimo

This Fortissimo experiment served as a starting point for gradual transition for current Delft3D users and growth model for new Delft3D users worldwide:

- transition from Delft3D on local desktops/clusters to remote computational resources,
- with no time spent on installation of hardware and software, and with scalability of HPC resources and scalable and optimized Delft3D

Fortissimo was needed to facilitate the first steps and bring partners together. An approach with eight tasks (see description in sections 4.1 and 4.2 of the report) was chosen such that separate tasks have several functions and interrelate with other tasks. Several showcases are used as test case for beta testing, for further optimization, and sharpening of the business case.

For the showcases we chose existing real life Delft3D applications that are typical for running large ensemble simulations, coupled modelling with different Delft3D modules for integrated studies, and high resolution modelling. These are typical applications that are used in practice e.g. for impact assessment (of hydrodynamics, morphology, water quality, and/or ecology) of construction works by construction industry, (landscape) architects, and engineering SMEs.

With our experiment we target the use of large scale HPC as this is necessary for high-resolution and integrated studies with Delft3D. As we see large scale High Performance Computing on supercomputers (currently starting at an order of thousands of computational cores) and Cloud Computing (like Amazon) approaching each other, we followed two tracks. The first track is on the current large scale HPC facility Cartesius of SURFsara, for which we developed shell-scripts for typical (more experienced) users to efficiently use the hardware and software. The other track is on the smaller HPC Cloud facility of SURFsara for the development and proof-of-concept of the portal. The idea is to merge the two tracks more and more during and after the experiment. In the near future, we intend to make a connection via a portal to the large scale HPC facility Cartesius of SURFsara. SURFsara has developed a basic

REST API to SAGAPython in WP2. The API can be used to submit jobs to Cartesius directly from the Fortissimo Marketplace or from any other platform or language that supports REST.

2.10.3 Impact and Business Benefits

For all partners the experiment resulted in new beneficial knowledge, business benefits are for

- Deltares: optimizing Delft3D for HPC, making DaaS operational, starting additional, new opportunities in combination with Delft3D (like large scale HPC).
- HKV: Experience with DaaS, providing own modelling as a service based on DaaS.
- SURFsara: providing Software as a Service, increasing the usage of their hardware by enabling use of Delft3D, and new knowledge on installing and optimizing Delft3D.

Exploitable output of this experiment is a computational service with the product Delft3D:

- quick & easy remote access to dedicated HPC resources for use of Delft3D,
- flexible scaling of HPC resources depending on Delft3D application,
- pre-installed, validated/certified, and optimized Delft3D installation on HPC,
- high quality and adequate customer support (both on HPC resources and Delft3D).

Potential end users are SMEs that require access to Delft3D on computational resources that

- allows to adapt more quickly to needs of clients and to improve quality of work,
- adds value to existing work methods and helps to increase the competitiveness.

DaaS opens new possibilities for SMEs, such as HKV, because it offers quick, efficient, and flexible access to HPC hardware resources for modelling and simulation using Delft3D. This Fortissimo experiment served as a starting point for gradual transition for current Delft3D users and growth model for new Delft3D users worldwide. Deltares and HKV themselves are already involved in further projects using Delft3D running on remote HPC systems.

Deltares expects additional revenues of about €70K per annum due to an increase in the use of (certified) Delft3D and of about €500K per annum due to an increase in Delft3D-related advisory and research projects by Deltares itself. With DaaS, Deltares expects an increase of business opportunities in data and forecasting services based on Delft3D and projects related to large scale computing with Delft3D, for example for dike safety assessments.

Due to the new possibilities of DaaS for large ensemble modelling and highly detailed modelling, HKV expects additional revenues of about €100K and €30K per annum, respectively. With DaaS, HKV expects an increase of business opportunities in add-on services based on Delft3D. Furthermore, DaaS will reduce risks in projects with a lot of Delft3D modelling, with the opportunity to spend more project time on creating added value for the client.

As a result of the use of DaaS, the increased revenue from the provision of additional computer resources by SURFsara is expected to be around €120K per annum.

It is planned to make DaaS available as a service not only via HPC systems at SURFsara, but also more widely through the Fortissimo Marketplace.

2.11 Experiment 611: Improved releasable buoy design with CFD on an HPC platform

2.11.1 Motivation

Today, CFD has demonstrated its capability to answer complex cases with great robustness. With the accessibility to computing resources growing and the trust gained in CFD solvers, numerical simulation is more and more commonplace. However, some very complex applications are still challenging. To compute the huge amount of data required for complex cases in a reasonable frame of time, HPC is required.

The simulation of the behaviour of a radio communication buoy released from a submarine during the launching phase is proposed as an experiment for the Fortissimo project. Indeed, numerical simulation is the only way to anticipate the buoy behaviour, as tests with submarines in a real environment are almost impossible.

This type of simulation involves fluid-structure interaction and overlaid meshes to obtain realistic results. The use of these technologies requires larges and fine meshes (several millions of cells). Computations are required to run for multiple days to converge. To compute such large and complex cases in a reasonable timeframe, simulation software must necessarily be run on an HPC system.

Today, SMEs designing and manufacturing innovative products, such as Alseamar, look for affordable solutions and easy HPC access to perform computations on their designs. K-Epsilon and Bull built together a cloud solution to simulate cases like that of Alseamar.

2.11.2 Relevance to Fortissimo

The consortium gathered for the experiment brings together all the required complementary expertise for carrying out the Fortissimo project involving a challenging case. Alseamar brings the design and manufacturer skills; K-EPSILON brings the CFD expertise, software and engineering, and Bull brings the HPC platform and HPC experts.

K-FSI and other supporting software has been ported to the BULL eXtreme factory HPC-as-a-Service to create an appropriate simulation model. An on-line solution monitor has been integrated with the eXtreme factory web interface. This monitor collects the information about computations running on eXtreme factory and sends them to a K-Epsilon web page accessible only by K-Epsilon staff.

Because naïve end-users such as Alseamar do not possess the skills to perform simulations of such complex cases, K-Epsilon makes use of the pay-per-use HPC cloud on their behalf. Specific workflows have been developed on the HPC system to reduce engineering time and to feed into the Alseamar design cycle

Fortissimo gave us the opportunity to collaborate on an industrial case to show the capabilities of the in-house tool of K-Epsilon on the HPC. Thanks to the obtained results, each partner can show to potential customers the maturity of the process.

2.11.3 Impact and Business Benefits

Thanks to this experiment, **Alseamar** achieved to launch the commercialization of a new product. The commercialization is planned for 2017. Alseamar estimate that 3 jobs will be created, and the turnover will increase by 20%. Through the project, Alseamar gained trust in using CFD technology, offering an alternative to real testing to improve efficiently their design.

The project presented the opportunity for **K-Epsilon** to integrate its in-house tool K-FSI on a HPC cloud, with a pay-per-use service. The results demonstrate the capabilities of K-Epsilon to address very complex cases with K-FSI. 2 jobs were created during the Fortissimo project, and K-Epsilon expects to create another 3 positions in a five-year plan. The annual turnover is expected to increase by 8% in the first year after the project, and by 65% in a 5-year plan.

For **Bull**, this experiment is an opportunity to reach new potential customers in the maritime market. From the exploitation plans, Bull will gain 20% of the turnover made by the K-Epsilon from studies, to provide the computational resources.

3 Concluding Remarks

The second set of open call experiments in Fortissimo cover a wide range of industry sectors and bring in many new partners, in particular SMEs to strengthen the consortium. The results will have the potential to enrich the Fortissimo marketplace and many of the experiments have concrete plans for offering services.

Collectively these experiments have shown that the Fortissimo approach of providing cloud-based HPC is one that allows business benefits of modeling and simulation to be enjoyed by companies that were previously unable to take advantage of such technology. The experiments showed that this approach can deliver value for all stakeholders, and in particular SMEs which are recognized by I4MS as vital for Europe's future economy.

Typical benefits reported by the partners include: reduced times to market; lower production costs; improved quality of manufactured products, and the opportunity to expand customer base. In most experiments the financial returns will exceed the investment of public funding, although not all benefits can or should be reduced to directly measurable monetary returns. The indirect financial impact of some of the benefits listed above can be even higher in the long term, and there is the potential for further societal and environmental impacts.

The approach of having small, focused experiments seeking to solve a particular business need proved to be effective. At the same time the experiments benefited from being part of the Fortissimo initiative as a whole. The experiments have served to bring inexperienced users to HPC, something unlikely to have happened without the support of the Fortissimo project.

As described earlier in this document, the experiments provided further requirements to Fortissimo marketplace and validated the approach taken and business processes developed. The experiments provide further success stories to the marketplace, strengthening its appeal and positive impact.