FORTISSIMO

D5.3

Open Call 1 Application Experiments Public Final Report

Workpackage:	5	Application Experiments	
Author(s):	Mark Sawyer (Editor)		UEDIN
	All experiments		
Authorized by	Mark Sawyer		UEDIN
Reviewer	Francis Wray		scapos
Reviewer	Jochen Buchholz		USTUTT
Reviewer	Matej Artac		Xlab
Dissemination Level	PU: Public		

Date	Author	Comments	Version	Status
2017-01-18	M Sawyer	Initial draft, without expt 518	V0.1	Draft
2017-01-30	M Sawyer	Following initial internal review comments	V0.2	Draft
2017-02-03	M Sawyer	For final internal review	V0.3	Draft
2017-03-13	M Sawyer	Approved	V1.0	Approved

Executive Summary

The Fortissimo project created the Fortissimo Marketplace. This provides one-stop, pay-per-use, on-demand access to advanced simulation and modelling resources including software, hardware and expertise.

The marketplace helps find novel solutions to your challenges, discover new opportunities and brings together all necessary actors to construct the exact solution that meets your business requirements.

In order to prove the concept of this approach, and to give service providers an opportunity to develop, test and offer services, a series of application experiments were carried out. The applications experiments were in three phases: an initial phase when the main project started, followed by two sets of experiments selected through open calls. The participants in an experiment typically consisted of an end-user, a software provider and an HPC expert and resource provider. Partners with specific domain expertise were also present in some experiments.

Each experiment set out to create a solution to an end-user defined problem, based on the use of cloud-based HPC and advanced simulation.

The experiments selected from the first open call (i.e. those reported on in this document) represent over 50 partners (not counting the core partners in Fortissimo such as the HPC centres), covering a wide range of business sectors and challenging applications.

The results show that the Fortissimo concept is well founded. Many experiments have produced results that will lead to production level services in the Fortissimo Marketplace that are proven in terms of technological feasibility and economic viability.

Fortissimo has also published compilations of the success stories which have been published. These are deliverables D10.13, D10.14 and D10.15 which are available from the Fortissimo project see www.fortissimo-project.eu.

Table of Contents

1 Objectives of the Experiments

1.1 Overview

This report is a compilation of the publishable information from 22 experiments that were carried out in the Fortissimo project following an open call for funding.

The objective of the Fortissimo project is to create the Fortissimo Marketplace, providing one-stop, pay-per-use, on-demand access to advanced simulation and modelling resources including software, hardware and expertise.

The Marketplace helps end-users to find novel solutions to business challenges, discover new opportunities and brings together all necessary actors to construct the exact solution that meets business requirements.

The experiments described in the report were carried out between October 2014 and December 2016. A total of over 50 partners, on addition to the Fortissimo core partners were involved, covering a diverse range of applications and industrial sectors.

The experiments have successfully demonstrated the business principle of using cloud-based HPC to enable new users and small companies to access advanced simulation technology in a cost-effective way. Significant technical hurdles have been overcome in many cases to enable services to be deployed in the Fortissimo Marketplace.

The exploitation of the results is an ongoing process, with the experiment partners committed to using the Fortissimo Marketplace to offer services with economic benefits to all stakeholders.

1.2 Management of the experiments

The experiments and the role of each partner are listed in Table 1. The objectives, achievements, work done and resources used are covered in more detail for each experiment in Section 2. Each experiment was assigned to a host centre, which was responsible for monitoring its progress and reporting to the WP5 management.

There were over 50 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	Partner short name (See list of full names in Appendix A)
Experiment 501: Cloud-based HPC platform for maps conversion	End User: SISENER Application Expert: INGECON ISV: INGECON HPC Expert: XLAB HPC Provider CESGA Host Centre: CESGA

Experiment Title	Partner short name (See list of full names in Appendix A)
Experiment 502: EASi-HPC - Electromagnetical Application Simulation on HPC	End User: SEEMI Application Expert: ATI HPC Expert: INRIA HPC Provider: BULL Host Centre: BULL
Experiment 503: castINcloud - Sustainable CLOUD Services for bringing High-Performance CASTINg Simulations	End User: FDR Application expert: QUANTECH HPC Expert: CIMNE ISV: QUANTECH HPC Provider: CESGA Host Centre: CESGA
Experiment 504: MarineCloud - On-Line Cloud-based Simulation Workflows in Renewable Marine energy for Tidal Energy Farms	End User: OOSAS Application Expert: ACTIVEEON ISV: ACTIVEEON HPC Expert: BULL HPC Provider: BULL Host Centre: BULL
Experiment 505: Improved and optimized design of high temperature exhaust gases concentric chimneys	End User: DINAK Application Expert: AIMEN HPC Expert: UDC HPC Provider: CESGA Host Centre: CESGA
Experiment 506: HPGA – High Performance Gear Analyzer	End User: VE&D Application Expert: UNIMORE HPC Expert: CINECA ISV: UNIMORE HPC Provider: CINECA Host Centre: CINECA
Experiment 507: HPC-Welding ff	End User: LBO Application Expert: LandW HPC Expert: USTUTT , SICOS HPC Provider: USTUTT Host Centre: USTUTT
Experiment 508: Drug-Target Binding Simulations	End User: TI Application Expert: TUD HPC Expert: HUA HPC Provider: UEDIN Host Centre: UEDIN
Experiment 509: VIC4CAM - Experimentation of VIrtual Metrology HPC Simulation Services for SME Production Process Control in Sustainable and Competitive CAmshaft Manufacturing	End User: EPC Application Expert: UNIMETRIK HPC Expert: CESGA ISV: DATAPIXEL HPC Provider: CESGA Host Centre: CESGA

Experiment Title	Partner short name (See list of full names in Appendix A)
Experiment 510: HighSea - High Performance Virtual Sea Experiment	End User: HYDROLIFT , INVENTAS HPC Expert: INVENTAS , SINTEF , BIBA ISV: HOLONIX , BIBA HPC Provider: CINECA Host Centre: CINECA
Experiment 511: TSEC - The Seismic Experiment Cloud	End Users: SHARP-AS , SIPLtd Application Experts: SHARP-GmbH, Fraunhofer ISV: SHARP-GmbH HPC Provider: BULL , USTUTT Host Centre: BULL
Experiment 512: Cloud-based simulation of pipeline components for the Oil and Gas Industry	End User: DRG Application Expert: ENGYS-UK HPC Expert: NAG ISV: ENGYS-UK) HPC Provider: UEDIN Host Centre: UEDIN
Experiment 513: Cloud-based Simulation for Antenna Design and Radar Signature Prediction	End User: LUNTECH Application Experts: NX HPC Expert: GENCI ISVs: ENTARES HPC Provider: BULL Host Centre: BULL
Experiment 514: CLEEN - CLoud based Environment ENgineering services	End User: eAmb , T2I Application Expert: PROGESI , eAmb HPC Expert: CINECA ISV: PROGESI HPC Provider:CINECA Host Centre: CINECA
Experiment 515: Virtual Automatic Rapid Prototyping Based on Fast Morphing on HPC Platforms	End User: HSL Application Expert: UTV HPC Expert: CINECA, UTV ISV: RBF Morph, ANSYS HPC Provider: CINECA Host Centre: CINECA
Experiment 516: StamHPC - High performance computing for the metal stamping industry.	End User: MATRICI Application Expert: QUANTECH HPC Expert: CESGA , Fraunhofer ISV: QUANTECH HPC Provider: CESGA Host Centre: CESGA

Experiment Title	Partner short name (See list of full names in Appendix A)
Experiment 517: Cloud-based Optimization platform for reinforcement steel cut industries	End User: SCHNELL Application Expert: UNIZAR HPC Expert: UNIZAR ISV: SCHNELL HPC Provider: CESGA Host Centre: CESGA
Experiment 518: cDES4SME - Cloud based Discrete Event Simulation for SME	End User: CERX Application Expert: DCU HPC Expert: UEDIN ISV: ICMR HPC Provider: UEDIN Host Centre: UEDIN
Experiment 519: SuREHPC - Sustainable & Renewable Energy HPC	End User: ZECO Application Expert: ENGINSOFT HPC Expert: CINECA ISV: ANSYS HPC Provider: CINECA Host Centre: CINECA
Experiment 520: Prediction of optical properties of dyes and application for the rational design of time-temperature integrators	End User: SCRIBA Application Experts: UNIMORE , UNIVAQ HPC Expert: CINECA HPC Provider: CINECA Host Centre: CINECA
Experiment 521: Multi-physics simulation of high temperature superconducting devices	End User: OXO , ICMAB Application Expert: ICMAB , CIMNE HPC Expert: CIMNE HPC Provider: CESGA Host Centre: CESGA
Experiment 522: SSSM - Sample, Simulate, Sample Map	End User: DFRC Application Expert: DFRC HPC Expert: DFRC ISV: DFRC HPC Provider: USTUTT Host Centre: USTUTT

Table 1: List of initial experiments in Fortissimo

2 The Experiments

This section contains a brief description of each experiment in terms of the motivation, expected outputs and impact.

2.1 Cloud4Maps

The objective of this experiment has been to establish a commercial web portal offering, on a SaaS basis, the interpolation of maps to increase their resolution. This is a new service enabled thanks to HPC, as currently PCs run out of memory in cases where the interpolation is calculated with high resolution (< 1 m). This interpolation service is an engineering support tool for the implementation of projects in sectors such as mining, building and infrastructures industry, energy facilities such as wind farms and solar FV plants, military and defence, waste management, environmental sector, universities and education. The service is based on the migration of a commercial software for PC used for the design of wind farms developed by the Spanish ICT company Ingeniería y Control Electrónico S.A. to an HPC platform.

To demonstrate the validity of the approach, this experiment engages all participants in the commercial value chain, including the software vendor (Ingeniería y Control Electrónico or INGECON), an engineering company as end-user (SISENER), a HPC infrastructure provider and a technology expert (CESGA) with experience in the Fortissimo platform.

2.1.1 Motivation

Many engineering projects in every industrial sector everywhere in the world need cartography covering a larger or smaller area during the tender, design and implementation phases. Getting accurate cartography increases project costs and can cause delays or even be difficult to subcontract depending on the part of the world where the project has to be implemented. Almost every civil engineering project requires a resolution of 1 meter or better. This demanding resolution could be achieved through software by applying a Kriging interpolation algorithm to a map with a lower resolution. This original map could be an existing one or one generated at a lower cost in time and money, increasing then the resolution by means of interpolation.

There are commercial software applications with a module enabling map transformations using Kriging interpolation algorithm such as INGECON's WindAST, the basis of this experiment. However, these applications are specific purpose packages (e.g.: to design wind farms), so their licences are expensive because they include functionality not needed in most of the projects in other engineering sectors. Kriging interpolation is very intensive in terms of computing resources, so enabling it on a SaaS platform using HPC makes sense especially for engineering SMEs.

For an ISV this is an efficient way to offer a software application to many new customers in different new sectors. The engineering companies will save time and money when dealing with cartography in their projects. Consequently, HPC centres will get more revenue by increasing the usage of their infrastructure.

2.1.2 Relevance to Fortissimo

As it has been mentioned, the Kriging algorithm is very compute intensive. Currently running a project using the Kriging algorithm using WindAST on PCs (4 GByte RAM) for a typical

wind farm design with a resolution of around 80 meters can take several hours (4 to 6 hours). Such an interpolation using the algorithm allows designers to make decisions on which wind turbines to install. Full CPU load on a PC prevents the engineer to do anything else on the PC in the meantime. Achieving the 1 meter resolution required for the detailed engineering project targeted in this experiment would require calculating 80*80=6400 times more points than if the resolution is of a mere 80 meters. The use of HPC has reduced the cases for wind farms to a few minutes of computing, and in other projects requiring even greater resolution to a few hours. Furthermore, such demanding jobs (1 meter resolution) could not be executed on a PC, because most of the test cases typically fail since there is not enough memory.

2.1.3 Impact and Business Benefits

During the evaluation process of the HPC system by SISENER, the company introduced the developed tool into the design process of the civil works for an electrical substation in steep terrain. The HPC system has been used as a time-saving tool, and significant reductions in time and costs were achieved.

Taking into consideration the context of wind farm engineering, accurate information for earthwork planning is required in the design process. Fortissimo helps to reduce time to obtain the precise topography for a project design.

The time reduction achieved getting the cartography in a substation layout design project is of up to 70% (in a process lasting 3-5 hours, savings are of 2-4 hours). The process time reduction is therefore considered as a Key Performance Indicator (KPI), and its value in this case shall be 70%.

The use of the Fortissimo HPC-Cloud in designing the earthworks for a Wind Farm substation has been quantified in a reduction of 88% of direct costs when not using the Fortissimo solution. This is a result from the time reduction of processing the maps (manually) and from the reduction of needed subcontracting in topography campaigns. The cost of staff and of the subcontracted topography studies is significantly reduced.

Correspondingly, indirect costs involve another 12% of the former process costs (engineering costs) due to time reduction.

These time/cost savings can be extrapolated to an annual period. A company like SISENER can manage 26 similar projects in a year, and therefore the total annual savings for an engineering company would be up to €55,000. These cost savings would be higher in the case of topographical companies which can apply the computational tool directly to almost all the projects in which the company may be involved.

The use of HPC for an engineering company, like SISENER, provides good information with less time spent and a subsequent cost saving during the engineering process.

For an ISV as INGECON, small engineering companies such as SISENER wouldn't buy a software licence to execute only a few projects per year, but can be targeted as customers of a pay per use system as the one designed in the project. Also it helps in the delivery of services such as deployment of new releases/updates, users' support and demos/trainings.

For a customer like SISENER, around 100 interpolations for their design projects per year can be expected. This means a yearly revenue of between €50 and €100 for INGECON per customer. This figure may seem small, but there are tens of thousands of prospective customers similar to SISENER.

In addition, there are already 2 more topography companies (which are also end-users providing services to engineering companies creating and selling topographic maps) using the solution before the project ends, leading to actual savings during 2016 of around €165,000 for the 3 end users.

With every new customer, pay back would be significantly increased from the end-user's perspective, and by the end of this year INGECON expects to have at least 10 customers.

2.2 Electromagnetical Application Simulation on HPC

2.2.1 Motivation

Manufacturers are increasing the use of electrical and electronic components in all kinds of products to provide new functions, improve performance and reduce costs. This increased use of electrical components can create electromagnetic vulnerabilities which in turn can disturb or disrupt equipment operations. This can happen in various conditions:

- Inside an electrical harness between power supply wire and command wire
- Between electrical harnesses
- Due to external sources (electrical equipment, engines, WiFi) or natural ones like lightning

There are different ways to deal with these problems, such as changing the position and/or routing of the wires and cables or cable shielding. These solutions can introduce additional costs and weight.

A wide range of industries and applications is affected by this including machine design, robotic assembly lines, devices for commercial buildings and public facilities, embedded systems (aircraft, trains, boats, tramways, drones), and in general, all automatic devices and electrical systems.

To save time and money, manufacturers need tools which can:

- Detect bad electromagnetic effects as soon as possible: before prototyping, during the design phase
- Avoid cable shielding when it is not necessary, leading to lighter equipment with lower manufacturing costs

An electromagnetic simulator, integrated with an electrical CAD software suite, used during the design phase, on a simple PC connected to HPC, will allow manufacturers to adapt the design to reduce or eliminate electromagnetic problems before building the first prototype.

2.2.2 Relevance to Fortissimo

Current practice in the manufacturing sector and particularly with SMEs is to proceed empirically by experience and then to solve electromagnetic issues when they arise. This is done during test and qualification phases and even quite often during installation on customer premises. A better approach would be to simulate electromagnetic vulnerability during the design phase on different cases to decide what should be the right routing of wires, if they should or should not shield some of them, and or take any appropriate action for that purpose. Therefore there is demand for a cost-effective way to carry out this analysis.

In design offices, engineers are used to work on PCs, getting immediate response from the software. Electromagnetic simulations require complex calculations that need large amounts of computing resources. Simulating a realistic design becomes impossible on a PC, as the time taken would be prohibitive. There is an additional risk of interruptions with the subsequent need to restart the calculation from the beginning.

In addition the calculations must be run thousands of times to simulate a reasonable range of frequencies, between 50 Hz and 2 GHz for example.

HPC has the potential to dramatically reduce the computation time from hours to seconds and so becomes essential for simulating electromagnetic vulnerability of equipment in any normal manufacturing context.

The users of the simulator are designers of electrical systems, and we target mainly SMEs which typically do not have any specific skills and expertise in HPC. Therefore the solution developed in this experiment must provide seamless access to HPC from a PC workstation. In this way the users could run simulation from their PC, without needing to be concerned with where it will run, and then get the results presented on their PC. This seamless access to HPC is essential to meet the needs of the targeted users.

Fortissimo HPC-Cloud provides easy access to HPC resources to quickly process electromagnetic simulations, something that is a crucial requirement for SMEs.

Ultimately the users would like to be able to have a cost-effective on-demand service and to get the result only a few seconds after service invocation. The partners aim to achieve such a result via an intermediary solution that can be incorporated into the Fortissimo Marketplace to create simulation as a service.

2.2.3 Impact and Business Benefits

The benefits established cover all the consortium project partners:

- Regarding Algo'Tech the benefit was to demonstrate the feasibility of integrating HPC in its offer in a transparent way for the user, thus demonstrating realistic electromagnetic simulations during the design phase. When it is ready for the Marketplace it will be offered in SaaS mode and will account for 10% of direct business plus will indirectly support 20% of the current business. This is expected to lead to overall business growth of 8%-10% per year.
- Seemi will be able to address electromagnetic issues at the design stage to save costs and time and to reduce problems for their customers. They are keen to use this tool as soon as it is ready for the Marketplace to improve and optimize their current processes in terms of electromagnetic vulnerability protection, and avoid issues on any new complex installation they will deliver.
- Inria did improve its Pastix solver and opened it to "non HPC specialist" users like Algo'Tech. This will create new opportunities for it to be used and further improved.
- Bull, as an HPC center, opened up a new HPC usage scenario. It allows them to adapt their offering to address new customers and they are looking forward to answer to this new need for "HPC on demand".

2.3 Sustainable CLOUDServices for bringing High Performance CASTINg Simulations to the SMEs (castINcloud)

The objective of the experiment was to develop and validate the castINcloud service layer, an affordable and easy to use service for metal casting simulations. CastINcloud will build flexibly on existing HPC-Cloud providers and offer casting design and simulation to SMEs under a pay-per-use service. The ultimate goal is the full, simple, efficient and affordable integration of available powerful high performance computing infrastructures with advanced casting simulation software for European SMEs. Main customers of the new service will be SMEs and large design departments of big companies.

2.3.1 Motivation

The casting industry is widely considered as a sector that exerts great influence in the development of the world economy. Because the foundry industry is predominantly an SME industry, with more than 80% of companies employing less than 250 people, the adoption of new information and communications technologies (ICT), and in particular simulation tools, by SMEs contributes to increased productivity and innovation capacity in the sector. It is necessary to note that the 80% of casting production is done in SMEs.

Despite the great advances in computing hardware and software, high-end computer simulation and engineering design tools (also known as computer-aided engineering (CAE)) are often hard to afford for SMEs. This is particularly true for HPC-Cloud simulation tools.

The two principal reasons for this are:

- **Commercial simulation software often does not fit the SME's requirements in terms of cost and usability**. Most of the major professional simulation packages have become progressively more expensive, based on a business model of creating comprehensive suites of ever more modules with richer and more complex features. The main objective is to attract large automotive and aeronautic companies who can afford the high price tag. As a result, simulation software is often over-dimensioned and expensive for SMEs, and requires additional investments in powerful workstations, in staff training, and in consultancy services.
- **Lack of scalability in some commercial simulation codes**. Up to now, most of the traditional commercial software packages are optimised to run on stand-alone computers and hence they do not scale well in high performance computer infrastructures with a limitation in the size and computation time of the problems they can solve. Nevertheless, to remain competitive, SMEs need to be able to solve ever larger and more complex design and engineering problems. This in turn requires greater computing capacities, which can be met by offering flexible HPC-Cloud services.

2.3.2 Relevance to Fortissimo

In the current scenario, the traditional CAE system installed as in-house software, means: a) a equipment workstation ranging from €1,500 to €3,000 b) a license cost of €6,000 for the first year, c) a maintenance of €1,500 per year, d) plus the number of working hours by the engineer.

A typical simulation work to assist in the design of a casting process, considering a medium-complex part, represents around 4 iterations, each of them needing 10 computing hours with a

standard cluster conventional workstation (4 cores, 4-8 GB of RAM). This is approximately a week of work for a specialized engineer, and implies keeping occupied a workstation for the same amount of time, which is not consistent with an efficient design process.

Given the complexity of the casting process to be simulated, a very fine finite element discretization is needed in order to obtain accurate results. Such a fine discretization involves significant computational resources. Fundiciones de Roda is a SME Spanish Foundry Company specialized in grey and ductile cast iron that does not possess the necessary computational infrastructure. The possibility of using Cloud-based HPC resources proved to be fundamental in addressing this specific industrial and scientific challenge.

Such a problem would either be too big for the in-house systems or would take too long to run to be part of an effective design process. HPC use enabled Fundiciones de Roda to obtain results of much more complex casting process simulations in a reasonable time.

Fortissimo Marketplace is a web-based portal that allows experiments and commercial users to access the Fortissimo HPC Cloud, establish projects with the correct expertise, applications and HPC resources, and also provide account management and other features over time.

The Fortissimo Marketplace will include information on the resources and expertise provided by the partners, including training and marketing information (such as success stories) to assist SMEs make clear decisions about using HPC in their daily business. Through the Experiments, initial proofs of concept and support for the provision and use of ISV or SME in-house applications into the Fortissimo infrastructure are conducted.

During the experiment QUANTECH's objective was to integrate its castINcloud service in the Fortissimo Marketplace. Once the different solutions proposed for this type of integration are in the production phase, they will be analysed in order to select those options that fit better with the experiment business model.

The Fortissimo marketplace will constitute a great opportunity to promote and commercialize Click2Cast software as a fast metal casting simulation solution for HPC-Cloud platforms.

2.3.3 Impact and Business Benefits

Creation of a new SaaS will provide end-users with the parallel processing capability required to accelerate time-to-solution and to solve the metal casting high fidelity problems (where small improvements will provide large costs savings).

The use cases investigated in the experiment addressed optimization of filling and feeding systems. The process of optimization of the filling and feeding systems, the use of Click2Cast simulation with HPC-Cloud allows the foundry to be faster in deciding which is the most efficient feeding and filling system in order to reduce the maximum quantity of iron of these systems. This aspect is essential in a foundry because it is important to pour as many pieces as possible from a given quantity of melted iron. In this way, the weight of filling and feeding systems is reduced as much as possible. This reduction is one of the facts that affect the foundry productivity.

The traditional approval of the pieces consists on making trials and seeing if there is any problem with them. This is called colloquially "trial and error" method. The use of Click2Cast simulation with HPC-Cloud allows virtual testing of the process and thus avoids the time and cost of intensive real trials. This process would reduce prototypes cost and homologation process time.

With the use of Click2Cast with HPC-Cloud it is possible to run at the same time several options of the filling and feeding systems being able to reduce the time of producing the prototype. Time reduction is about 10% which means a reduction of design costs of 10%. Considering that in a year a small and medium size company like F. de Roda foundry performs 200 design studies in order to make offers to customers, the reduction of designing cost would be around €3,200 /year.

The use of Click2Cast with HPC-Cloud allows the foundries to have a greater speed and agility to develop the offers for customers as it is explained above. This has a positive impact in the awarded contracts arising from offers made and it is estimated as an increment of 20%. This means the % of awarded contracts would move from 12% to 15%. In 2015 a 10% of the whole production of the foundry were pieces related to awarded contracts in 2014, then with HPC-Cloud it is possible to increase production in 0.3%. Consequently, sales would increase in 0.3%. Considering this % the annual billing would increase €19,500 year.

Support provision in technology to industry, in particular SMEs is a strategic part of CESGA's mission. The development of industrial HPC gateways and graphical user interfaces for industrial workflows will allow CESGA to increase and improve its services for SMEs requiring HPC integration within their business processes. Furthermore CESGA has gained new valuable experience on the integration of industrial desktop applications with remote HPC resources.

QUANTECH could use the computing services offered by CESGA and potentially others offered by the Fortissimo Marketplace providing SaaS option to customers. CESGA's resources will be used by Quantech in order to execute the model developed in the experiment 503 and possibly for moving new software executions from the SME computers to the HPC resources.

Finally, one of the main results of the experiment is to provide the fundamentals of a metal casting simulation service to end-users through the Fortissimo marketplace with a cost-effective access to the service, providing new business opportunities to SMEs and showing that the CAE technology has become essential for the foundry industry.

2.4 MarineCloud

2.4.1 Motivation

The ocean possesses a tremendous amount of energy. It has been estimated that if less than 0.1% of the energy available in the oceans could be captured and converted into electricity, it would satisfy the present global demand for energy more than five times over. Specifically, Tidal Farms, a group of multiple tidal stream generators assembled at the same location, are very promising power plants for the production of electric power as they can benefit from the knowledge and experience acquired in the domain of wind energy, but are based on a more predictable and regular resource: tidal currents.

However, such farms are very difficult to engineer. Given the extreme oceanic weather conditions, the cost associated with such offshore infrastructures is very high, and a small error on production assessment can have a major impact on profitability. In turn, the actual production of energy strongly depends on many factors: ocean variability at daily scale and over 20-year tidal cycles, global to local effects, turbines geometry, array effect and turbulence effects due to interactions between generators competing for the ocean energy.

Open Ocean's purpose is to bring innovative solutions to Tidal Farm developers, in order to help them assess the oceanic environment and boost the development of this promising technology. MarineCloud's experiment was aimed at developing a new product able to produce Tidal Farm yield estimates from high-resolution oceanic current data in less than 24 hours.

2.4.2 Relevance to Fortissimo

As such, High Performance Computing (HPC) is facing a new challenge. Current preliminary simulations are not capable of producing a realistic timely result. On Open Ocean's current 32 cores cluster, it takes about 3 days of CPU time to simulate 1 year of ocean variability, depending on the spatial and temporal resolutions of the model. A higher spatial (or temporal) resolution means a reduced uncertainty on the energy production of the tidal farm, but a much longer computation time. Ideally, several tidal farm configurations need to be tested before choosing the optimal one. Thus, there is a strong interest in reducing the computation time while increasing the accuracy of the model.

Moreover, there was a strong need to automate the workflows involved in the simulation, optimise the execution, and make it flexible and modular.

An easy-to-use flexible cloud environment provided through Fortissimo is a logical path to follow. The service prototyped during the experiment MarineCloud Fortissimo Experiment met our expectations.

First, we have optimised existing building blocks to accelerate the simulations. Then, we have built dedicated Tidal Farms simulation workflows that were also subject to intensive benchmarking and optimisations. Finally, we have developed a simple interface to launch the workflow and get the result, seamlessly executing on HPC Clouds.

2.4.3 Impact and Business Benefits

A simple interface was developed, allowing a user to launch a high-resolution numerical simulation of three-dimensional oceanic current on a period ranging from 1 year to 10 years, at the Alderney Race offshore Normandy in France.

The main challenges were:

- to be able to produce **a numerical simulation of 1 year of 3D oceanic current in less than 24 hours** without compromising the quality of the data (a standard threshold of 5% uncertainty on the production assessment was selected),
- to **reduce the number of inputs needed**. Indeed, the inputs of a numerical model can be very numerous and complex to apprehend, especially to users who are not expert in ocean modelling.

This interface lays the base for a **new kind of product** which will:

- **reduce the difficulty to access accurate oceanic datasets**, as the user will themselves be able to launch their own computations and retrieve the results in 24 hours,
- **let the user select the area of interest**
- thus allow for more thorough analyses and studies,
- target all kinds of offshore industries as 3-dimensional current data is needed in a variety of fields.

By reducing the time needed to model and analyse environmental data, the MarineCloud experiment improves Open Ocean's workflow, and the company becomes more competitive in the market of oceanic studies for renewable energies. The improvement done on the yield estimate computation time can easily be applied to all generic site characterisation statistics needed for such offshore projects. Open Ocean now has, as a result of the experiment, a good experience in workflow parallelisation. It has greatly improved Open Ocean productivity.

The MarineCloud experiment was a milestone for **Open Ocean** in its transition from marine energy consultancy to marine data intelligence Software as a Service (SaaS) provider.

2.5 Improved and optimized design of high temperature exhaust gases concentric chimneys

2.5.1 Motivation

DINAK is an SME expert in designing, manufacturing and installing domestic and industrial chimneys and ventilation systems. They need a simple and powerful tool to analyse and test their designs. This tool should help them to improve the design of concentric chimneys and gain understanding of the physical phenomena involved in exhaust processes.

The reduction of emissions requires optimized design of chimneys, and simulation activities will play an important role in the design of new chimneys. If a stove is installed in a building, it will be necessary to install a ventilation system to assure an effective and regulations-compliant exhaust system and the proper air renovation ratio. The concentric chimney design proposed in these applications is a countercurrent design, where both gases involved have different directions: The inner tube leads hot combustion gases to the exterior and the external cylinder leads fresh air from the exterior into the stove providing oxygen. If the chimney is not properly designed, not enough oxygen will reach the furnace and the combustion will be inefficient.

This design has to manage the thermal transfer between the hot gases from the furnace and the cold gases from the exterior. Since there are many variables involved in the optimization of the design of a chimney and physical testing is not feasible on the grounds of cost and time, it is necessary to use advanced numerical tools to improve it. To optimize the design of the insulators, chimney geometry and suction systems for each application, a computational fluid-dynamics (CFD) software should be used. However, the problem is really complex because there are many variables and the solution from CFD should be sufficiently accurate (and thus detailed), so high performance computing (HPC) is required to find the optimal design.

AIMEN, as a simulation service provider deployed and adapted OpenFOAM to solve the specific problem, and UDC, as expert in HPC developed an application with a user friendly interface and BlackBox operation for HPC using the Fortissimo architecture. AIMEN has improved its CFD knowledge and the understanding of HPC services with its participation in this Fortissimo experiment, and UDC has acquired better knowledge about the personalization of technical applications for industrial sectors. Finally, CESGA has tested and implemented a new visualization service based on ParaViewWeb.

Once the numerical model is calibrated, DINAK uses a simple and intuitive application to submit the CFD model to the HPC architecture to design new customized concentric chimneys for high temperature gases which are adapted to each operation conditions and comply with the new and more restrictive energy efficiency legislation.

2.5.2 Relevance to Fortissimo

From a financial standpoint, it is indeed unthinkable for a SME such as DINAK to shoulder the regular investments needed to maintain an operational and up-to-date HPC cluster which can provide the computing infrastructure required to execute the CFD simulations of their chimneys.

Furthermore, the need for computational capacity might be variable, with high yet sporadic demands. The design of a chimney might require the simulation of different design

configurations and different use scenarios in order to optimize the final design. Thus, some simulations must be executed in short periods of time, and there could be fairly long periods in which no simulations tasks are required. HPC cloud offers fast response and the required number of resources for each case.

The Fortissimo infrastructure together with the development of the WP505 experiment will allow DINAK to improve chimney design and gain comprehension and insight for each case. The Fortissimo infrastructure provides the best possible technological solution available to satisfy DINAK specific needs today. This refers not only to the highly scalable computing resources it provides, but also to the knowledgeable human capital accrued by the application and HPC experts available to us whenever needed.

With the simulation model developed in the experiment, DINAK shall be able to conduct analysis sufficient to optimize the design of the concentric chimneys and adapt it for each operation conditions.

2.5.3 Impact and Business Benefits

A key benefit of using the Fortissimo HPC Cloud will be the reduction of costs and time in chimney design. The frontend application allows DINAK to accelerate the global design process of concentric chimneys and optimize the design adapted to the operation conditions in each case. Having a faster design of each product will allow DINAK to enter into every new emerging market in its starting point, a very important aspect to increase its competitiveness. Experience in chimney systems shows that being the first solution to a new problem class can lead to an extra 5-10% market capture. Currently, DINAK develops around 3-4 new products per year and this advantage would increase their turnover by approximately €100,000.

Before this experiment, DINAK required approximately a month of work for the design and testing processes of a new chimney. Every new product implied the work of 3 specialized engineers and 2 factory workers to decide the different options, design prototypes, manufacture them and test complete chimneys to verify the initial hypotheses. With a reliable simulation application DINAK can reduce the whole process down to one week (depending on the case). The use of the simulation can be handled by only one engineer and will allow DINAK to avoid the use of prototypes and trial phases and to save both time and personnel. This fact will realise a saving of €50,000 per year.

Additionally, the fact of having a more accurate knowledge of the designed product, will allow DINAK to pass the CE Mark tests with a lower possibility of failure. Every repeated test (in average 1-2 a year), generates an additional cost for DINAK of €5,000-€7,000.

Finally, DINAK will be able to offer a consulting/simulation service to their customers which is not available to date.

Other benefits that DINAK will achieve from its participation in this experiment are:

- An improvement in the company's knowledge of CFD calculation.
- Turn a "based-on experience" activity into a "knowledge-based activity".
- To further improve and optimize tools and procedures in chimneys manufacturing.
- Improve the performance of exhaust systems already installed.
- New scientific and technical knowledge about a key business activity.
- A new tool with an easy interface that will help to improve the design activity.

- To gain access to computing technologies, reduce the "learning curve" and improve the technical background of the company engineers.
- To sound out new business lines: Offer services based on Finite Element Method (FEM) and HPC to third parties.
- To grow and stress differentiating factors to set the company apart from competitors.
- To collaborate with other organisations, not involved in our line of business, but important to improve our knowledge.

2.6 HPGA – High Performance Gear Analyzer

2.6.1 Motivation

The gearbox market in Europe earned revenues of €2,928.1 million in 2010. The market will reach €3,721.15 million in 2017. In Italy a large number of gear manufacturers is present, both Large Enterprises (LEs) and SMEs operate on the field of gear production, gear design and gearboxes.

The HPGA experiment aims to furnish a new technology for supporting the design of reliable and efficient gears without the need of big investments in terms of: computational resources, expensive software licenses, long and expensive trainings. In our vision, HPGA will provide new innovation opportunities and service for European gear manufacturers.

The HPGA is developed starting from the needs of a modern gear designer, who is generally an expert on gears and traditional design tools (based on standards and codes, simple tables or database implemented on spread-sheets or commercial software, and CAD software); this kind of designers generally has basic knowledge about software for structural analysis and only scarce knowledge of specialized applications.

The past experience of UNIMORE in developing new computational tools for gear analysis and optimization has shown the limitations of the implementation on personal computers and workstations; the need for a great increase of the computational capabilities was clear in order to obtain a computational tool able to satisfy the needs of the designer in a reasonable time.

The end user VE&D has a long time cooperation with UNIMORE, in particular in the field of mechanical transmissions. Therefore, when the HPGA project was conceived VE&D was identified immediately as an ideal partner. Indeed, VE&D has been working in the field of automotive engineering since 50 years furnishing services and technologies to its industrial partners and cooperating with the University for the development of new technologies. Their point of view was extremely important in drawing the guidelines for HPGA, and their role in the exploitation of HPGA will also be of primary importance.

UNIMORE and CINECA are strategic partners in different kinds of research projects; starting from several successful collaborations, the idea of developing HPGA was first discussed with CINECA which analysed the feasibility of the HPGA implementation on their HPC facilities and its effectiveness in terms of computational efficiency.

2.6.2 Relevance to Fortissimo

The development of HPGA draws on more than ten years of research in the field of gear transmissions. The research group of UNIMORE developed its research in close cooperation with several industrial partners. Based on this experience UNIMORE developed several computational tools for gear analysis and optimization. Recently the further development was impacted by the insufficient computational power of standard Workstations, which limited further developments. It was clear that only HPC Cloud technologies would be able to make our software available for any design engineer with good performance.

Starting from the previous premise, the HPGA experiment has implemented a software developed in MATLAB language on the CINECA HPC facilities. The software appears with a simple interface where the final user finds all standard input data of gears datasheets; in addition some popup menus are devoted to specific operations: create the geometry and

check data coherence; create the model and perform analyses or optimizations; present results in a standard way acceptable for the world of gearing.

Typically, SME gear manufacturer are lacking skills and resources to develop complex models, to buy expensive software licenses to perform large-scale computations and hire highly skilled people having experience in stress analysis and gear design. The potential impact of the HPC Cloud based High Performance Gear Analyzer (HPGA) will allow SMEs to reap the benefits of the most advanced methods for gear analysis.

2.6.3 Impact and Business Benefits

The number of users for HPGA is potentially huge as shown by the dimensions of the global market of gearboxes. On the other hand, we are perfectly aware about the difficulties of introducing new design tools in this specific industrial sector that is characterized by a large use of standards and codes and a certain traditionalism in the design activities. This is nowadays mitigated by the extreme need for increasing competitiveness due to the presence of new manufacturers from emerging countries. There is a clear need for improving the efficiency of products in order to compete on the ground of innovation instead of price.

In this context HPGA can play a role, since it offers a new way for applying and using sophisticated design methods without the need for big investments; this can be appealing for SMEs but also for LEs. The HPC Cloud characteristics of HPGA seem to fit with the typical needs of SMEs manufacturers, engineering companies and design divisions of LEs. No need for expensive software licenses, no need to own complex computing infrastructures, no need for long training for engineers: these are the keywords of HPGA.

Based on the previous considerations and from a good knowledge of the potential users requirements, we forecast a slow but constant ramp-up in the use of the HPGA software during the next five years. As a SME engineering company VE&D predicts a 15% improvement of their costs thanks to HPGA, this would represent a good success for a highly skilled and efficient company.

UNIMORE forecasts an initial increase of its turnover regarding gear activities (industrial projects and service) of 100% for the first year, starting for the actual small turnover of about €20,000, with a possible slow transition that could reach €100,000 in five years.

These forecasts are supported by the direct feedback from industrial partners who attended the “The Gear Day” event organized in Modena by UNIMORE (Gear Day at UNIMORE website) with about 100 participants from more than 40 gear industries. Both LE and SME manifested great interest for the HPGA technology.

2.7 HPC-Welding ff

2.7.1 Motivation

Much of the parts integrated in automobiles and machine tools are welded components. The mechanical requirements on machine elements are in continuous increase. Welded components suffer high temperature loads in the manufacturing process. Internal tensions and weak points in this components result as consequence of this temperature load. The requirements to the simulation currently are oriented to consider these manufacturing flaws in the evaluation to the component durability.

In questions concerning a concrete welding process, whether for the production of a new component or for the optimization of an existing part, there is hardly an alternative to welding tests. However, those trials are costly and time-intensive. In order to check the quality of the weld seam, the specimens have to be cut, polished and sanded to get microsections. In addition, the work piece is destroyed by the findings. The costs are difficult to estimate a priori, thus long response times are inevitable.

CAE analyses of welds seams and weld processes could dramatically reduce those response times. A simulation shows new approaches and helps to optimize all relevant parameters. Expensive prototypes can be avoided. In addition, the two most important parameters are obtained, the welding seam depth and heat propagation in the tool during the welding process. By using only welding samples, these values can only be determined afterwards and by time-consuming findings. To analyse a weld seam by using CAE simulation takes only a few hours. However, this fails as there are hardly any suitable simulation methods validated by welding tests.

The aim of this Fortissimo experiment was to develop such a reproducible, independent simulation methodology to predict results of welding processes.

2.7.2 Relevance to Fortissimo

Each CAE simulation requires computing power. With the size of a model, i.e. discretization and the number of degrees of freedom, the demand for computing power increases exponentially. If other factors such as non-linear material behaviour or transient conditions are added, conventional analyses on standard computing clusters are no longer possible. The response times would be much too long, the time advantage against welding attempts void. An SME, however, can hardly afford a supercomputing cluster, as a HPC centre does. The costs of acquisition and maintenance exceed the annual turnover by far.

Thanks to Fortissimo, SME get access to such HPC Clouds. With their supercomputing power highly complex CAE simulations, such as welding processes, can be analysed and improved using computer-aided engineering. This significantly reduces costs and response times as no expensive trials are necessary. In addition, CAE analyses can help to avoid negative side effects, such as excessive heat input or excessive welding penetration depth. For end users, this means, in addition to the cost saving of the unnecessary welding samples, the service life of the products can be prolonged and failures can be avoided if a better weld quality can be found by simulation.

The major achievement for L&W is the experience in the application of HPC. The access to HPC opens for L&W the possibility to perform projects that in the past were not possible

because an excessive computing time. The advantageous use of the HPC requires however higher investments in Software-Licenses in order to be able to perform calculations with a higher level of parallelization (amount of CPU's that the software license allow).

Another great success of Fortissimo is the merging of the partners in this experiment, which certainly does not end with this report. In the future, LBO and L&W together with the HPC experts of the HLRS will be cooperating to provide their customers a consulting service for all welding issues. That will reduce development costs for products significantly due to the fact, that a lot of prototypes with long lead times can be omitted.

2.7.3 Impact and Business Benefits

The new found simulation method enables LBO to serve its customers much faster and more cost-effectively for inquiries regarding the laser welding of components. The customer is saving by avoiding expensive prototypes and extensive welding tests. Reliable statements on safety or feasibility can be made very quickly; the risk of failures in the weld seam is assessable. LBO is able to advise its customers and potential new ones competently through the gained knowledge about the welding processes and their parameters. This applies both for the improvement of existing products and the evaluation of an optimal welding process for new components in advance.

L&W has developed a methodology to simulate the laser welding process by the Finite Element Method gaining a lot of know-how regarding the energy input into metallic materials. This new simulation method broadens its product portfolio. L&W will also be able to address and serve new customers, who have also specialized in welding processes of all kinds. With only two to three new customer projects, the company's revenue can be increased by 5% to 10%. In addition, a powerful partnership has been established with HLRS, which supports complex and time-intensive CAE analyses. This is not limited to simulations to welding processes, but rather to any CAE analysis. In future it could be profitable to give up cost-intensive in-house clusters and to use HPC clouds only for all simulations. The principle of "pay-on-demand" means huge cost saving potentials.

2.8 Drug Target Binding Simulations

2.8.1 Motivation

The journey for a drug from invention to market is a long one. It has been estimated that the time required to develop a new drug de novo ranges between 10 and 17 years that is, if it ever makes it. The chance for a new drug to actually make it to market is only 1:5,000. These slim chances are accompanied by a high cost for developing a new drug -which may reach an average of US$ 403 million per new drug. As these spiralling costs threaten to make the development of new drugs increasingly unaffordable for both companies and consumers, it is clear that efforts should be made to address this problem.

Repositioning existing drugs for new indications (i.e., new diseases) could deliver the productivity increases that the industry needs. A prerequisite for drug repurposing is drug promiscuity (polypharmacology) –a drug's ability to bind to several targets. . Research indicates that there is a correlation between promiscuity and structural similarity as well as binding site similarity of protein targets.

In this experiment, we employed a pipeline of algorithms for measuring structural similarity between proteins and consequently infer drug off-target interactions (side-effects) and identify potential therapeutic features of existing drugs.

The pipeline identifies the correlation between drug promiscuity and structural similarity of binding areas to different protein targets. More specifically, promiscuity in medicine is defined as the ability of a compound to bind to multiple targets and elicit polypharmacological effects.

Binding of the same compound, which has a specific structure, to different targets requires that these target share similarities in structure too. Even if these similarities do not apply to the whole macromolecule structure, it is highly probable that the sites where drugs usually bind (ligands and pockets formed in the molecule structure) are very similar. Of course, the process of finding structural similarities among parts of composite three-dimensional structures is complex and tedious. It is usually performed pairwise (query and target) and first requires an alignment of the compared structures. The alignment is either global, based on the protein backbone, or local focusing on a specific sub-structure of interest (e.g. a protein chain or a ligand) and results in a 3D transformation that must be applied to the query compound (usually protein) in order to match the target compound (usually another protein).

Based on the transformation information, a pair of proteins is aligned and consequently all the respective parts, which are potential binding sites for drugs are examined.

To give a more practical example, let's think of all proteins that are related to malaria. These proteins are known drug targets of malaria and can be retrieved from related biomedical resources such as DrugBank . If we are able to compare all these malaria related proteins with all other proteins in Protein Data Bank then it will be possible to build a database with proteins that have very similar binding sites to malaria related proteins. If any of these proteins is targeted by another known drug compound (not known to treat malaria) then this drug can be added to the list of candidates that treat malaria. In the opposite, the malaria drugs that target the specific proteins will also be good candidates for treating other diseases. As of January 2016 PDB contained more than 115,000 biological micro-molecular structure making the aforementioned computation task really big and resource demanding.

We employed the case of malaria as a test case and relevant drug compounds and proteins. To give a more concrete example in the malaria case, we performed a smaller scale evaluation on the EPCC infrastructure. We have chosen only 10 malaria related proteins (out of a few thousand retrieved from DrugBank database, which are related to known malaria compounds) and queried them over a small sample of Protein Data Bank comprising 800 proteins out of the 115,000 macromolecules currently recorded in PDB. Even for this small portion of computation (800x10 protein pairs) the total CPU time was 1900 CPUh, which corresponds to an average of 0.25CPUh per protein pair.

Within this experiment, we leveraged on the HPC Cloud infrastructure offered by EPCC, in order to improve computation time, which may scale up to 115,000x3,000x0.25 hours of using a single core of the HPC infrastructure for a single evaluation of a systematic study of drug promiscuity. The cost for this computational effort of 86.25 $x10^6$ CPUh is about 2.5M euros. At the same time we adopted a more financially viable computational approach leveraging on cloud properties and taking full advantage of CPU time considering also the memory requirements of the jobs that are executed in parallel in the same HPC node.

Compared to the theoretical upper bound that defines the time needed to execute our small experiment on a single core processor (1900 hours) it can be significantly improved when more processing cores are used in parallel. A simple parallelization that assigns each task as a whole to a single core and the existence of an unlimited number of cores (or at least 8000) is expected to minimize the total execution time to that of the slowest pair. However, due to a large imbalance to the size of the examined macromolecules the execution time may exceed 5 or 6 hours, may require a large amount of memory to complete the various tasks (alignment, maximum common subgraph detection, similarity computation etc.) for specific protein pairs and may lead to unsolvable bottleneck and underusage of the available resources. When the number of processing cores increases it becomes crucial to split the processing pipelines to smaller individual tasks that are distributed across nodes and are interleaved in order to take advantage of the available processing power. In the same time, memory management must be performed in order to optimize memory usage, without falling into virtual memory, or having starvation (due to insufficient memory in a node) of a process over competing processes in the same node.

It is interesting that in our experiment with the 10x800 protein combinations we achieved a 77% usage of the processing cores in the case of 64 cores, whereas this ratio dropped to 50% when 512 cores are employed.

It is anticipated that such improvements would boost the competitive advantage of SMEs, which can perform these analyses on behalf of pharmas that wish to reduce the cost of wet lab tests, whilst finding new targets for their compounds, thus receiving a share from the market of drug development and patenting.

2.8.2 Relevance to Fortissimo

The execution of the application on an HPC Cloud infrastructure presented an excellent opportunity to employ more sophisticated algorithms that allowed us to improve performance and subsequently reduce the cost. This was achieved through parallelization of the individual tasks of the pipeline and by employing certain structural properties of the models, the computation of which allowed us to swiftly eliminate large numbers of upcoming computations. A simple parallelization that does not take advantage of the ability to interleave tasks and maximize resources usage, and does not early prioritizes and balances

slow jobs to the available processors, manages to create long queues of slow jobs in one processor and large idle periods in others. In the experiments we performed, using 64 cores it took more than 90 hours to finish a 1900CPUh job, which corresponds to 33% usage of the allocated processing cores, By leveraging on the elasticity property of the HPC cloud services and intelligently shifting resources to the more complex computations, we achieved an improved performance and a control over the computation time, which ranges between 50 and 77% usage of the allocated processing cores (ranging from 512 to 64 respectively), thus allowing a more accurate estimation of the expected cost for resources.

2.8.3 Impact and Business Benefits

Generally we see many fields of applications of the technology developed in Fortissimo in slightly adopted forms:

- Gene and protein matching (based on www.projects.biotec.tu-dresden.de/gogene/gogene/)
- Orphan drug development, for rare diseases.
- General text-mining on biomedical documents relating diseases and treatments (based on www.GoPubMed.com)
- Endpoint search in alternatives for animal trials (based on www.Go3R.org)
- Gravity and magnetics modelling (based on www.potentialGS.com)
- Particle tracking (based on www.kalaimoscope .com)

We estimate that 80% of necessary technology is developed for points 3 to 6 (100% for points 1 and 2) both from this experiment but also from code that we have developed for other projects and the technological background acquired through this experiment. So rather little effort is necessary in order to provide interesting product extensions to the whole range of our product portfolio.

Our application areas address life sciences, health care, and drug discovery more specifically. Healthcare is a sizable industry for Europe, with estimates of upwards of 700K people employed in the European pharmaceutical sector (http://www.efpia.eu/facts-figures) with 3 or 4 times more related jobs as a result of pharma investment and related investment of upwards of 30 billion Euros in the EC (http://www.efpia.eu/facts-figures). Our ability to contribute to this sector in terms of providing reliable services, training skilled personnel emerging from this project with experience, will all contribute to the aim of high quality and efficient healthcare services.

Recent trends in drug development indicate that the value of orphan drug development is a niche business strategy for many pharma companies. Profit margins for orphan drugs are higher than blockbuster drugs due to a small patient pool resulting in smaller clinical trials and a higher price point support for orphan drugs.

The current rate of drug repurposing activity raises the expectation that a substantial percentage of rare diseases if not all 8000 rare diseases might be treatable with drugs in the current pharmacopeia (Muthyala, 2012). As new targets are discovered due to human genetics program, the repurposed chemical entities could serve as sources for screening new indications.

Based on the service that we developed in this experiment, companies will be able to run in silico experiments before reaching their wet labs. They will be able to evaluate the potential of high promiscuity drugs to bind to proteins related to the rare disease, to create their own proprietary compounds and test them against the genes of interest. The effective applications

of repurposing technologies should enable major companies significantly enhance their development pipelines, especially for rare diseases caused by single gene mutations. Therefore, the repurposing of drugs and drug-like molecules should be anticipated to have a promising future.

2.9 Experimentation of VIrtual Metrology HPC Simulation Services for SME Production Process Control in Sustainable and Competitive CAmshaft Manufacturing (VIC4CAM)

2.9.1 Motivation

Dimensional quality control has become a critical task within the manufacturing chain, representing added value and a proof of competitiveness for the manufacturers. So, these companies are investing in new equipment and solutions to reduce the impact of these systems in the manufacturing process and, at the same time, extract as much information as possible in order to detect and prevent defects and deviations involving direct and brand costs.

In this framework, the integration and exploitation of 3D optical scanning systems for dimensional quality control in manufacturing industry generates significant benefits in terms of time consuming and information generated compared to the traditional tactile technologies. However, the usage of these systems is also emerging technical problems when dealing with the huge amount of data acquired in terms of processing, analytics and storage. For instance, a typical size of the files involved in the experiment is around 300 MB, representing 15 million of points. This means a single company generates several Terabytes of information in short periods of time (30-50 factor may be applied for a service provider like UNIMETRIK). For that reason, metrology software developers like DATAPIXEL have also to work on the optimization of the processing algorithms enabling quicker access to the information contained in the pointclouds (3D digital version of the physical part formed by collected data from the object surface).

The objective of this Case Study is to develop a data processing service which enables manufacturing companies, particularly SMEs, to control manufacturing processes to a very high level of accuracy. This requires intelligent, fast and intensive analysis of the manufacturing quality using 3D digital information of the parts to be manufactured. The combination of scanning, measurement and analysis system enables the early identification of deviation from the design parameters in the manufacturing process and of the necessary corrective measures to be taken.

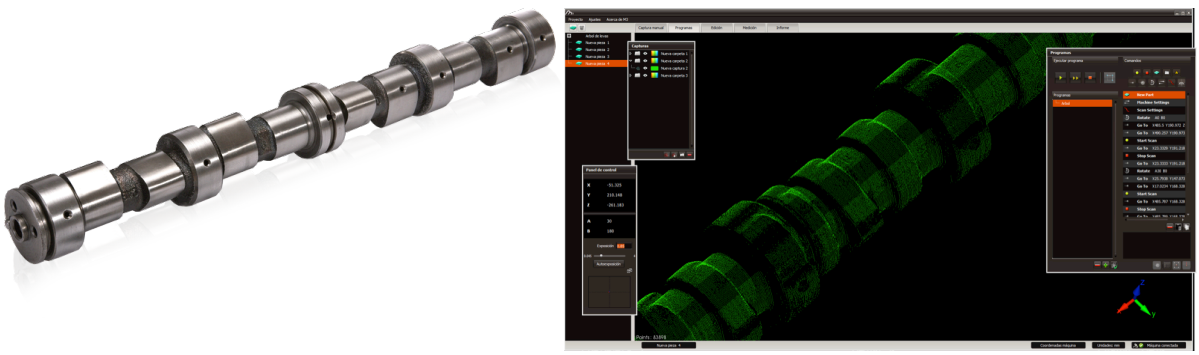

Figure 1: Physical part and pointcloud after scanning for advance processing and analysis in dimensional quality control

To implement such a framework, the proposed service involves the processing of very large data files comprising Terabytes of data which requires the use of cloud-based HPC. This Case Study has developed the necessary functionality to provide an HPC-based simulation service for the detection of defects and deviations and the generation of new functionalities such as reverse engineering, which represent the most computing consuming process. This experiment has worked on the production of a camshaft (critical component of high power engines), where the generation of the 3D model from the acquired pointcloud has been optimised.

2.9.2 Relevance to Fortissimo

VIC4CAM proposed an experiment of Virtual Metrology HPC simulation service evolving the M3 (multi-sensor massive measurement) platform and capitalising on in-line 3D scanning information acquisition systems to support manufacturing SMEs in (a) performing 100% control of produced parts (b) mastering production processes by intelligent, fast and massive analysis services of 3D digital part information; thereby supporting early identification of deviation sources from the expected production behaviour. VIC4CAM targets a highly demanding market segment with strict manufacturing tolerances, i.e. cylindrical parts and camshaft production, to establish a solid pillar that facilitates a fast and smooth adoption of the VIC4CAM HPC simulation services by other clients and market segments in the automotive and aeronautic sectors.

As mentioned before, the integration of 3D optical systems for the digitalization of the dimensional quality control has increased exponentially the amount of data available. So, now the manufacturing companies and services providers have to deal with new problems related to data processing and analytics.

Figure 2: 3D dimensional quality control equipment used for camshaft digitalization

By the exploitation of HPC resources, these companies, mainly SMEs, are able to exploit all the capabilities of the optical systems and extract all the potential information contained in the pointclouds. In this way, new analysis such as massive geometry extraction and temporal analysis of the dimensional quality of large batches are now possible. Moreover, traditional tasks such as reverse engineering are now optimized enabling the generation of outputs much faster.

The improvements generated by the use of HPC Cloud have affected to all the manufacturing value chain: domain expert and service provider (UNIMETRIK), ISV (DATAPIXEL) and end user (EPC).

2.9.3 Impact and Business Benefits

Depending on the role and activity of each partner in VIC4CAM experiment, the business benefits related to develop high-tech products and services based on HPC technologies are different:

- UNIMETRIK as Domain Expert will increase its services for manufacturing companies with large parts through the generation of new remote services for intensive dimensional measurements. This service delivery is expected to have an impact in the incomes of €450,000 in five years frame and new job positions.

- DATAPIXEL as ISV will be able to implement new capabilities in M3 SW platform (e.g. 4D Visualization tool) and enable the metrology SW integration with HPC services, especially by Data structuring process. In terms of economic benefits, the commercialization of the M3-HPC module will have an impact of €750,000 over the next 5 years period.

- EPC as end-user, will improve the quality of its products to reach 0% defective part delivery. This will allow generating vast knowledge for both camshaft new and re-design as well as machinery engineering and maintenance. All these developments will enable

the company to achieve the zero defects delivery, saving €1,500,000 to the company during the next five years.

- CESGA will be able to offer new services in manufacturing domain. In particular, it will exploit HPC applications in virtual metrology field.

2.10 HighSea - High Performance Virtual Sea Experiment

2.10.1 Motivation

The maritime sector has a long tradition of designing boats. Boat design is often based on experience, assumptions and know-how. The boat architect is often seen as an artist, an inventor, and, finally, an engineer. Feedback from captains and boat-owners is usually anecdotal, without real data as the foundation for engineering decisions. Boats have sensors, but, usually, the resulting data are neither collected nor transmitted to the boat manufacturer.

Simulation, in this sector, is still seen as difficult/time-consuming and usually only used extensively for the design of racing boats or for large firms. With limited data to define the scenario, the setup of a simulation is often difficult requiring the development of an appropriate simulation model. Furthermore, the computational power required for such simulations is often beyond the capabilities of the SMEs who design and manufacture boats. For designers, the process of gathering feedback from simulations is still considered too long and expensive to be really helpful within the design process. HighSea has addressed this by an integrated approach where both data from usage, data from prototypes tests and from simulations are used to design hulls and structures.

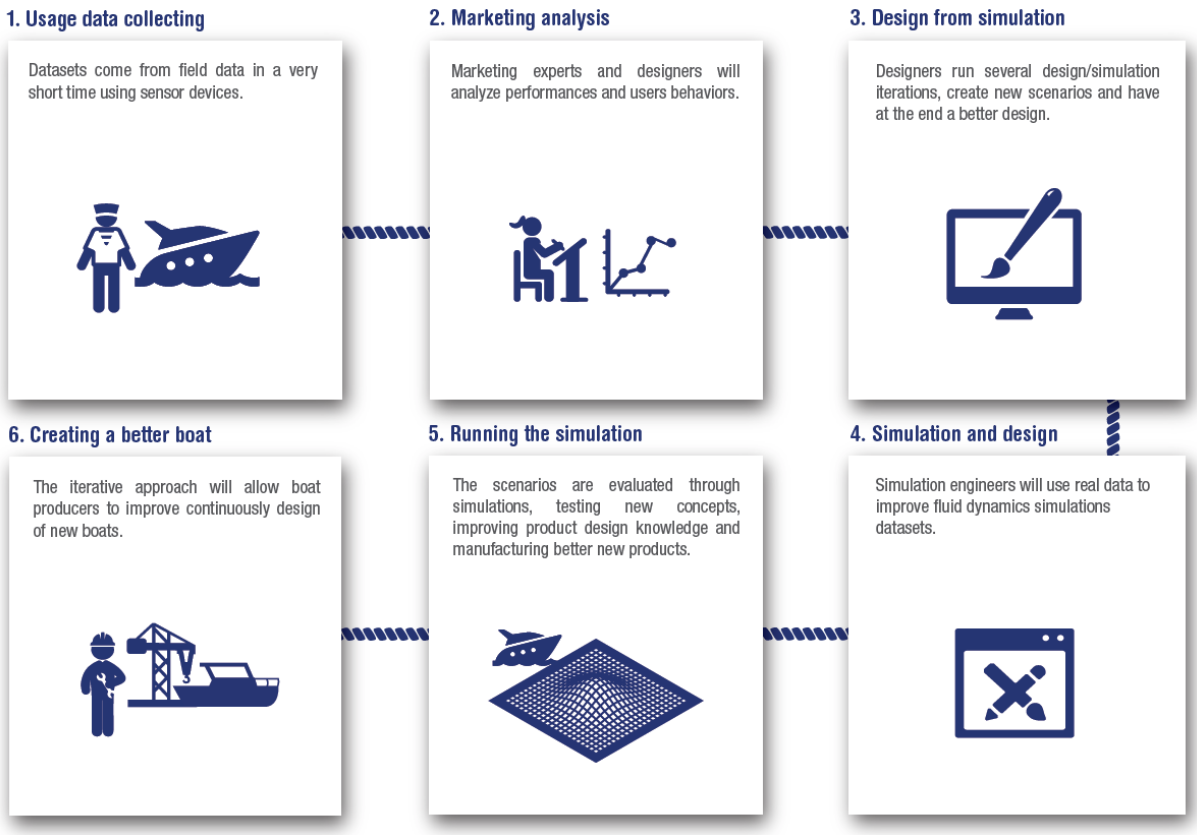

Figure 1 The information value chain for HighSea

The HighSea consortium's industrial is Hydrolift which is a Norwegian boat designer and manufacturer. For Hydrolift, the Highsea's simulation of flow around a boat hull under different sea conditions and of the behaviour of structures such as the captain's chair is very important in order to improve their products. HighSea has analysed both real sea and

customer usage data. For Hydrolift the use of Cloud-based-HPC to speed up fluid and structural simulations in the design of boats and provide a boat-design service has also been an important aspect of the project where the aim has been how to give boat manufacturers a competitive advantage through shorter development times and improved boat design.

The aim for Hydrolift through this experiment has been to use 15% less resources on tests and prototypes for new boat models. Further, by the automatic data gathering and transfer capabilities implemented in HighSeas, the aim has been 30% time saving into the test processes of new models.

2.10.2 Relevance to Fortissimo

The Fortissimo HPC offering has enabled the HighSea Experiment consortium to provide a cost effective and efficient solution to support the design of new boat models based on real usage data and hydrodynamic simulations.

Both the introduction to HPC technology as well as the extensive employment of hydrodynamic simulations are hindered by implementation barriers in terms of costs and effort that prevent most SMEs from fully tapping the potential of these technologies. The Fortissimo offering helped the boat designer Hydrolift by creating the opportunity to use CINECA HPC facilities in the design of a boat supported by the domain expertise of Inventas, Holonix, BIBA and SINTEF and bringing together computing resources and appropriate simulation software. This combination of domain expertise, HPC resources and software will enable the consortium to provide a cloud-based boat-design service to small boat designers and producers.

Utilisation of simulation implies a reduction of prototype tests – saving in time, materials and tests. Even though a prototype will still be built, the repetitive and time and costs consuming modification can be eradicated. From this a cut of 30% of the changes depending on the boat's complexity can be expected.

2.10.3 Impact and Business Benefits

The Fortissimo HighSea Experiment has delivered many important results. However, the industrial objectives were of course not achieved during the short lifespan of the experiment. But, the findings and experiences gained in the project is thought to enable the sought-after industrial reductions in resource-usage on new models.

ISV results

The ISVs in the Fortissimo HighSea Experiment have used the experiment to enhance their products and increase the sustainability of their business models. The iLike-Designer and the Universal Marine Gateway have significantly improved their TRL and are creating new business opportunities for the respective owners individually as well as mutually.

Application Expert results

The Fortissimo HighSea Experiment application experts have increased their experience both in the maritime industry and in the implementation and utilisation of HPC technology thus strengthening their business models.

What is expected when the Fortissimo marketplace is launched are a 15% time saving for simulation setup and 20% time saving for computation. It is also believed that the know how

developed within the Fortissimo HighSea experiment has shown that one can achieve overall faster process due to well established processes and availability of real data. This business effect is estimated to have an effect of €12,000 in total for each new project and it is foreseen that the experience build-up from new model to new model will add additional effects. It is also expected that the availability of data and a defined process helps to reduce the overall time to market in the range of 20% less time.

End User results

For the end users of the Fortissimo HighSea Experiment the design for the "right quality" i.e. reduction of over-quality will result in a reduction of 10% of the costs (monetary value of course dependant on the boat size) for each boat. The Hydrolift boats are in the extreme segment and so annual production is not high, however, for other boat manufacturers with a high-volume production this will yield significantly to the bottom-line and competitiveness. E.g. a medium-large shipyard producing 300 small boats, with a turnover of €15-20,000,000; will with a saving of €3,000 - €5,000. per boat mean €900,000 total saving.

The HighSea results for end users is also believed to improve brand perception as what is designed is what the boaters really need since the design is based on facts. Due to the short time span of the experiment it is at the end of HighSea estimated to result in 5% more sales. On a general basis, boat manufacturers get part of their overall turnover from selling boats and the rest from maintenance and possibly reselling boats that they have taken on from customers buying a new boat. As such, the expected increase in overall turnover should therefore be seen in this light. E.g. with a 50/50 ratio between selling new boats and other activities, a 2.5% turnover increase can be expected.

2.11 TSEC - The Seismic Experiment Cloud

2.11.1 Motivation

New geological insights, new technologies and better seismic imaging methods have led to a strong increase in oil and gas exploration in the North Sea and around the world.

The numerical methods to reconstruct the subsurface structure from acoustic measurements play an ever increasing role in the detection and surveillance of oil and gas reservoirs. This is mainly driven by the increasing performance of HPC hardware, which makes it feasible to use new numerical methods. After weeks of computing time on HPC systems these seismic imaging methods lead typically to a 4D result that describes the seismic reflectivity and reveals the subsurface structure and their physical properties.

The 4D results are called “pre-stack” since they are in a subsequent process summed up (stacked) to become the 3D image of the subsurface. In a subsequent process interpreters look at the data to identify possible prospects and calculate the risk of drilling wells. Following the first exploration wells the rock properties are identified by an interpreter whose work is usually done on workstations using the 3D stacked data sets. In most cases this is an iterative process – since the data shows inconsistencies and, for example, the sound-velocity field needs to be improved.

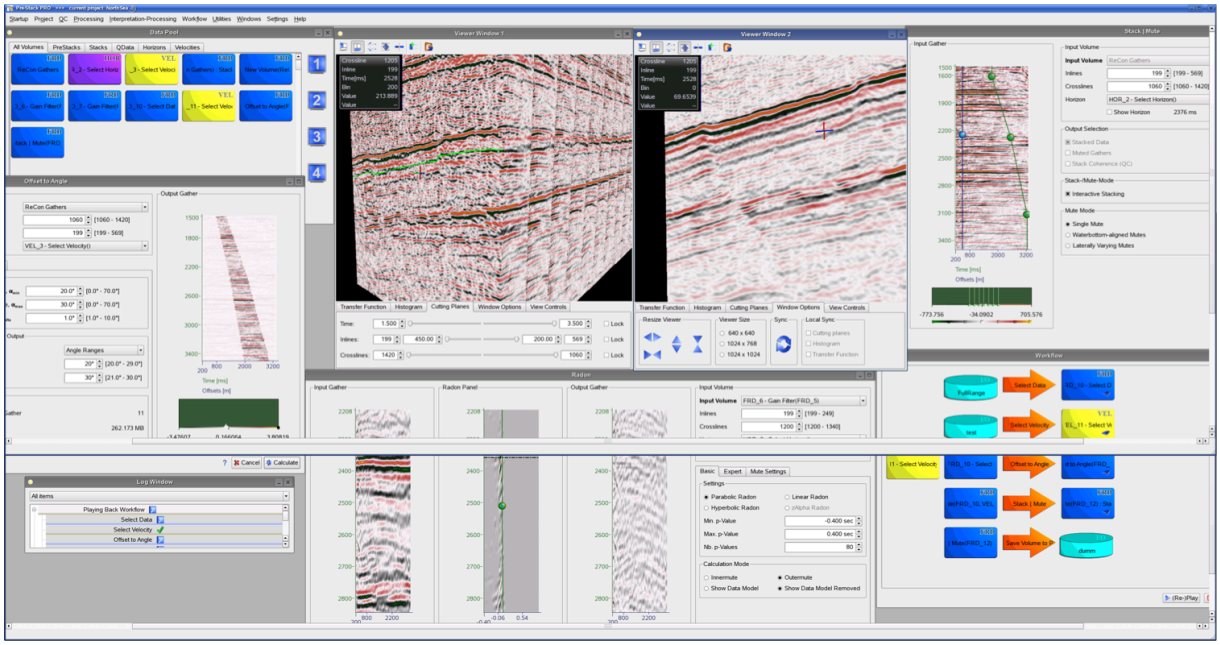

Fig. 1 Interactive 3D visualization with Pre-Stack PRO

Pre-StackPRO is a software system that links the 3D stacked results to the pre-stack results and offers numerical methods like coherence enhancing diffusion filters or demultiple algorithms that remove ghost effects from the data. The software gives the interpreter a chance to look at the pre-stack data sets and generates optimized stacks. Seismic imaging is an ill posed inverse numerical problem. Pre-StackPRO provides a link between interpretation and processing, offers a new way to improve the results, gets a better geological picture and reduces the risks of drilling.

One of the main advantages of Pre-StackPRO is its core architecture, which is based of the Global address space Programming Interface (GPI-2) [2]. GPI-2 has proven many times to

work with extreme scale applications and up to 4096 processing nodes[3]. Fig. 2 shows a benchmark of different Pre-StackPRO workflows tested on extreme factory by Bull on up to 16 computing nodes. It shows very good scalability for the Radon filter and the 2 and 3 dimensional Parallel Edge- and Coherence-Enhancing Anisotropic Diffusion Filter (Parallel ECED) that are two algorithm offered by Pre-StackPRO and part of the denoising workflow. One can see from the Partial Stacks workflow, that the I/O intense algorithm is limited by the bandwidth of the parallel filesystem.

Workflows like these are used in an interactive fashion to increase the quality of the subsurface images. Therefore, the reduction in time to solution will speed up production works significantly.

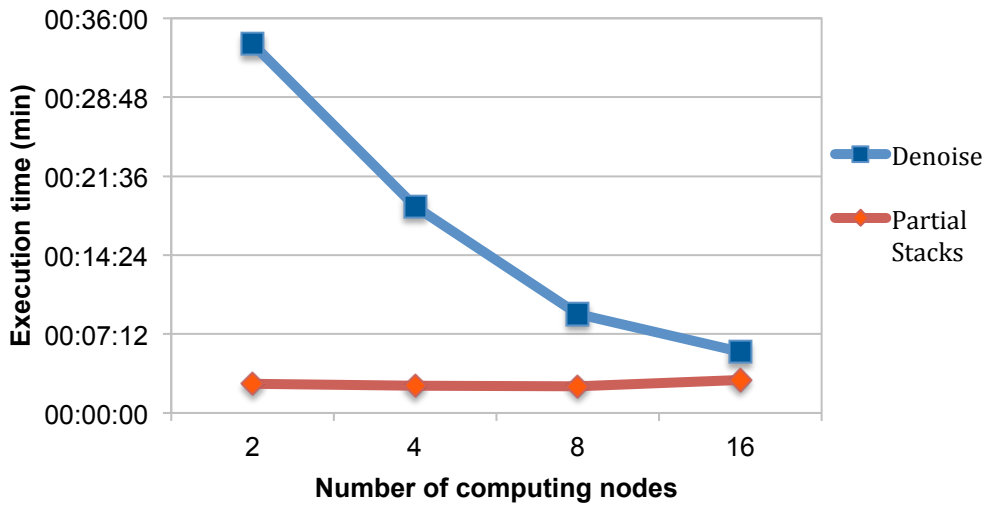

Fig. 2 Execution time for denoising and partial stacks workflow on extreme factory by Bull

2.11.2 Relevance to Fortissimo

The bigger European companies such as Total, BP, Shell, ENI, Repsol and Statoil usually maintain their own large computing centres. However, there are a lot of small and medium size companies and many small service companies in all European countries working in this field. Such SMEs typically do not have the financial capability to run and maintain their own HPC cluster.

Pre-StackPRO is currently the only software on this market that scales across many nodes and combines interactive visualization with parallel processing. The use of Pre-StackPRO in the Fortissimo HPC Cloud enables SMEs to leverage the performance potential of Pre-StackPRO on leading HPC hardware without the requirement to invest in their own hardware.

A pay-per-use hourly or monthly based hardware and software billing model of cloud based computing is ideal for cost accounting in highly volatile workloads and enables cooperative works in consulting projects as well as easy demonstrations in remote locations.

TSEC provides to Fortissimo a complete HPC offer that is available to Oil&Gas European SMEs. This enables Fortissimo access to new markets and hence increasing their economic benefits in Europe.

2.11.3 Impact and Business Benefits

The experiment adapted the underlying architecture of Pre-StackPRO to be able to run on HPC cloud environments. Further it identified and disseminated the available data staging processes for large seismic data sets to and from the datacentres and their security concepts. Both are essential to integrate an HPC cloud solution into a production workflow.

This way the ISV Sharp Reflections GmbH is now able to expand their business model and offer Pre-StackPRO as HPC cloud product to more SMEs. With the results of this experiment the ISV, together with the datacentres, are also able to offer consulting regarding the whole seismic workflow. In a conservative business model Pre-StackPRO as Software-as-a-Service (SaaS) will contribute with about €1,000,000 equivalent to 10% of total revenues in 2017, increasing to €4,000,000 in 2022. Sharp Reflections is also preparing for a scenario where 50%, or more, of future revenues comes from SaaS. Bull, as a HPC centre involved in this experiment benefits now of access to a range of customers in the Oil&Gas sector that was previously unaddressed by its extreme factory HPC offer. Expected revenues are between €200,000 in 2017 and €800,000 in 2022.

Most of the leading software vendors in the post-stack market offer pure workstation based solutions and the post-processing of the pre-stack data is done in separate batch oriented software packages. The necessary hardware increases the costs and therefore risks for SMEs, which are very sensitive to spending especially in times of low oil prices. Hence, this cloud solution of Pre-StackPRO offers SMEs, all-round the world, to benefit from the advanced capabilities of Pre-StackPRO on HPC hardware. This way the full scalability of Pre-StackPRO can be leveraged at low risk and full cost control. End-users SIP and Sharp Reflections AS can now process larger seismic projects they couldn't before because of financial restrictions regarding the costs of on-premises hardware. This results directly in faster processing times, real-time 3D visualization and processing of large seismic datasets and therefore higher quality images and a shorter time to solution. An analysis shows that depending on the number and size of seismic projects the potential saving for SMEs by using the Bull cloud infrastructure compared to on-premises hardware is about €20,000-€30,000 per year. This may lead directly to more competitive pricing.

SMEs further profit from frequent hardware updates at the datacentres and the location within the European Union that guarantees the strict European data regulations standards, which are highly important for security sensitive domains such as the Oil&Gas industry.

This way SMEs can expand their business models and integrate the Pre-StackPRO cloud solution into their production workflow – e.g. collaboration with customers, demoing on conventions and trainings etc.

2.12 Cloud-based simulation of pipeline components for the Oil and Gas Industry

Fortissimo experiment 512 is concerned with the provision of a cloud-based technical solution to enable in-depth CFD simulations to be used within the context of oil & gas industry. In particular, two representative pipeline component simulations were performed. DRG, an SME that provides engineering consulting services to leading oil & gas customers globally, relies on ENGYS's software solutions for its CFD needs. This experiment focused on enhancing ENGYS's flagship HELYX CFD software (an enterprise-class open-source based CFD software package for general purpose applications) to incorporate a client-server module that allows cloud-based simulations to be run interactively and seamlessly on remote HPC systems.

2.12.1 Motivation

For many SMEs in the engineering and manufacturing sectors, in-house non-HPC computing hardware is usually insufficient for solving large problems, such as the kind of CFD simulations required by the end user of this experiment. Initial investment for an in-house HPC resource is often prohibitively expensive, in particular for those businesses with only occasional CFD usage. On-demand cloud-based HPC solutions, combined with software based on open-source technologies, can offer a cost-effective alternative.

Before this Fortissimo experiment, DRG had access to local computing resources with limited parallel capability. Although there is in-house expertise to run large remote parallel jobs, HPC resources have to be arranged, and jobs have to be manually assembled and submitted, which can be a time-consuming and error-prone process.

During this experiment, the partners have developed a new cloud-based technical solution. At the end of the experiment, the HELYX software has been enhanced with a fully functional client-server module that allows remote job submission and management, in addition to its existing job preparation capability. This means that DRG has gained better and easier access to HPC resources on an on-demand basis, allowing more accurate and computationally intensive simulations to be performed in a timely fashion, as demonstrated by the two simulations of oil & gas pipeline components performed as part of this experiment. The new client-server software in HELYX will be commercialised by ENGYS via direct sales and HPC on-demand service providers, including platforms such as the new Fortissimo Marketplace.

2.12.2 Relevance to Fortissimo

Fortissimo is a perfect platform to bring all parties together. It brings the HPC resources (HPC provider) and know-how (HPC expert) in one project, helping the ISV partner (ENGYS) to enhance its software solution. For the end user, the Fortissimo experiment is a low-risk opportunity to assess a new technology for on-demand cloud-based scientific computing. All parties can benefit from the development of new value-added services, which can then be promoted and sold via the Fortissimo Marketplace.

As part of this Fortissimo experiment, ENGYS developed and tested a novel client-server framework for their CFD software HELYX with the help of NAG and DRG. The new client-server framework allows end users to perform CFD simulations on remote HPC hardware

directly from a Graphical User Interface (GUI), which is very relevant to this project as an active enabling technology to facilitate the access and effective use of HPC resources. The introduction of the client-server module in HELYX also opens the possibility of providing HELYX as an on-demand service on a short-term licence basis, which could be promoted and delivered via the Fortissimo Marketplace and other similar platforms.

2.12.3 Impact and Business Benefits

From the end user's perspective, the client-server solution developed in this experiment allows CFD simulations for the oil & gas industry to be performed in parallel using remote HPC resources on-demand. The extended hardware resources available in the HPC platform enables the end user to either decrease simulation times when running same size models or perform more complex simulations on larger grids to achieve higher accuracy of results. The reduction of lead times in consulting projects and the ability to produce better results for clients has a positive impact on competitiveness, which ultimately leads to the provision of more cost-effective solutions, increased project profits and improved client satisfaction.

The ISV partner benefits directly from this experiment by introducing the client-server framework in all its software products, which is expected to increase sale opportunities by 20% in the short term. Deployment of this cloud-based solution on regional HPC on-demand providers can also help increase the visibility of HELYX and attract further potential users. On-demand usage of the software, made possible via the new client-server interface, also offers a cost-effective solution to attract occasional users of CFD.

The involvement in this Fortissimo experiment means the HPC expert partner can develop case studies and marketing materials to showcase its software engineering and HPC capabilities to attract new consulting business. The experiment also allows the HPC expert to develop experience in more domain specific fields.

The HPC provider can increase the commercial use of its HPC facility through this Fortissimo experiment and create opportunities to develop new HPC services through collaborations.

2.13 Cloud-based Simulation for Antenna Design and Radar Signature Prediction

2.13.1 Motivation

Lun'tech is a French SME that designs radar reflectors based on Luneburg principles. For the design of a new Luneburg reflector, Lun'tech uses in-house software which is limited in terms of function and accuracy. Lun'tech then manufactures a prototype of the simulated reflectors and makes a RCS (Radar Cross Section) measurement in its anechoic chamber.

Lun'tech also adapts existing Luneburg reflectors. In this case the design process is mainly based on prototyping two or three units to meet the desired specification. This method takes time and is therefore expensive.

To reduce the number of prototypes and therefore the time-to-market, Lun'tech would like to use more powerful simulation software during the design phase. Electromagnetic simulation generally requires a lot of memory and computation resources, so the use of an HPC compute platform becomes mandatory. Lun'tech needs to carry out simulations only a few times per year. Therefore, a Cloud-HPC platform with a pay-per-use model is more interesting compared to software with a permanent licence.

Nexio Simulation is a software vendor and markets the simulation software CAPITOLE-EM for antenna design and the calculation of RCSs. Today, the software is sold with a permanent license and with a yearly maintenance contract that includes updates and technical support. This model is suitable for large companies but is not for SMEs, Nexio Simulation wants to develop this segment of the market with a Cloud-HPC offer.

Nexio, another subsidiary of Nexio group, is an engineering company which provides expertise in the antenna and RCS domains.

During this experiment, Lun'tech, Nexio Simulation and Nexio worked in partnership to test the Cloud-HPC solution. The simulation software CAPITOLE-EM was installed on Bull's HPC platform. Lun'tech could use the software via this platform to perform the required electromagnetic simulations. Nexio then helped Lun'tech to analyse the results of the simulations.

2.13.2 Relevance to Fortissimo

This project was an opportunity for Lun'tech to test the use of high-fidelity electromagnetic simulation.

Usually electromagnetic simulation requires a large compute server, especially for RCS calculations where the frequencies are high. This is because the numerical model is then composed of small mesh elements with a size related to the wavelength of the electromagnetic field.

The HPC-Cloud solution is interesting to SMEs because its cost is lower than that of buying an appropriate compute server. Also, the pay-per-use basis is a more efficient way to use software when simulations are needed only a few times per year.

The main interest for Nexio Simulation was to test a new HPC-Cloud offer of its software CAPITOLE-EM to an end-user. Direct feedback from this test has enabled Nexio Simulation

to adapt its offer before any official launching. Another interest for Nexio Simulation was to test the software on an HPC platform.

Finally, the availability of the Fortissimo Marketplace will allow Nexio Simulation and Nexio to be available via an effective platform and to access to a large number of potential customers.

2.13.3 Impact and Business Benefits

The cost of a permanent licence for commercial high-fidelity electromagnetic simulation software is 36,500 and an additional €5,500 every year for the support and software update. To this amount, the cost of a compute server (tens of thousands) must be added. When the software is used only several times per year, the cost of the simulation is too high and would not be profitable in a short period by an SME like Lun'tech.

The first benefit of this experiment for Lun'tech was to use Cloud-HPC electromagnetic simulation on a pay-per-used model to drastically reduce the cost of hardware and simulation software. The benefit of using the simulation was a 30% time saving in the design phase and a 50% cost saving during the test phase, because it allows the simulation of many configurations of a new product with a reduction in the number of prototypes needed.

Lun'tech is designing one new product per year and manufactures 2 prototypes to validate the new product design. The average cost of a set of molds for a new product design, including testing, is €37,600. Thanks to the HPC simulation, the total costs saving per year is €12,250

There are 2 others benefits for Lun'tech :

- Luneburg Antenna sales increase: the performances of our Luneberg antennas are today lower than expected by our customers. This is the reason why the sales on this type of products are low. The complexity of Luneburg antennas (large diameters, specific materials for high frequencies) requires us to go through a simulation phase using powerful tools (software and time optimized calculations). Once the performances are achieved, we expect to increase our sales by a factor of 10 (from €10,000 to €100,000 / year). Consequently, the total turnover for Lun'tech would rise from €450,000 to €550,000.
- Simulation services that can be proposed to our customers: Lun'tech will be able to propose simulation services. We estimate that it will represent 5% of our 2015 turnover (€22,000/year).

The total sales increase will finally be €122,000/year. The total investment for LUNTECH has been €21,000 including €16,000 of European taxepayer.

For Nexio Simulation, the direct benefit was to integrate CAPITOLE-EM software into the extreme factory HPC cloud platform. This allows Nexio Simulation to market antenna or RCS simulations with CAPITOLE-EM on extreme factory platform.

This project has been a good opportunity to work on a totally new Cloud offer of CAPITOLE-EM. The new offer will be based on a pay-per-use basis. This is different from all competitors that propose Cloud-HPC solution where the customer needs to buy a permanent license to use the software. With a pay-per-use offer, electromagnetic simulation using CAPITOLE-EM will be more accessible to SMEs.

2.14 CLoud based Environment ENgineering services

2.14.1 Motivation

One of the most important business areas of consultancy for services companies, dealing with environmental issues, is represented by the authorization procedures, an obliged step due to European Directives (2014/52/UE, 2011/92/UE and 2008/1/CE). From small and medium-sized enterprises (SMEs) to the biggest industrial plants, in fact, there is a considerable demand for environmental consulting services, in order to reduce and possibly avoid every kind of pollution risk.

The CLEEN experiment aims at overcoming the existing limits of the environmental modelling tools, i.e. long processing time, low data elaboration quality and focusing on a single scenario. The main aim of the CLEEN experiment is therefore ***to set up and test an innovative service for SMEs, public sector*** (i.e. environmental agencies) ***and private stakeholders*** (i.e. consultancy companies, research centres, engineering facilities) ***through a single access-point/platform***.

The consortium was set-up in order to include the required skills and expertise: eAmbiente, leader in environmental indicators and modelling tools; T2i, leader in stakeholders involvement, CINECA one of the worldwide largest super-computing centre, and Progesi, software expert.

The final user has, thanks to the HPC Cloud-based service, a simultaneous view of impacts of air, soil and noise pollution, together with a health risk assessment.

2.14.2 Relevance to Fortissimo

After the end of the experiment, the aim is to offer a service through the Marketplace structured in two ways: an 'ON-LINE' service (through a Cloud middleware that will launch, and finally aggregate the results, different models in parallel) and an 'OFF-LINE' service (through a dedicated site where augmented reality and virtual reality facilities will be used to better evaluate and interact the platform results).

This service is targeted to designers, working on Environmental Impact Assessment (EIA) procedures, Environmental Consulting companies, Environmental Managers of large factories having a considerable environmental impact to consider and manage, and Public Administrations, which are involved in the validation process.

The use of CLEEN simulation via the Fortissimo HPC Cloud will help customers to rapidly evaluate substantial changes in their production cycles by quickly calculating the changes in their expected environmental impacts. At the same time it can reduce the costs of design of new plants providing an innovative service that will be used for new ***multiple scenario-based*** design due to computational power and the integration between different tools. A *leap forward* made possible by FORTISSIMO Project thanks to interoperability among different skills (i.e. computing, applied research, environmental engineering, consulting) that would hardly be seated at the same table otherwise.

2.14.3 Impact and Business Benefits

All the Environmental assessment stakeholders will benefit from the use of the CLEEN service.

Savings, for the end – users (e.g. designers, architects, consultants) will be mainly represented from a reduced time-to-result (-80% less) and from the reduced investments in hardware and software licenses (quantifiable in about €4,000/yr for the amortization of a powerful workstation, and €10,000-20,000 in licenses).

At the operational level, thanks to the use of the Fortissimo Cloud infrastructure, they will find all the tools needed for a complete environmental Evaluation Impact Assessment integrated in a single workflow, available on a pay-per-use basis. We estimate the end-user will pay for an EIA around €6,500.

Due to these improvements, eAmbiente expects to increase its market with around €400,000 of additional business over the next five years corresponding to a +28% in the EIA sector per year. An increase in employees is also estimated, in 2 new employees over the next five year and finally an increase in competitiveness even at European level, since the workflow is easily customizable to non-Italian environmental legislation.

T2i will develop a new EIA – related service through its "offline facility", increasing its skills and its institutional activities. Thanks to these improvements, T2i estimate a 5% increase in commercial revenues, in each year 2017 – 2019.

Finally this experiment offers a success story for CINECA, in the application field of environmental service outside the field of weather forecasting where it is already a recognized player, that is estimated to bring at least one new customer per year, with an approximate 5% increase in commercial services revenues (including operational CLEEN revenues).

2.15 Virtual Automatic Rapid Prototyping Based on Fast Morphing on HPC Platforms

2.15.1 Motivation

It is only in the recent years that Additive Manufacturing (AM) emerged as a viable mainstream production technology. The overcome of technical and bureaucratic obstacles has allowed 3D printing to grow as a cost effective option for small and medium scale production, able to produce complex shapes not achievable with standard manufacturing processes.

This design elasticity allows to optimize components design, cutting by almost a third manufacturing time and halving production costs by reducing energy and material waste. Current design tools however were developed targeting traditional manufacturing procedures and are not expressive enough, limiting the full potential of 3D printing.

From this point of view CAE tools are able to suggest new shapes and accurately predict the components behaviour making them a natural choice in the design chain. However, and especially when dealing with complex Computational Fluid Dynamic simulations (CFD), shape optimization can be an unaffordable task for SMEs, requiring also to apply shape variations in cascade to all the numerical models used to carry the desired study.

Mesh morphing is emerging as a meaningful answer to the challenges posed by shape optimisation problems, especially if product performance evaluation requires heavy numerical modelling as in the case of computational fluid dynamics (CFD) and computational structural mechanics CSM computational meshes. Fast Radial Basis Functions (RBF) enable accurate shape control of complex parts.

The target of this experiment is the development of an HPC tool dedicated to CFD optimization with special regard to 3D printed geometries using a cloud infrastructure.

Cloud-based HPC can be a key-enabler in maintaining and improving a SME market share in this field of application for more than one reason. Computationally expensive CFD simulations can be adopted accelerating calculation times, complex problems can now be tackled not being tied to the limitations of an in-house infrastructure and a more flexible cost of a pay-per-use service can be faced. Moreover the innovation intrinsically enabled by the cloud infrastructure, i.e. always available on-demand data and a collaborative cloud interface, can be a winning feature both to promote the technology and as a source of new client acquisition.

2.15.2 Relevance to Fortissimo

Numerical grid parameterization using a mesh morpher allows to avoid the time consuming task of mesh generation (that can take up to 70% of the total analysis cost), access to CFD simulation through the Fortissimo HPC Cloud allows to further speed-up the calculation times reducing the time to market and return of investment. Using a collaborative interactive cloud interface helps also analysts and clients to work together and to be integrated in the value chain, increasing customer satisfaction and building better products.

ISV RBF Morph (RBF Morph) sponsored the project by giving access to RBF Morph and ANSYS Fluent licenses free of charge and CINECA, the HPC centre, made available part of its Tier-1 cluster, Galileo, through a cloud-based access.

2.15.3 Impact and Business Benefits

This experiment managed to demonstrate the validity of the service by optimising a prospect industrial case, a Lamborghini 12 cylinders airbox, taking advantage on the synergic collaboration between consortium partners HSL, leading SME in the AM and rapid prototyping field, University of Rome Tor Vergata domain expert, RBF Morph ISV and leader in morphing solutions and CINECA the HPC provider.

The innovative CAE workflow designed and tested with HPC during the Experiment has allowed HSL to build a new service with significant business potential for existing and new clients. HSL owns a wide range of clients in the automotive sector and has built over the years a strong reputation in advanced rapid prototyping services. Core-business of the company consists in designing and producing car components with high performance requirements, both for the racing context and for GT car firms.

Having access to the RBF morphing tool combined with CFD analysis and powered by HPC opens a wide range of business opportunities. In parallel with existing rapid prototyping services HSL can now propose to a client alternative component designs enhanced with valuable performance indicators.

From the point of view of HSL offering a shape optimisation service in parallel with existing core business rapid prototyping activities, represents an opportunity to establish customer loyalty over a range of key R&D tasks. HSL is ready to offer the developed virtual tool to a range of existing car firm clients, projecting for the next 2 years a revenue growth of 16%.

Given the engine performance improvement outputted by the Experiment simulations, it was forecasted that Lamborghini, first potential client of HSL for the implemented virtual tool, would benefit of a ROI[2] equal to 7.56.

UTV has deepened its knowledge in HPC and consolidated its leadership in the field of mesh morphing and optimization. It is estimated that thanks to the new know how acquired the interested department will increase the number of industrial research services. The economic benefit is estimated to be in the order of €40,000-€70,000 per year in a 5 years plan. Finally this experiment offers a success story for CINECA, in the application field of high fidelity CFD, that is estimated to bring at least two new customer SMEs per year, with an approximate 5% increase in commercial services revenues.

2.16 High Performance Computing For The Metal Stamping Industry (StamHPC)

The objective of the experiment was to develop a software solution that allows industry to simulate metal forming with higher efficiency and ease of use than possible using today's state-of-the-art commercial codes.

Stampack is a simulation code for Windows available from QUANTECH which models the forming of sheet metal panels. Its simulations enable engineers to concentrate on engineering problems and their solution. The major challenge of this experiment was to develop a high-performance version of Stampack (StamHPC) able to run effectively in a Cloud of HPC Linux resources, made available on a pay-per-use basis. The goal is the full, simple, efficient and affordable integration of available powerful high-performance computing infrastructures with advanced simulation software.

2.16.1 Motivation

The sheet metal forming industry is widely considered as a sector with great influence in the development of the world economy. HPC computing will have a considerable impact on several manufacturing companies, where current high-end computing capabilities are deemed grossly insufficient.

The main outcome of StamHPC will be a new software solution available on a pay-per-use basis that allows the sheet metal forming industry to solve metal forming simulation problems on the next generation of HPC computers with higher efficiency and ease of use than today's state-of-the-art commercial codes.

High-end computer simulation and computer-aided engineering (CAE) tools are often hard to afford for SMEs. The two main drawbacks for this are:

- **Cost and usability**. Most of the major commercial simulation software packages have increased progressively their prices because of the creation of comprehensive suites of ever more modules with richer and more complex functionalities. The main objective is to attract large companies that can afford the high price tag. However, these software packages are often over-dimensioned and too expensive for SMEs, and require additional investments in powerful workstations, in staff training, and in consultancy services.
- **Code scalability**. Up to now, some of the traditional commercial software packages have been designed to be executed on workstations therefore they do not offer a good scalability when they are used on HPC resources. This lack of scalability limits the sizes of the problems that can be solved and avoid a faster time to solution. However, metal forming SMEs need to be able to solve larger and more complex designs in order to in order to remain competitive in markets

The aforementioned drawbacks will be addressed by implementing, adapting, and parallelizing Stampack code [2], developed and commercialized by QUANTECH, to really exploit the intrinsic capabilities of the HPC infrastructures.

2.16.2 Relevance to Fortissimo

Metal Forming is a complex process and its simulation requires a very fine finite element discretization in order to obtain accurate results. Such a fine discretization involves significant computational resources. MATRICI is a sheet metal forming industrial company with expertise in developing world-class product-process of all kinds of BIW-panels (body in white) in the automotive sector, but does not have the necessary computational infrastructure. The possibility of using remote HPC resources has been proven to be fundamental in addressing this specific industrial and scientific challenge.

Traditional CAE systems are usually installed as in-house software and it requires a computing equipment (€1,500 - €3,000, license cost (around €40,000 first year) and a maintenance fee (around €6,000/year). Additionally the SMEs' engineers need a specific training in the software usage.

The simulation of a metal forming process, considering a medium-complex part, represents around 50 iterations, each of which need 20 computing hours with a standard conventional workstation (8 cores, 16-32 GB of RAM). These kind of studies represent 10 weeks of work involving a dedicated workstation and an specialized engineer. Such a problem either would be too big for the in-house systems of MATRICI or would take too long to run to be part of an effective design process.

A Cloud-based version of Stampack software (StamHPC) has been adapted, developed and validated. Its performance and usability have been evaluated in an industrial setting. Using the StamHPC solution within an HPC-Cloud it is possible to run, at the same time, several options of the feasibility design concepts. This allows the end-user to reduce the time to design a prototype.

The graphical interface of the solution provides an easy and intuitive use in the metal forming industry. This allows any end-user, even without HPC expertise, to launch a remote calculation and get results with an appropriate response time. Furthermore an appropriate licensing server has been developed which supports the availability of StamHPC on a pay-per-use basis.

The Fortissimo Marketplace will constitute a great opportunity for QUANTECH to promote and commercialize StamHPC solution as a fast metal forming simulation solution for remote HPC platforms.

2.16.3 Impact and Business Benefits

The experiment tested the feasibility of using a Cloud-based HPC simulation environment for the forming of sheet metal parts.

StamHPC is a SaaS solution which will provide the metal forming industry with the parallel processing capability required to accelerate time-to-solution and to solve the metal forming high fidelity problems. With the use of StamHPC solution on HPC-Cloud it is possible to reduce the time of producing the prototypes. Time reduction is about 50%, which means a reduction of engineering costs of 50%. Considering that in a year a die Maker company like MATRICI performs 200 design studies in order to make offers to customers, the reduction of design cost variability, plus the reduction of trial-and-error cases would represent savings around €1,500,000 /year (2.5% of current company turnover).

An additional benefit of using StamHPC will be the improvement in speed and agility to develop the offers for the metal-forming industry customers. This has a positive impact on the awarded contracts arising from proposals made, which is estimated as an increase of 30%.

The parallelization of the commercial code Stampack has allowed CESGA to improve its knowledge about specific industrial workflows, and its problems and applications. This experience will contribute to the CESGA's services portfolio. Additionally CESGA has gained new valuable experience in the integration of industrial desktop applications with remote HPC resources and has increased the provision of computing hours. CESGA's resources will be used by QUANTECH in order to execute StamHPC and possibly for moving additional software runs from the SME computers to the HPC resources.

QUANTECH could use the computing services offered by CESGA and potentially others offered by the Fortissimo Marketplace providing a SaaS option to customers.

The objective of Fraunhofer SCAI is to support SME ISVs with a flexible but cost-effective solution for licensing their products - elasticLM [3]- and to offer their solutions to their customers also in Cloud environments. elasticLM is a novel product for protection of ISVs' IPR, aka software licensing, especially designed for use in distributed computing environments. The Fortissimo Marketplace is considered an excellent place for making elasticLM accessible for a greater number of interested SME ISVs and to jointly attract new customers of the ISV.

The fundamentals of a metal forming simulation service can be offered to end-users through the Fortissimo Marketplace with cost-effective access to the service, this will bring to SMEs new business opportunities and shows that CAE technology and HPC infrastructures are key for the metal forming industry.

2.17 Cloud-based Optimization platform for reinforcement steel cut industries

2.17.1 Motivation

Schnell Software S.L. designs specialized CAD-CAM software for steel cut and bend companies and develops software applications which optimize the elaboration process of iron for reinforced concrete.

In 2014, it detected that many software apps on the market offered only partial solutions in the detailing of pieces and the production process of the cut and bend steel industries (recipients of its clients´ information). Another discovery was that the sources of information in the sector such as construction and engineering companies, work with software tools that are adapted to their requirements but differ from those used in information receivers´ industries.

This required availability of specific data import and export tools on the market for communication between both groups. These tools proved to be quite efficient although in many cases they did not avoid unnecessary task duplication that was undertaken by both the sender and receiver of the information. Moreover, the scenario became even more complicated when a cut and bend plant received information from multiple engineering/construction companies that had all used a variety of designs and tools. There were even some people working in the same engineering group using different tools, IT apps or small personalized programs.

Consequently, Schnell Software detected the necessity to enhance company communications and also standardize the scheduling work tools for the forming of different Bar Bending Schedule (BBS). The Bar Bending Scheduling (BBS) is defined as a list of reinforcement bars that is presented in an easy visual form and summarizes all the needed particulars of bars: diameter, shape of bending, length of each bent and straight portions, angles of bending, total length of each bar, and number of each type of bar. The scheduling work or the detailing work is understood as the realization of these lists. The lists come therefore from the orders that the steel plants receive from their customers to make the cut.

The search for these necessary improvements plus the current lack of a sufficiently simple, graphic, powerful, flexible Web-tool in the market that would upgrade the work process on an international scale, inspired Schnell Software to amplify its product portfolio and create Rebar Web (www.rebarweb.com). Thus it pioneered the launching of an international product for the detailing of pieces in the cloud for the steel sector that would generate a social Web of communication at a sectorial level.

Rebar Web offered its users attractive economic savings and benefits:

- Possess a professional tool at a greatly reduced cost. No costs for the installation in situ.
- Time saved in the designing of BBS.
- Savings in management and work organization costs.
- Time saved in revision and quality, given the possibility of transmitting the information directly to the productive process.

- Ready access to the information in the case of necessary modifications with a technician in situ. All this, with no additional costs of software licenses or hardware due to available access to the internet on site.

However, in 2015, Schnell Software decided to go one step further in the market and attempt to give Rebar Web a new additional function: the optimization of steel cutting. Schnell already possessed optimization software (**Optimo**) in its portfolio, which had previously developed with UNIZAR-BIFI and this new challenge consisted in adapting this system of optimization to its execution in the Cloud. They were taking into account the international character of the web, which implied that a large number of users might use the Cloud optimization service at the same time.

The value of the optimization, which is based on complex algorithms used in the investigation on physics, would provide Rebar Web and its clients with great assets. The users would be able to optimize their schedules by diameter and obtain reports with the results. In this way, they would obtain the best possible combination of their orders and maintain scrap to a minimum in the cutting process, save time in the analysis of their production orders and raw material while obtaining valuable support for the management of their reusable products.

Rebar Web would serve as a database portal to optimize functions in the Cloud and the clients would be able to carry out a real simulation of a cutting process with minimal cost and effort.

Besides, for some small companies, the acquisition of an optimization system that guarantees a reliable cut of high quality is economically unfeasible. Rebar Web will present them with the possibility of using this tool at a reasonable price plus the opportunity of testing the software before its purchase.

The optimized cutting process applied in a plant that produces 2000 tons per month would reduce waste material by 2% and personnel expenses by 10%. This means that each Schnell's customer may save approximately 480 tons per year.

The principal advantages the user obtains with the optimization in the Cloud are:

- Accessibility: All users can access with no necessary installations.
- Response time in the calculation process: If the calculation process is performed on multiple cores, the parallelism enables the results to be received in record time.
- Quality of the optimization process: the higher the number of interactions realized in the optimized process, the greater the efficiency and quality of the solution.

In Figure 1, we can see the execution of 1000 jobs for a casting optimization of 60 tons. In the Y axis we observe the percentage of scrap and in the X axis the number of jobs.

The lower the point, the better the solution. This example would be equivalent to 1000 executions and would last for a very long period. If only one solution is executed, the local probability would be very close to the average represented by the blue line between 7.5% and 8%. In the case of 1000 executions, the best solution is a point very near 5%. Thus a 2·5% improvement is observed which can be translated into a saving of 2 tons of steel depending on the size of the optimized order.

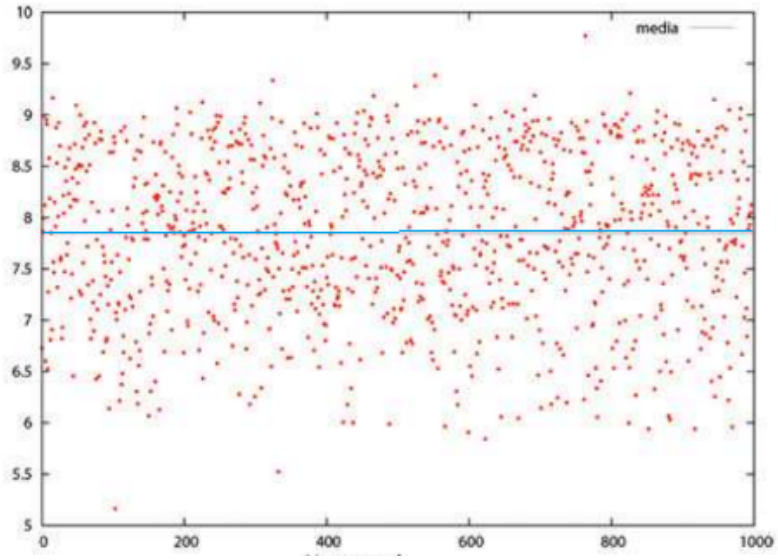

Figure 1 Percentage of scrap vs number of jobs.

Regarding the three previous points, Schnell Software analysed its international competitors and saw there were companies that offered other products of optimization, which however, were less efficient due to the calculation process used. These were restricted to local PC, limited hardware resources and in any case they didn't operating in the Cloud.

SCHNELL was in possession of an advantageous inception which enabled it to benefit from the possibilities that its innovative technology presented in contrast with the current systems. It likewise considered that this form of working could not easily be introduced by its competitors, who haven't much experience in cutting optimization systems.

Consequently, with the newly implied differences between Schnell and its counterparts regarding BBS detailing and optimization services in the Cloud, it would consolidate its position in the sector and benefit from the advantages entailed with the pioneering and highly technological services offered on the Web. Thus, Schnell market potential would be noticeably strengthened.

2.17.2 Relevance to Fortissimo

The Fortissimo project offers the usage of their computing resources in a pay-per-use Cloud approach, which is a key point for the porting of the optimization service.

- It avoids that SCHNELL has to invest a great initial amount of money in its own hardware, which would be a great effort for such an SME.
- It is also remarkable that with this approach SCHNELL does need neither specialized personnel to manage the hardware composing the simulation cluster nor investing in a specific room and its resources as cooling, electricity, UPS, etc.
- Thus the pay-per-use model allows SCHNELL to offer to its customers a computing platform to optimize their orders with the SaaS model.

Fortissimo also offers a valuable knowledge pool in which different experts from different computational fields can help to improve the approach, design and final setup of the optimization service.

Experts from UNIZAR-BIFI and CESGA provide the technical knowledge for the design of a good architecture of on-demand dynamic HPC cluster simulation on the Cloud, using their years of experience in managing HPC and distributed computing infrastructures. Without this capability, SCHNELL Cloud solution is unfeasible because it cannot return results on time and cannot serve several customers at the same time, except if a large investment in hardware is done.

2.17.3 Impact and Business Benefits

The new service of optimization on the Web conveys Schnell Software with the following benefits:

- A greater commercial control with an application that is also a marketing tool. The company will be more visible in the sector, which will result in a superior market coverage and a potential increase of sales.
- Increased software module options offered by the company, reaching new customers that were previously inaccessible and thus increasing sales.
- Reduction of software installation time/expenses and obtain greater profit margins.
- Enhanced agility and control of its technical support service based on the possibility of knowing what is making the end user without the need of visiting in situ.
- Have at its disposal an advanced technology that enables it to increase the difference over its competitors and improve its sales possibilities.
- Offer its clients a service of additional value in their maintenance contracts; that is to say, the optimization on the web will be included thus making regular maintenance even more attractive for them. This will also allow it to ensure a minimum billing level.

On the other hand, the end users perceive the following advantages:

- Have at their disposal a powerful optimization tool (a new software module more closely customized to their requirements) without having to make a substantial initial investment, thus enabling them to reduce their IT expenses and risks.
- Reduce their information storage costs.
- Improve their optimization quality.
- Diminish time in budgets preparation and viability analysis. This will make their projects more profitable.
- A more responsible consumption of raw-material resources thanks to the reduction of wastage, which will moreover decrease CO2 emissions.

2.18 cDES4SME - Cloud based Discrete Event Simulation for SME

2.18.1 Motivation

For SME's in the manufacturing sector, significant inefficiencies arise in the operation of the production lines due to the interaction of raw material, operators and equipment. For large multinational organisations the use of analytical tools to predict the complex interactions and stochastic events relating to the flow of product is realised through the use of licensed software used by skilled modellers and analysts. SME's do not have the capital (financial or human) to use these optimisation tools in their plant, so management must use their experience to run the plant as effectively as possible.

2.18.2 Relevance to Fortissimo

The use of cloud-based HPC to deliver discrete event simulation based (DES) optimisation under a SaaS style of ownership is attractive in reducing the cost of ownership. The Fortissimo approach of a marketplace accompanied by the availability of HPC to back it up combines the two key ingredients in enabling what has been hitherto a single point of access approach.

Further to this, DES based simulation requires intense calculations, many of which could occur in parallel. The stochastic nature of the analysis means that to provide a complete answer to a single set of control parameters can require a significant number of replications under differing random conditions. These can be processed in parallel when simulation is used to provide an evaluation of the effectiveness of a particular set of control parameters for an optimisation algorithm. The systems being modelled have multiple control parameters, leading to a large search space for optimisation algorithms. The most efficient means of searching the solution space is often to evaluate a trial set of parameter inputs, evaluate the performance of the system and then develop a new generation of parameter inputs based on the best results. In this way the algorithm reinforces the best solutions and discards poorly performing options. Nevertheless, in each generation, some novel combinations must be included in the evaluation to avoid the results tending towards a local optimum while missing a better global solution.

2.18.3 Impact and Business Benefits

This Fortissimo experiment probably came a little early in the development of the system, and would have suited software much closer to market. As the experiment progressed, while functionality was added to the modelling element of the software to address the challenges identified in the end-user use case and API tools to allow the calculation engine to take advantage of the cloud-based HPC scaling were developed, the expected development of the user interface and optimisation algorithms encountered difficulties which meant that the full evaluation of the business case was not possible within the human resources available. However, the requirement to include a consultant role in the business model was identified and this has been incorporated into the business plan.

2.19 SureHPC: Sustainable & Renewable Energy HPC

There are many companies involved in the renewable energy sector in Europe. Many of these are small and medium-sized enterprises (SMEs). There is significant political and industrial demand for the development of new efficient systems which are able to increase the exploitation of renewable energy resources: solar, wind and hydro power. Among these, water turbines are the oldest renewable energy system, as they are employed since XIX century. Nowadays this sector is gaining more and more interest because it represents at the same time an efficient, reliable and low-impact energy system. Focus is on small and micro plants, which are able to exploit a larger part of the natural hydro power potential with a very low environmental impact.

The activity in this experiment consists on the development of a customized tool for water turbines design, based on *Computational Fluid Dynamics* (CFD) simulations on HPC cloud infrastructure. New operation models for small size water turbines are proposed, which are able, compared to conventional plants, to exploit a larger share of the hydro power potential in both developed and emerging countries.

The goal is achieved starting from the project requisite supplied by the end user. Initial geometry is inserted in a *Computer Aided Engineering* (CAE) automatic process where a parametric approach is used for a simulation driven optimization. The result is the identification of the best configuration, customized on the user request.

Consortium partners in this Experiment are Zeco, the water turbine manufacturer and SME, EnginSoft, the CFD application expert, and CINECA, the HPC provider.

2.19.1 Motivation

Current practice in the hydro power sector is to determine empirically the suitable plant in a series of time-consuming experiments. However SMEs in this sector have to face private and public tenders to sell their turbines in both national and global markets, where the competition is very strong and the development time very short.

Kaplan water turbines are widely used because of their easy adaption to different installation conditions, preserving high efficiency. Indeed the possibility to regulate both stator and rotor blades makes the Kaplan turbines able to keep high performances even in off-design conditions, hence they are able to work efficiently in a wider range of operating conditions compared to other turbine types (Francis, Pelton). However hydro power plants usually require significant civil works and costs that can be a serious obstacle to small and micro installations. Kaplan turbines for example usually are fed by radial inlet systems which are much more expensive than axial feed ones. The development of such systems can be now part of a dynamic and profitable market. They can reduce installation costs increasing the exploitation of hydro power resources at a lower cost. One of the most important problem is to adapt the axial Kaplan turbine system at different installation conditions, preserving the high efficiency and avoiding the occurrence of critical issues, like cavitation.

Computational Fluid Dynamics (CFD) simulation can dramatically improve the turbine design process and reduce the number of trials needed to set-up the final product. These simulations, however, are CPU-intensive and require the use of HPC and need the support of domain specific expertise. Nevertheless, their use can improve competitiveness and reduce the 'time-to-market' for new products, increasing moreover the reliability.

Furthermore the use of physical complex models, like multi-phase approach, and the large dimensions of the domain simulated, makes the HPC mandatory to simulate in a short time such a plant.

2.19.2 Relevance to Fortissimo

The use of CFD simulation via the Fortissimo HPC Cloud helps SMEs in the hydro power sector increase their productivity by reducing the costs related to installation, design and maintenance by up to 25%, and the time to market by up to 50%. A further benefit is the full prediction of undesired issues like cavitation, which is responsible for the largest part of the overall maintenance costs.

The traditional trial-and-error approach of European SMEs to the design of hydro power turbines does not easily support the characterization of cavitation and transient phenomena, which is more commonly an approach used by premium global manufacturers. This reduces the competitiveness of European SMEs in the global market. CFD simulation codes are useful tools for the design of water turbines particularly when high challenging aspects like cavitation have to be taken into account. However, in many cases, such codes are too complicated to be used by SMEs with limited resources and require access to supercomputer resources. The use of the Fortissimo one-stop shop which brings together supercomputing resources, domain specific expertise and licensed simulation packages can overcome these barriers. This enables European SMEs to compete globally through better design and quicker times to market.

EnginSoft, the application expert, provided the SW licences and developed the customized virtual tool, which is used by Zeco within the project. CINECA, the HPC centre, made available part of its Tier-1 cluster, Galileo, through a cloud-based access.

2.19.3 Impact and Business Benefits

Benefits cover all the consortium project partners.

Regarding Zeco, thanks to the virtual tool based on high fidelity CFD simulations on cloud HPC, the turbine design can be quickly customized on client requests, reducing significantly the time to market. Also design costs are lower than the standard workflow as the simulation can reduce the number of prototypes needed for real testing. The on cloud solution is also an innovative *pay-per-use* approach which avoids large up-front investments of hardware and software costs.

The benefits for Zeco obtainable by the use of the Fortissimo HPC-Cloud have been quantified as a 75% reduction on simulation time, a 50% shortening of the time to market, a Return On Innovation Investments (ROI^2) of 17%. Due to these improvements, Zeco expects to increase its market with around €2,000,000 of additional business over the next five years.

EnginSoft will be able to offer to other SMEs in the hydro power sector the tool developed in the Experiment through the Fortissimo market place, with the possibility to become a key partner in design process innovation. Furthermore, as cloud technology is getting more and more relevant in the CAE (Computer Aided Engineering) sector, the experiment will give to the application expert (EnginSoft) a competitive edge gaining expertise with this technology.

Due to the increased market for advanced simulation using HPC, EnginSoft expects a growth of 10% in its business related to the turbo-machinery market sector.

Finally this experiment offers a success story for CINECA, in the application field of high fidelity CFD, that is estimated to bring at least three new customer SMEs per year, with an approximate 5% increase in commercial services revenues.

2.20 Prediction of optical properties of dyes and application for the rational design of time temperature integrators

Time temperature integrators (TTIs) are devices recording their thermal history. Placed in proximity of perishable products, they can be used to monitor the thermal history of packaging and storage conditions. In this sense, such devices represent an important aspect of cold chain logistics, in a world where production is considered a global feature. Cold chain logistics is also addressed by regulators because the quality of products and goods is greatly affected by potential excursion in the storage temperature, along the distribution chain. Specifically cold chain is relevant for the safety of consumer, but most of all for the cost of energy spent for transport and for management of returned goods. Cold chain logistics is a field where new technology solutions may become real applications in a short amount of time. Investors are willing to bet on new multifunctional materials, i.e. phase change materials for packaging are brought to the market with high speed.

2.20.1 Motivation

As well as for controlling the temperature, there is also great interest in instruments for measuring the temperature in real time. Indeed, awareness of the real-time shipment temperature allows one to intervene in order to mitigate an adverse event. This potentially saves money and is able to save also the products, because logistic operators may put in place actions before the spoilage of large quantity of materials takes place.

Regulators have issued several good distribution practices for medicines in the European Union (European Commission, Available: http://ec.europa.eu/health/human-use/good_distribution_practice/index_en.htm) and in the United States. International Associations, such as Parenteral Drug Associations (PDA Technical Report No. 58 (TR 58) Risk Management for Temperature-Controlled Distribution) or World Health Organization (WHO Technical Report Series, No.961, 2011), increasingly address the real time control of temperature of shipping and define also the chain of responsibility when the quality measures have not been taken.

There is therefore a market demand for new time temperature integrators that are up-to-date in terms of accuracy and capability of data sharing, but at the same time with a reduced cost for unit package. Smart labels, containing the TTIs, could be incoprated on unit packaging and not on tertiary packages or large cartons, which may be subject to changes in temperature with a gradient that is not a fine measure for the status of the product inside the carton. Time temperature integrators should be put as near as possible to the product, because the temperature outside may change very differently with respect to the temperature of the product itself.

2.20.2 Relevance to Fortissimo

Scriba is developing a cost effective solution for smart time temperature integrators, that can be miniaturized and detected for readout by electronic devices such as smartphones. The mechanism of detection is based on the optical contrast and materials providing the information on the thermal history of the product are phase transition materials. In the Scriba TTI architecture label TTAG, the overpassing is recorded by a mechanism of wetting of nanostructured surface such as holographic surface. Therefore, Scriba is interested in defining a class of materials that have phase transition temperatures in a certain range, that present

optical properties that can be measured. These materials consist of mixtures of lipid phase moieties and chromophores or fluorophores. The behaviour of these materials inside the TTAG architecture is generally being assessed by experimental laboratory tests. However, a significant research effort has been employed in finding the correct materials and the correct mixtures.

Molecular dynamics simulations together with algorithms that predict the optical properties of dyes within phase material matrix, represent the objective of the Fortissimo Experiment 520 which greatly reduces the time required by Scriba for material assessment. The procedure involves constructing a workflow for the simulation of the dye molecule which is then analysed by the perturbed matrix method to calculate the absorption of the dye.

The writing and deployment of such calculation codes, in particular molecular dynamics, requires a background in theoretical chemistry that cannot be sourced internally by an SME such as Scriba, which is active in manufacturing and software for user apps. Therefore, the collaboration with application experts in UNIMORE and UNIVAQ, and CINECA HPC expertise and computer provision has been essential to test and implement the strategy of lipid materials and dyes to be used as thermosensitive materials. Moreover, only HPC providers can sustain the calculation resources required by molecular dynamics, in order to provide effective solutions in an accelerated manner. The Fortissimo Marketplace appears to be the correct infrastructure to promote and distribute this calculation service, in order to be accessible and exploitable also by companies acting in different fields, such as biotech companies developing immunosensing kits and protocols, or pharmaceutical companies.

UNIMORE and UNIVAQ, the application experts, provided the code for piping the molecular dynamics and perturbed matrix method algorithm on standard workstations. CINECA, the HPC expert and provider, implemented the cluster and cloud version of the calculation workflow and developed the web interface. Moreover, CINECA made the Galileo cluster available for running test calculations, through a cloud based access.

2.20.3 Impact and Business Benefits

Scriba Nanotecnologie is developing an innovative time temperature integrator for smart packaging which can be accessed with a smartphone application. The simulations performed with Experiment 520 have defined a library of materials which can be used in Scriba's TTI architecture, reducing the time of customization in laboratory and allowing to start custom validation with pilot studies in relevant environments. This advantage has contributed to increase the technology readiness level of Scriba's TTI solution and corroborated the activity of fund raising for starting industrial production with automatic machinery developed in collaboration with industrial partners.

Savings on the research for customization of reference temperature and total integration time is estimated at around a year of trained personnel, which sums up to cost savings in the optical readout customization. The return of investment on innovation, estimated after two years of industrial production with current commercial contacts, will be approximately of 20% (ROI^2 = 1.2), since the savings to achieve the customization of the thermosensitive material are estimated in €90,000 for the first customer and €70,000 for the subsequent. Looking at the revenues, one positive outcome of Fortissimo Experiment would be a largely improved capability to satisfy customer requests in time, allowing to estimate a potential revenue of €400,000 for the Time temperature integrators by Scriba each year.

2.21 Multi-physics simulation of high temperature superconducting devices

2.21.1 Motivation

The high degree of development achieved by the High Temperature Superconductors (HTS) is well supported by the increasing of the number of manufacturers and the huge effort in the development of applications, essentially, in the electro-technical area: from generators and motors to cables, current limiters, and magnets for energy storage, image diagnosis, fusion reactors or large accelerators.

In any case, the unique characteristics of the HTS materials require specific design tools for a better understanding and optimization of their function in devices and systems based on them. These design tools should deal with mechanical, thermal and electromagnetic parameters and performances of the superconductors allowing a simplification of the design process and an increasing in the ability of new engineers to access this new technology and its correspondent market.

From the electromagnetic point of view, HTS are strongly non-linear materials. They exhibit hysteresis and some of their properties present abrupt changes. In addition, thanks to the explicit time dependence that is exhibited in the Maxwell equations formulation, its hysteretic behaviour imposes the computation of a time dependent process in order to achieve any state. Both, time dependences in the HTS material modelling and strong nonlinearity lead to a very complex and time consuming computing process. HPC (High Performance Computing) tools as FEMPAR (**F**inite **E**lement **M**ulti-physics and massively **PAR**allel software package) should be available for an efficient design of devices and systems based on superconductivity.

In the state of the art, the lack of specialized codes has forced manufacturers to develop adequate procedures and formulations that can be used at small scale generating experience and knowledge but the leap to larger scale is just starting.

The FORTISSIMO experiment is a step forward in such a development and gives to the company the added value for having a good connection with the customer with the knowledge and the engineering aids which can offer.

2.21.2 Relevance to Fortissimo

From the point of view of the developers of superconducting materials, products and their applications, the implementation of a flexible and powerful 3D design tool, able to deal with superconducting components and parts and their behaviour when integrated in systems, able also to include complex geometries, is indispensable. The opening of the market of superconducting devices is clearly in the way and pushing with increasing force, day by day, contributing also to the need of operative capacity for computing and modelling efficiently in medium and large scale. The design requires a multi-physics scope including thermal, electromagnetic and mechanical studies where all of them interact because the dependence of the HTS materials on the three types of physics.

There exist some configurable computing codes that can help but the inclusion in HPC is not developed as an extended working framework.

FORTISSIMO has successfully contributed to the first steps in the development of such a kind of computing tool and an experienced team able to continue in the enhancement of its abilities. The contribution of HPC centre has been a key, providing the necessary facilities for development.

2.21.3 Impact and Business Benefits

The main identified benefits are:

- CIMNE has improved its simulation software FEMPAR and has developed a solution based on it for HTS.
- Increased turnover for OXOLUTIA. In 1-3 years, it is expected to reach €500,000 related to HTS devices. Better visibility of the activities of the company. Positioning within the community of Applied Superconductivity at international level.
- Training of key staff within OXOLUTIA in HPC and parallelization. Knowledge of HPC as an important tool for competitiveness of SMEs and related methodologies and actors.
- ICMAB has increased its capacity for participating in collaborative projects with private and public institutions. For example, the role of the ICMAB in the EUROFUSION project has been designed based on the use of FEMPAR-HTS code. Taking into account the new open opportunities this institution could achieve, an incoming in the range of €45,000 for the next 3 years is forecasted.
- CESGA has promoted HPC and opened their infrastructure and knowledge to SMEs and ISVs following government guidelines and CESGA's strategic plan.

2.22 SSSM – Sample, Simulate, Sample Map

2.22.1 Motivation

DFRC AG is the operator of a service called LBASense, which is able to map crowd behaviour on a citywide scale. In order to provide this service, DFRC is deploying two types of mobile phones' detectors — long range (several per city) and short range (several at key locations inside the city). Based on the detections that are collected from the sensors, a mapping process that is performed as part of the system installation and data fusion algorithm, LBASense is able to locate anonymously the number of people in each part of the city as well as the flow of the people within the city. This information is highly valuable for services such as transportation planning, tourism promotion, and public safety applications.

The service, which is currently deployed in many cities in Europe and Asia, initially was operated on the cloud using Amazon Elastic Cloud services. LBASense key bottleneck was the deployment process, which requires an extensive process of "fingerprinting" the cellular network digital signature. This process was done by temporary deployment of special measurement tools in multiple locations within the city (using a special car) and post-processing the results. For each point, the car needed to stop for an hour, take measurements, and then continue to the next measurement point. A single car was able to measure up to 10 points per day; a small city such as Bern required around 100 points.

In practice, the process was more complex and less efficient. While the measurement points were selected in advance in a way that would be optimal for the system, in reality, the mapping process was highly affected by the deployment of the cellular network over the city. The result was that some of the points were almost useless for the fingerprinting process, while in other areas, we might find that our system did not have sufficient data, and therefore, we needed to send our team to perform additional measurements. The process of system deployment in a new city was very long (2 to 4 weeks per medium-sized city) and expensive.

This main limitation in scaling up LBASense service was overcome by using HPC resources in order to optimize the sampling process through a combination of simulation tools and actual measurements.

2.22.2 Relevance to Fortissimo

The goal of SSSM (Sample, Simulate, Sample Map) was to use high-performance simulations in order to speed up the LBASense deployment process. In the new scenario - estimating new measurement points on the fly - we need approximately 1000 times more computation power for each iteration, as intermediate simulation is required. Furthermore, the computation resources for large cities are higher by a factor of 10-100 times.

Clouds are not sufficient to cover these needs, thus HPC is mandatory. Using HPC simulation tools was the only way to make the process computationally sustainable and scalable, rather than just fast.

Given a small set of measurement points, DFRC estimated the location of the base station and its coverage, subsequently verifying the accuracy. Simulating the accuracy for different sets of measurements and calculating total accuracy errors helped identifying points with potentially high inaccuracy. The process was parallelised, repeating the estimation of the

coverage map on a grid of variable size, for various signal strength values, with different accuracy coefficients.

Using one of the HPC clusters at HLRS, the simulation of a complex scenario could be achieved in only 500 seconds with 8 processes, compared with the original computing time of 3500 seconds.

2.22.3 Impact and Business Benefits

As the adoption of mobile phones spreads world-wide, the amount of data transferred over cellular and digital networks increases dramatically every day; the Big Data era requires incredible storage and processing capabilities. As a company that maps the cellular network to create statistical crowd figures: DFRC needs to quickly identify where to take significant signals samples, measure and interpolate them in order to locate the source by triangulation.

LBASense is a full ecosystem: end users, the local LBASense operator responsible for the operation and marketing, solution providers who are providing value-added domain-specific applications using LBASense infrastructure and services, to the system operator (DFRC), responsible for the technology development of the operation of the system.

As the system cost is one of the most important factors in this value chain, it was critical to reduce the deployment costs to a minimum. While the hardware cost of the system is relatively low, the installation costs were becoming the main cost for system deployment, especially when the deployment was done abroad. Reducing installation cost directly translated into lower system costs affecting the whole value chain.

Using HPC, DFRC is being able to speed up the whole process of mapping a city (i.e. 10000 base stations) to an astonishing “matter of hours”.

The ability to access cost-effective and one stop shop HPC service, is enabling DFRC to significantly reduce the system’s deployment effort: we estimate SSSM saves approximately two weeks of two engineers per deployment (Approx. €25,000/deployment including travel costs and depend on the location of the deployment).

This will allow DFRC to offer cheaper, faster and more targeted/focused service and so to be more competitive with respect to cellular operators. DFRC expects to gain new market share, especially by the capacity of reducing time to market.

DFRC foresees the SSSM applications in location-based systems mainly smart cities, critical infrastructure, crowd management, retail, tourism and advertisement.

3 Concluding Remarks

The first 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, and their results will have the potential enrich the Fortissimo marketplace.

The results show that the Fortissimo concept is well founded. Many experiments have produced results that will lead to production level services in the Fortissimo Marketplace that are proven in terms of technological feasibility and economic viability.

The partners are continuing to exploit the results of their work using the opportunities created by the Fortissimo Marketplace.

Appendix A: List of participants:

Short name	Full name	Country
ACTIVEEON	Activeeon	France
ARCTUR	Arctur Racunalniski Inzeniring Doo	Slovenia
ATI	Algo'tech Informatique	France
BIBA	Biba - Bremer Institut Fuer Produktion Und Logistik Gmbh	Germany
BULL	Bull SAS	France
CERX	Ceramix Ireland Ltd	Ireland
CESGA	Fundacion Centro Tecnologico De Supercomputacion De Galicia	Spain
CIMNE	Centre Internacional De Metodes Numerics En Enginyeria	Spain
CINECA	Consorzio Interuniversitario Cineca	Italy
DATAPIXEL	Datapixel Sl	Spain
DCU	Dublin City University	Ireland
DFRC	DTRC Ag	Switzerland
DINAK	Dinak S.A.	Spain
DRG	Dynaflow Research Group Bv	Netherlands
eAmb	Eambiente SRL	Italy
ENGYS-UK	Engys Ltd	United Kingdom
EPC	Engine Power Components Group Europe Sl	Spain
FDR	Fundiciones De Roda S.A.	Spain
GENCI	Grand Equipement National De Calcul Intensif	France
GOMPUTE	Gridcore Ab	Sweden
HOLONIX	Holonix Srl-Spin Off Del Politecnico Di Milano	Italy
HSL	Hsl Srl A Socio Unico	Italy
HUA	Harokopio University	Greece
HYDROLIFT	Hydrolift As	Norway
ICMAB	Agencia Estatal Consejo Superior De Investigacionescientificas	Spain
INGECON	Ingenieria Y Control Electronico Sa	Spain
INRIA	Institut National De Recherche En Informatique Et En Automatique	France
INTEL	Intel Gmbh	Germany
INVENTAS	Inventas Kristiansand As	Norway
LandW	Lauer & Weiss Gmbh	Germany
LBO	Lasersystemtechnik Bollinger & Ohr Ug	Germany
LUNTECH	Lun'tech	France
MATRICI	Matrici S.Coop.	Spain
NAG	Numerical Algorithms Group Ltd	United Kingdom
NEXIOSIM	Nexio Simulation	France
NX	Nexio Sas	France
OOSAS	Open Ocean Sas	France

OXO	Oxolutia Sl	Spain
QUANTECH	Quantech Atz Sa	Spain
ROGESI	Progesi Spa P	Italy
SARA	Surfsara Bv	Netherlands
SCAPOS	Scapos Ag	Germany
SCHNELL	Schnell Software Sl	Spain
SCRIBA	Scriba Nanotecnologie Srl	Italy
SEEMI	Societe D'etudes D'equipement De Modernisationindustrielle	France
SHARP-AS	Sharp Reflections As	Norway
SHARP-GmbH	Sharp Reflections Gmbh	Germany
SICOS	Sicos Bw Gmbh	Germany
SINTEF	Stiftelsen Sintef	Norway
SIPLtd	Seismic Image Processing Ltd	United Kingdom
SISENER	Sisener Ingenieros Sl	Spain
T2I	T2i - Trasferimento Tecnologico E Innovazione S.C.A R.L.	Italy
TI	Transinsight Gmbh	Germany
TUD	Technische Universitaet Dresden	Germany
UDC	Universidade Da Coruna	Spain
UEDIN	The University Of Edinburgh	United Kingdom
UNIMETRIK	Unimetrik Sa	Spain
UNIMORE	3.1.1.1.1 Universita Degli Studi Di Modena E Reggio Emilia	Italy
UNIVAQ	Universita Degli Studi Dell'aquila	Italy
UNIZAR	Universidad De Zaragoza	Spain
USTUTT	Universitaet Stuttgart	Germany
UTV	Universita Degli Studi Di Roma Torvergata	Italy
VE&D	Vehicle engineering and design s.r.l.	Italy
XLAB	Xlab Razvoj Programske Opreme In Svetovanje D.O.O.	Slovenia
ZECO	3.1.1.1.2 Zeco Di Zerbaro E Costa E C Srl	Italy