SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures

INFRA-2012-2.3.1 – Third Implementation Phase of the European High Performance Computing (HPC) service PRACE

PRACE-3IP

PRACE Third Implementation Phase Project

Grant Agreement Number: RI-312763

D5.3.3
Report on the SHAPE Implementation

Final

Version: 1.0
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Date: 30.01.2015

Project and Deliverable Information Sheet

PRACE Project	**Project Ref. №: RI-312763**	
	Project Title: PRACE Third Implementation Phase Project	
	Project Web Site: http://www.prace-project.eu	
	Deliverable ID: D5.3.3	
	Deliverable Nature: Report	
	Deliverable Level: PU *	**Contractual Date of Delivery:** 31 / January / 2015
		Actual Date of Delivery: 31 / January / 2015
	EC Project Officer: Leonardo Flores Añover	

* - The dissemination level are indicated as follows: **PU** – Public, **PP** – Restricted to other participants (including the Commission Services), **RE** – Restricted to a group specified by the consortium (including the Commission Services). **CO** – Confidential, only for members of the consortium (including the Commission Services).

Document Control Sheet

Document	**Title: Report on the SHAPE Implementation**	
	ID: D5.3.3	
	Version: 1.00	**Status:** ***Final***
	Available at: http://www.prace-project.eu	
	Software Tool: Microsoft Word 2007	
	File(s): D5.3.3.docx	
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	Approved by:	MB/TB

Document Status Sheet

Version	Date	Status	Comments
0.1	6/November/2014	Draft	Structure and first elements of the document
0.2	20/November/2014	Draft	First draft of the 2nd SHAPE Call
0.3	2/December/2014	Draft	Agreed the final structure of the document
0.4	16/December/2014	Draft	Contributions from the SHAPE Pilot
0.5	28/December/2014	Draft	Completion of the SHAPE Pilot contributions
0.6	09/January/2014	Draft	Final polishing and editing
1.0	31/January/2015	Final version	Final version ready for EC submission

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure, industrial Access, SME, SHAPE

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List of Acronyms and Abbreviations

AISBL	Association Internationale Sans But Lucratif (legal form of the PRACE RI)
AMETH	Applied Mechatronic Engineering & Technologies
BSC	Barcelona Supercomputing Center (Spain)
BPI	Banque Publique d'Investissement
CAE	Computer Aided Engineering
CALMIP	CALcul en MIdi-Pyrenees
CEA	Commissariat à l'énergie atomique et aux énergies alternatives (France)
CEO	Chief Executive Officer
CFD	Computational Fluid Dynamics
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
CNR	Centro Nazionale delle Ricerche (National Research Center of Italy)
CPU	Central Processing Unit
CRM	Customer Relationship Management
CSC	Finnish IT Centre for Science (Finland)
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres
DMP	Distributed Memory Processing
EC	European Commission
EESI	European Exascale Software Initiative
EPCC	Edinburg Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)
ETP4HPH	European Technology Platform for High Performance Computing
ESFRI	European Strategy Forum on Research Infrastructures; created roadmap for pan-European Research Infrastructure
FE	Finite Elements
FZJ	Forschungszentrum Jülich (Germany)
GENCI	Grand Equipement National de Calcul Intensif (France)
GmbH	Gesellschaft mit beschränkter Haftung (Limited Liability Company in Germany)
GPU	Graphics Processing Unit
GRNET	Greek Research and Technology Network S.A. (Greece)
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HLRS	High Performance Computing Center Stuttgart (Germany)
IAC	Industrial Advisory Committee
IAP	Integrated Access Programme
ICHEC	Irish Centre for High-End Computing (Ireland)
IDC	International Data Corporation
INRIA	Institut national de recherche en informatique et en automatique
INSEAN	Istituto Nazionale per Studi ed Esperienze di Architettura Navale
IPR	Intellectual Property Rights
IRIT	Institut de Recherche en Informatique de Toulouse
ISC	International Supercomputing Conference
ISV	Independent Software Vendors
IT	Information Technology
JSC	Jülich Supercomputing Centre (FZJ, Germany)
JYD	Juan Yacht Design SL
KI	knowledge and innovation

KPI	Key Performance Indicators
KTH	Kungliga Tekniska Högskolan (Royal Institute of Technology of Sweden)
LES	Large Eddy Simulation
MoM	Method of Moments
MoU	Memorandum of Understanding
MKL	Intel Math Kernel Library
MLACA	Multi Level Adaptive Cross Approximation
MPI	Message Passing Interface
MSCBD	Multi Scale Block Decomposition Method
NDA	Non-Disclosure Agreement. Typically signed between vendors and customers working together on products prior to their general availability or announcement
NNMF	Non Negative Matrix Factorizzation
OEM	Original Equipment Manufacturer
OpenFOAM	Open Field Operation and Manipulation
OpenMP	Open MultiProcessing
OS	Operating System
PETSc	Portable, Extensible Toolkit for Scientific Computation
PM	Person Month
PATC	PRACE Advanced Training Center
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE-1IP	PRACE First Implementation Phase Project
PRACE-2IP	PRACE Second Implementation Phase Project
PRACE-3IP	PRACE Third Implementation Phase Project
PRACE-4IP	PRACE Fourth Implementation Phase Project
Q	Quarter (e.g. Q1 2015 = First Quarter of 2015)
RAM	Random Access Memory
RANS	Reynolds-averaged Navier–Stokes equation
RI	Research Infrastructure
ROI	Return on Investment
ROSPA	RObustness in Safety Performances Analysis
R&D	Research and Development
SaaS	Software as a Service
SC	Super Computing conference
SCRL	Società cooperativa a responsabilità limitata (Cooperative Limited Liability company in Italy)
SHAPE	SME HPC Adoption Programme in Europe
SL	Sociedad Limitadad (Limited Liability Company in Spain)
SME	Small Medium Enterprises
SMM	Small and Medium sized Manufacturers
SRL	Società a Responsabilità Limitata (Limited Liability company in Italy)
SSC	Scientific Steering Committtee
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1
TTR	Time To Result
UC-LCA	University of Coimbra - Laboratório de Computação Avançada (Portugal)
URL	Uniform Resource Locator
WP	Work Package

Executive Summary

SHAPE (SME HPC Adoption Programme in Europe) is a programme defined by PRACE-3IP WP5. The mission of the SHAPE programme is to help SMEs to demonstrate a tangible Return on Investment (ROI) from assessing and adopting solutions supported by HPC, thus facilitating innovation and/or increased operational efficiency in their businesses. Within this programme, selected PRACE partners can provide expertise, training (e.g. through the PATC network) and resources (within regular PRACE Preparatory Calls) to SMEs in order to overcome the barriers to HPC adoption: lack of expertise, high entry cost and excessive risk of trying out new solutions.

After a successful pilot phase, the SHAPE Programme is now operated as a permanent service by the PRACE aisbl with the support of adequate resources of the Project.

During the PRACE-3IP extension[1] period PRACE-3IP WP5 performed a follow-up action toward the SMEs involved in the SHAPE pilot, in order to monitor the benefits of participating in the pilot and evaluate possible ROI and business impact obtained by the SMEs by means of the HPC adoption. The follow up action pointed out that in almost all the cases the pilot has been of real value to the SMEs with tangible measures of the return on investment for the SHAPE work, as presented in this deliverable.

Furthermore, the deliverable presents the work done by WP5 to assist the PRACE aisbl in launching and disseminating the official call of the SHAPE programme, after the conclusion of the pilot, including the support to the evaluation committee during the review process of the submitted applications. The call has been launched on November 10th 2014 and closes on January 15th 2015. At the closing of the call 12 Applications have been submitted: four from France, four from Italy and one each from Finland, Germany, Spain, and Switzerland.

[1] PRACE-3IP Extension denotes the period of M25-M31 extending the work of WP2 – WP7 by seven month in order to ensure a seamless and continuous support of the project for the PRACE RI prior to the planned start of the PRACE-4IP project in H2020.

1 Introduction

The SME HPC Adoption Programme in Europe (SHAPE) is a pan-European programme to support the adoption of High Performance Computing (HPC) by European small to medium-size enterprises (SMEs) developed by PRACE [1] under its PRACE-3IP European Commission funded project.

The SHAPE programme has been designed in the PRACE-3IP Deliverable 5.2 [2] and just after that, a smaller-scale SHAPE pilot programme was conducted to assess and refine the SHAPE offering as documented in the PRACE-3IP Deliverable 5.3.1 [3]. At the conclusion of the pilot, PRACE-3IP WP5 recommended to PRACE aisbl the implementation of the programme on a permanent basis. See Deliverable 5.3.2 [4].

The PRACE Council on 3-4 June, 2014 decided to operate the SHAPE Programme as a permanent service. The decision established that the Programme should be run by PRACE aisbl with the support of adequate resources of the Project, involving PRACE Members with SME-related expertise. Furthermore, the involvement of the Tier-1 centres, relying on existing national initiatives towards SMEs was judged of key importance for the success of the Programme.

During the PRACE-3IP extension period (1 July, 2014 – 31 January, 2015) WP5 was granted with some resources to assist PRACE aisbl in running the official call of the SHAPE programme after the conclusion of the Pilot and assist the evaluation committee in selecting the applications presented by SMEs. This deliverable describes the work done by PRACE-3IP WP5 in this context.

Section 2 describes the results of a follow-up action issued with the SMEs involved in the initial SHAPE Pilot, some month after the conclusion of the pilot itself. The objective of this follow-up was to better understand how taking part in the pilot has affected these SMEs, whether they are planning to use HPC solutions, how these are provided and to evaluate if a possible return on investment (ROI) and business impact has been obtained.

Section 3 presents the activity done to assist the PRACE aisbl to launch the SHAPE second call (the first call being the pilot), disseminate the information and help the SMEs in the submission of the applications. Finally Section 4 draws some conclusions.

The Deliverable is intended to support the PRACE aisbl in the permanent implementation of the SHAPE programme. The intended audience is primarily the PRACE RI, the SMEs, industrial users and stakeholders who consider access to HPC expertise and resources an important instrument to enhance their competitiveness. The information in this deliverable, mainly the ones related to ROI and feedback from the SMEs, are important also for the ETP4HPC platform as this information can influence suppliers of HPC.

In addition, the service providers involved in HPC activities can find in this deliverable information allowing them to cooperate with SMEs after the SHAPE experience, issuing a synergetic action with SHAPE and SMEs.

2 Follow-up to the initial SHAPE Pilot

In this section the projects which participated in the inaugural SHAPE programme are revisited. This is in order to quantify the success of the SHAPE pilot programme: have the participating SMEs adopted HPC, have they a measurable return on investment as a consequence, do they see cost savings or reduction in lead times through their use of HPC, and so on.

The material in this section is based primarily on feedback obtained directly from the SME partners and as such represents a realistic picture of the outcomes of the pilot. These outcomes are summarised in the final subsection.

2.1 Thesan: Design Improvement of a rotary turbine supply chamber through CFD analysis

Company name: Thesan srl (Italy)
SHAPE contact: Roberto Vadori (Thesan), vadori@thesan.com
Technical partners: CINECA (Italy)

2.1.1 *Project Overview*

The project involved Thesan srl, a small Italian company active in the field of renewable energy production, and CINECA as the participating HPC Centre.

This work dealt with the optimization of a volumetric machine that would have opened a totally new market for the company. Thesan had the machine under active development, with a prototype working and fully monitored in an experimental mock-loop setup. This prototype operated under controlled conditions on a workbench, giving as an output the efficiency of the machine itself, much lower than the design target.

The main goal was to obtain increased efficiency through the design and realization of the moving chambers in which fluid flows thanks to an extensive CFD modelling and simulation campaign. This required performing virtual tests on different design solutions to measure the physical quantities and assessing the performance of a given geometry. The final goal was to design a better geometry of the different components, mainly the supply and exhaust chambers, cutting down time and resources needed to build a physical prototype and to limit the physical realization only on a single geometry of choice.

The CFD modelling allowed, through scientific visualization, to perform a detailed characterization of the fluid dynamics patterns present within the prototype and to identify the main geometrical parameters able to drive the optimal configuration. High Performance Computing facilities and Open-Source tools, such as OpenFOAM, were of prime interest to handle the complex physical model under consideration and to perform a sufficient amount of design configuration analysis. For more information see [5].

2.1.2 *HPC Usage*

Following the experience of the SHAPE pilot project, Thesan has redesigned and re-implemented its design cycles, mainly in CFD activities. Even if an investment in terms of hardware is not planned in the near future, Thesan will actively seek opportunities offered by the EC to obtain CPU time and support from the experts at PRACE Centres, with HPC activities being part of the design process from now on. Thesan chose to focus on the development of in-house expertise in the use of open-source CFD codes and automatic launching procedures, leaving the burden of optimizing HPC procedures elsewhere.

A junior engineer was hired, received training through the PATC offering at CINECA, and the collaboration with CINECA experts during the project was an important step for on-the-job training.

2.1.3 *Business impact of the pilot*

As the pilot applied to a prototype of a machine not yet on the market, and a totally new market opener for the company, it is hard to make an estimation of expected revenues.

It is however possible to estimate the ROIs in term of money saved using in-silico models instead of physical prototypes. To develop the first physical prototype and to perform the experimental measurement campaign Thesan spent between 20 and 30 thousand Euros and this involved about 8 months of effort for a team of skilled personnel. Building each new physical prototype to test new configurations in successive design iteration cycles would cost about 8 thousand Euro and it will involve personnel activity for about 4 months.

This pilot project showed that CFD-based prototyping using open-source tools on HPC systems allows a dramatic reduction in costs. A complete analysis of a new configuration requires about 15-20 thousand core hours (for a rough estimate of 4 thousand Euros in computing costs at market value) and only 1 month for data achievement (here data interpretation and decision making is the main bottleneck).

The Thesan SHAPE pilot has been awarded the *IDC (International Data Corporation) HPC Innovation Excellence Award*, on June 24th 2014 during the ISC 2014 conference in Leipzig, (https://www.hpcuserforum.com/innovationaward/winners.html). These awards are granted twice per year (in June and November during the ISC and SC conferences respectively) to success stories involving HPC in science and industry, demonstrating ROI of adopting HPC and justify HPC investments, especially for SMEs.

2.2 AlbaTERN: Numerical Simulation of Extremely Large Interconnected WaveNET Arrays

Company name: AlbaTERN (UK)
SHAPE contact: Bill Edwards (AlbaTERN), bill.edwards@albatern.co.uk
Technical partners: EPCC (UK)

2.2.1 *Project Overview*

Albatern develop novel interconnected offshore marine renewable energy devices. The goal of the project was to formulate a multibody dynamics code capable of simulating a large scale WaveNET array (100 or more devices, including over 1300 interconnected bodies) using HPC techniques to extensively parallelise the solution in collaboration with EPCC at the University of Edinburgh.

Albatern focussed on prototyping a full physics simulation of a Squid renewable energy device. EPCC developed a parallel implementation of simplified physics simulation suitable for execution on distributed memory processing (DMP).

Albatern created a prototype impulse based multibody dynamics simulator, following an approach suitable for parallelisation on DMP machines. The prototype solver was constructed in MATLAB as a technology demonstrator and proof of concept. The principal challenges in the development of the solver were maintaining numerical stability while managing error correction and managing computational effort. For more information see [6].

2.2.2 *HPC usage*

Currently Albatern are working on implementing their prototype solver in the manner demonstrated by the EPCC prototype solver that was developed during the SHAPE project.

A requirement of the project is to produce a cross-platform compatible software solution that is capable of parallelisation on distributed computing platforms. While Albatern use Windows OS exclusively for simulation and analysis work, the majority of distributed computing is performed on a Linux OS. Therefore, to be able to produce software capable of running in both environments is a considerable advantage.

Adapting the Albatern prototype solver to utilise the PETSc parallel computing libraries in the same manner as the solver developed by EPCC is the current principle activity. Without an example implementation using the EPCC supercomputer, Archer, it would be difficult to for Albatern to understand how to implement an appropriate solution.

However, it has been found that PETSc requires a high level of technical expertise to use it effectively and has poor support for compilation on Windows OS. As an alternative to the PETSc library, Albatern are also evaluating an open source multi-physics library called Chronos Engine, also with support for distributed parallel computing through MPI on Windows and Linux OSes.

When an appropriate solver is complete it will be possible to estimate the compute resources required for the various different scales of simulation Albatern wish to undertake. Affordable distributed computing such as the HPC facilities at EPCC will be evaluated as well as other cloud computing resources such as Microsoft Azure.

Ultimately, HPC and cloud computing services are an important consideration for Albatern in the long-term as they reduce the need for IT infrastructure investment and maintenance and can be used in service style.

2.2.3 *Business impact of the pilot*

Albatern is engaged in a long term research and development program to develop WaveNET wave energy technology. The use of HPC computing capabilities is seen as a necessary tool to predict the combined system behaviour of large arrays. In some respects, this is a future proofing exercise for the company as large arrays are not expected to be deployed for several years and will in any case be conditional on the success of the current ‘Small Array’ demonstration program.

The pilot project has allowed Albatern to add definition to the technology development road map, providing a clearer route to market and further investment. The capabilities demonstrated during the pilot project will form the basis of an ongoing software development project that will, once complete and producing verifiable results, dramatically reduce the time to assess system loads and performance for new wave energy projects and therefore the time to bring new wave energy capacity on line. In combination with Albatern’s proprietary technology, this will give the company a powerful commercial advantage within this new market sector.

2.3 NSilico: High performance computation for short read alignments

Company name: NSilico (Ireland)
SHAPE contact: Paul Walsh (NSilico), paul.walsh@nsilico.com
Technical partners: ICHEC (Ireland), GENCI (France)

2.3.1 *Project Overview*

NSilico is an Irish based SME that develops software for the life sciences sector, providing bioinformatics and medical informatics systems to a range of clients. One of the major challenges that their users face is the exponential growth of high-throughput genomic sequence data and the associated computational demands to process such data in a fast and efficient manner. Genomic sequences contain gigabytes of nucleotide data that require detailed comparison with similar sequences in order to determine the nature of functional, structural and evolutionary relationships. The project aimed to identify relevant bioinformatics codes, followed by parallelisation and porting work using many-core technology that is of interest to Nsilico. The project identified a portable C++ library for implementing the Smith-Waterman algorithm. The library was then parallelised using OpenMP and ported to run on Intel Xeon Phi co-processors. This process has also generated useful documentation and valuable experience for Nsilico. For more information see [7].

2.3.2 *HPC usage*

Nsilico has taken a keen interest in HPC adoption, including the use of in-house many-core technology. As the final code from the project still requires more work and next-generation hardware to realise performance benefits, there has been discussions on potential future opportunities for follow-on work, potentially in collaboration with HPC experts from PRACE partners, on the next generation of the Intel Xeon Phi co-processor.

2.3.3 *Business impact of the pilot*

Nsilico has gained access and experience working on the Spanish PRACE Tier-0 system (MareNostrum) as part of this project, as well as their in-house system. The company has learnt both the limitations and the potential of many-core technology, including deployment issues and general challenges that one faces when porting codes onto specialised HPC hardware. This knowledge and experience have been of tremendous value to the company going forward.

2.4 Audionamix: Unmix Up

Company name: Audionamix (France)
SHAPE contact: Pierre Leveau (Audionamix), pierre.leveau@audionamix.com
Technical partners: GENCI (France)

2.4.1 *Project Overview*

Audionamix is a technology company developing audio unmixing technology, which relies on computationally intensive optimization algorithms. The source separation technology developed by Audionamix requires a significant amount of computation. To increase the speed of the technology, several High Performance Computing libraries for linear algebra have been benchmarked with two applications: a simple matrix multiplication and a Non-Negative Matrix Factorization. The benchmarked libraries were Eigen, Armadillo, MKL and the GPU library Magma. The benchmark returned that for both applications the GPU-based solution performed better than the other solutions. But among CPU based solutions, Eigen performed better on a complex task than MKL. Thus, the Magma library as an Eigen back-end seems to have a good potential for HPC-based linear algebra, since this solution would benefit at the same time from the GPU-accelerated computation of Magma and from Eigen's optimized data transfer. For more information see [8].

2.4.2 *HPC usage*

HPC has been integrated in the technological core of the company: the unmixing technology can now be compiled with a GPU-powered factorization engine. The intern who was working on the topic is now hired as a permanent employee. Further work on HPC will be triggered depending on the new algorithms that will be produced by R&D.

2.4.3 *Business impact of the pilot*

The GPU solution has not been deployed in production yet due to time constraints and other competing projects. Deployment is expected in Q1 2015. The main expected outcomes are an improvement user experience for our customers (getting results faster), and possibly a reduction of the costs (less servers to operate). The real value of the pilot will be evaluated in the light of the new business results, both in terms of existing product sales that will benefit from these advances, and also of licensing opportunities.

2.5 Juan Yacht Design: Testing LES turbulence models in race boat sails

Company name: Juan Yacht Design SL (Spain)
SHAPE contact: Gonzalo Kouyoumdjian (JYD), gonzalo.k@juanyachtdesign.com
Technical partners: BSC (Spain)

2.5.1 *Project Overview*

The objective of this project was to implement Large Eddy Simulation (LES) turbulence models outside the academic world to simulate flow around sails to replace RANS models that are the standard in the industry. The implementation and testing in the finite code ALYA was performed by the Barcelona Supercomputing Center so that Juan Yacht Design SL (JYD) could appreciate the advantages of using a LES formulation for their problem. The results showed that LES can provide significant advantages over RANS simulation, at least for the cases studied. There is a significant difference in the predicted forces that can be related to the fact that RANS cannot accurately capture two vortices created at the top and bottom of the genoa sail. For more information see [9].

2.5.2 *HPC usage*

To implement LES simulations more parallel computing resources are required, to reduce not only computing time but to increase memory available since LES requires denser meshes. The in-house HPC capacity was not increased but JYD invested in upgrading to Infiniband in order to use all their computing cores and RAM memory available in each simulation rather than running several simulations simultaneously in a lower number of CPUs and memory.

They use their own HPC resources but are considering buying computing time from outside suppliers when there are peaks of workload. HPC has been a key intrinsic part of their business and will continue to be, this explains the importance for JYD to have access to the latest technology and developments. This also explains why such a SME has in-house expertise on HPC.

2.5.3 *Business impact of the pilot*

The use of RANS turbulence models – a pioneering adoption of Computational Fluids Dynamics (CFD) – has enabled Juan Yacht Design to put aside the need for towing tank experimental tests, a key competitive advantage in a cut-throat industry.

One of the main findings of the project is a concrete evaluation of the advantage of using LES over RANS: the latter not accurately capturing the two vortices created at the top and bottom of the genoa sail, a problem that LES adequately resolves.

"With the support of the technical experts at the Barcelona Supercomputing Centre and the use of their in-house multi-physics simulation code, Alya, we were able to scale out our models up to 1024 cores of the MareNostrum machine and run the simulations there more efficiently than would ever be possible on our own machine," says Mr.Juan Kouyoumdjian, CEO of Juan Yacht Design. "The experience gained in this project will put us ahead of our competitors, having now a tool to simulate the aero around the sails in great detail and services our customers better with the results."

JYD are rerunning the case on their own HPC system and testing the LES models and configurations in other cases in order to have it implemented. At the same time they are modifying their systems so that the LES runs can be executed automatically without human intervention similar to the situation right now for the RANS cases. They expect to use LES simulations on their projects in the upcoming months. The results were so encouraging that JYD are planning on offering it to projects other than those of JYD. This would require increasing the HPC capacity. It is difficult to measure return on investment when using what was developed and learned on projects that JYD would have had even without LES or to measure how much of the revenue in the future could come from the benefit of using LES. Certainly there would be a contribution since one of the reasons clients come to JYD is because of the ability to simulate accurately. However, when opened for use in projects outside JYD as planned in the next 12 months the revenue generated would be mostly due to the LES capability developed on this SHAPE pilot project.

2.6 OPTIMA Pharma GmbH: Enhanced airflow simulations around filling machines in clean rooms

Company name: OPTIMA Pharma GmbH (Germany)
SHAPE contact: Ralph Eisenschmid (OPTIMA Pharma GmbH)
ralph.eisenschmid@optima-pharma.com
Technical partners: HLRS (Germany)

2.6.1 *Project Overview*

OPTIMA pharma GmbH (Schwäbisch Hall, Germany) produces and develops filling and packaging machines for pharmaceutical products. Sterile filling lines are enclosed in clean rooms, and a detailed and reliable knowledge of the airflow in the clean rooms enhances the design of the filling machines according to the customers' requirements. During this SHAPE project, the open source CFD software OpenFOAM® was instrumented on the Tier-0 system

Cray XE6 ("Hermit") at HLRS for running airflow simulations meeting the requirements of industrial production. For more information see [10].

2.6.2 *HPC Usage*

The SHAPE project enabled OPTIMA pharma to run their airflow simulations on a Tier-0 system and to enhance the quality of these simulations so that they are a regular and important part of the CAE process now. In the future, OPTIMA pharma, as a customer of HLRS, will utilize the acquired knowledge and experience in order to simulate airflows in clean rooms on Tier-0 systems at HLRS.

2.6.3 *Business impact of the pilot*

The work done during the SHAPE project substantially enhanced OPTIMA pharma's market position. Due to the SHAPE project, the airflow simulations are much faster and cheaper than before and are commonly utilized in the internal R&D processes now. Furthermore, OPTIMA pharma has offered major customers specific simulations of ordered filling machines for the customers' marketing policies.

2.7 AMET: Robustness in safety performances analysis

Company name: AMET srl (Italy)
SHAPE contact: Paolo Cavallo (AMET srl) paolo.cavallo@amet.it
Technical partners: CINECA (Italy)

2.7.1 *Project Overview*

Project ROSPA (Robustness in safety performances analysis) was performed by AMET and CINECA; AMET is a high-tech engineering company, active in the design and development of mechanic and mechatronic products and processes, based on numerical simulation. AMET, the acronym of Applied Mechatronic Engineering & Technologies, was established in 1999, as a spin-off of the Mechatronics Laboratory of the Politecnico di Torino. AMET and CINECA have partnered within the framework of the SHAPE Pilot to investigate the direct and mutual influence of the characteristic parameters that constitute the material card of a composite material, as used in commercial Finite Elements (FE) codes, in order to have a better understanding of these phenomena with the final aim of being able to deal with development projects with a higher confidence in the numerical results, thus reducing the costs of the experimental tests. The project outcome allowed AMET to fortify previously obtained results, extending their field of application to more standard problems and confirming tendencies and mutual relationships among parameters. For more information see [11].

2.7.2 *HPC usage*

HPC was the key to the success of the pilot project ROSPA: only through massive calculations has it been possible to investigate the mechanical behaviour of materials in the case of impacts, taking into account all the possible mutual relationships. The pilot project has clearly shown to AMET management the possibilities of HPC, and it has fortified the growing plans through a mixed use of resources (in-house for standard applications, HPC providers for high-end applications).

For the Pilot purposes, 32,768 runs (using the Altair Radioss solver) with 8 parallel threads were performed on CINECA Tier-1 system PLX, using a total of about 300,000 CPU hours. We acknowledge the support from Altair Engineering, which provided a license for the project aims. The number of parallel threads for the single runs was not dictated by software scalability, but as an equilibrium between software efficiency and cluster availability, due to the high number of runs.

It was estimated that with their in-house computing capability, AMET would have taken more than 7,000 days to perform the computational analysis.

2.7.3 *Business impact of the pilot*

The pilot project has greatly improved knowledge about the numerical representation of composite materials concerning impact behaviour; this gained knowledge will allow AMET to offer their high-end customers (Ferrari, McLaren, Dallara, etc.) a more robust approach when dealing with crash analysis of sport vehicles. This competence will put AMET in a better position when bidding for new projects, and moreover it will allow a way for more efficient management of the work once the project has started. No direct ROI was expected by the pilot; the focus was on increasing competence, and this was fully accomplished.

At the end of the Pilot, AMET has signed an open contract with CINECA to further pursue this project, and they will continue to rely on CINECA experts for any further HPC application.

2.8 Nexio Simulation (formerly ENTARES Engineering): *Electromagnetic simulation for large model using HPC*

Company name: Nexio Simulation Group (formerly ENTARES Engineering) (France)
SHAPE contact: Pascal de Resseguier (Nexio) pascal.de-resseguier@entares.com
Technical partners: GENCI (France)

2.8.1 *Project Overview*

The objective of the project was to adapt the electromagnetic software CAPITOLE developed at Nexio Simulation (ex-ENTARES Engineering) to HPC machines. This has been possible with the aid of the SHAPE pilot project, which has provided HPC expertise and computation hours on MareNostrum III. Two numerical methods have been investigated to solve the resulting dense MoM linear system, MSCBD and MLACA. A new implementation based on asynchronous tasks has been performed for the direct method MSCBD. Dependencies between tasks need to be well defined before moving to a runtime scheduling such as STAR-PU. As for the iterative method MLACA, a hybrid MPI-OpenMP parallelization has been implemented with excellent results. So far, electromagnetic models up to 6 million unknowns have been properly solved. For more information see [12].

2.8.2 *HPC usage*

This project has helped Nexio to continue developing the HPC version of their program. The main work is to test it on larger and larger models and optimize the computational time, scalability and the use of memory.

Nexio had some interesting discussions with research teams from different laboratories specializing in HPC (IRIT, INRIA, CALMIP) and it has been a very useful help for them. Their use of libraries (like TSCOTCH, MUMPS, STAR-PU) has greatly increased, as they are already optimized for HPC machines which reduces the development time and increases performance.

2.8.3 *Business impact of the pilot*

While the maximum size of simulation was about 500,000 unknowns in 2011, Nexio Simulation was able to simulate 6 million unknowns thanks to the use of PRACE Tier-0 resources and support in the context of the SHAPE project. This major improvement allowed Nexio Simulation to win two major contracts with Japanese aerospace companies and to port their application on Cloud Services using the Fortissimo project.

Furthermore, on 18 November 2014, International Data Corporation (IDC) awarded Nexio Simulation the HPC Innovation Excellence Award at the SC'14 high performance computing (HPC) conference in New Orleans, Louisiana, increasing their international visibility. See: http://www.idc.com/getdoc.jsp?containerId=prUS25250214

The expected business impact is to commercialize the HPC version of the CAPITOLE software all over the world. It is expected that half of the sales of CAPITOLE in the future will be with the HPC version. Nexio have observed an increasing demand to solve bigger models and an increase in the operating frequency of telecommunication devices.

2.9 Lapcos: Virtual Test Bench for Centrifugal Pump

Company name: Lapcos SCRL (Italy)
SHAPE contact: Daniele Bucci (Lapcos SCRL), daniele.bucci@lapcos.it
Technical partners: CINECA (Italy)

2.9.1 *Project Overview*

The goal of the Lapcos pilot project was to adapt an existing software solution for a specific engineering problem to run on a HPC facility, and make this accessible with a remote interface for end users as a SaaS platform. It has succeeded in (a) reducing the computational time and (b) simplifying for the end user the set-up and installation of such tool. The OpenPump application, developed by Lapcos was successfully compiled and installed on a CINECA supercomputer and integrated with the platform. The application was made accessible from the webcompute portal available at CINECA. A scalability analysis was conducted in order to correctly size the simulations. With the current software and hardware architecture, a speed-up of 20x can be achieved in compute-intensive simulations with the potential to significant reduce the time-to- market for centrifugal pump manufacturers. For more information see [13].

2.9.2 *HPC usage*

Lapcos Scrl is an SME-sized engineering firm that supports its customers in performing product development and R&D. Their HPC usage was established well before the participation in the SHAPE experiment. Indeed, one of their customers, a centrifugal pumps manufacturer, experienced very effective reduction in time-to-results (TTRs) by using HPC infrastructure without any other restriction due to excessive license fees. The "cloudification" of the specific task developed during the experiment is leading this end user to adopt HPC in its internal process by buying cycles. The completeness and the agility of the proposed solution were key factors for its adoption. A similar business model will be adapted with another pump manufacturer in the Northern Italy area.

2.9.3 *Business impact of the pilot*

The outcome of the project, a tailored virtual test bench for centrifugal pumps based on CFD simulation run on HPC infrastructure with a technician-friendly user interface, has been successfully demonstrated to a Lapcos customer and they are striving to adopt it as a production tool for virtual prototyping purposes. The solution, hosted in CINECA, is then sold by Lapcos, who provide technical support and training to its customers. This beta testing phase is still on-going but it can be considered successful.

At the same time, the OpenPump application might be marketed jointly by CINECA and Lapcos as a vertical solution based for the pump manufacturers. A market research exercise has been carried out and it is estimated that in Italy alone there are a hundred active companies that could be interested. The potential market, estimated in terms of licensing and compute cycle sales could range between 1 to 5 million €: the benefits for the end users are the reduction of TTRs, which lead to a consequent reduction in a time to market which is a key aspect in a very competitive market such as centrifugal pumps.

2.10 Monotricat Srl: Hull resistance simulation for an innovative hull using OpenFOAM

Company name: MONOTRICAT s.r.l (Italy)
SHAPE contact: Luigi Mascellaro (Monotricat s.r.l), monotricat@hotmail.com
Technical partners: KTH (Sweden); CINECA (Italy)

2.10.1 *Project Overview*

MONOTRICAT SRL is an Italian company that designs an innovative type of hull (MONOTRICAT), which is characterized by being highly efficient in hydrodynamic terms compared to other types of hulls. The aim of MONOTRICAT´s hull architecture is to obtain higher efficiency and larger load capacity. However the design and development processes for new hulls are very expensive and time consuming. In order to obtain extensive measurements relating to the performance of a new or improved hull, a robust and thorough test phase is required. For the MONOTRICAT hull, tests were run in the naval basins of Rome (CNR-INSEAN) and Trieste using a large number of models, and thus with a large expenditure of time and effort, and with resulting high costs.

The aim of this particular PRACE SHAPE project was to develop accurate and reliable CFD tools that MONOTRICAT can use to replace the highly expensive field tests. Moreover the project has produced a tool that can be used to better understand the hydrodynamic behavior of hulls and that also provides a quick, easily accessible and scalable HPC-based service that will optimize the research and development costs for the company. In this project not only the performance analysis was conducted, but also whole hull simulation processing, e.g. mesh generation of complex geometries, efficient solvers with various turbulence models and optimized parameters as well as visualization. These projects created a possibility for MONOTRICAT to take advantage of HPC enabled simulation tools and potentially replace the traditional methods. For more information see [14].

2.10.2 *HPC usage*

Thanks to the study conducted by the SHAPE PRACE project, MONOTRICAT has seen that the results obtained with HPC are comparable with those obtained in a Towing Tank within a good approximation. This allows MONOTRICAT to continue the project more rationally as it allows changing the design of the model and immediately observing the results that are new and which directly improve the product.

It became obvious that there is a need to make many changes in this hull. From previous experience it is known that it can be especially improved in the range of medium to high speeds, in order to use this hull in fast passenger transport. MONOTRICAT would be happy to make use of any future opportunities to use HPC via PRACE.

2.10.3 *Business impact of the pilot*

So far there has not been a direct measurable return on investment because, differently from other commercial products, a boat, after a a first proposal to the owners, requires a number of CFD studies that demonstrate not only towing but also self-propulsion, in order to verify the developmental ability, the capability to face adverse weather conditions (seakeeping) and many other tests designed to attain a certification that allow its use in the sea.

However, HPC has enabled a reduction in costs as MONOTRICAT can now exclude certain models and testing tank sessions.

In conclusion MONOTRICAT felt that the SHAPE PRACE project was of real value for the company.

2.11 Summary of the Project Outcomes

It is apparent from the reports described above that there have been many positive outcomes for the businesses involved in the SHAPE pilot. This section will briefly summarise highlights of those outcomes.

Thesan – have hired a junior engineer. Physical prototyping can be replaced with CFD-based prototyping reducing costs and time from approximately 30,000 Euros, 8 months effort, to 4000 Euros, 1 month effort.

Albatern – have now been exposed to HPC and are continuing to develop their model, with the expectation of using Cloud/HPC in the future to reduce time to assess system loads and performance and thus the time to bring new wave energy capacity on line.

Nsilico – exposed to HPC and are investigating follow-up projects to further enhance the code produced in the pilot.

Audionamix – intern hired for the SHAPE pilot is now a permanent employee. The production code should be released Q1 2015, with expectation of faster results for users and potentially lower costs (less servers to operate). Potential for future HPC work as new algorithms are developed.

Juan Yacht Design – the new LES capability developed in the pilot has allowed them to offer their customers more detailed and accurate results of the aero-sail simulations. Upgrading their inhouse HPC facilities. Good future revenue potential for the LES capability.

OPTIMA Pharma – will continue to use HPC facilities via PRACE partners. Their simulations can now be run much faster and cheaper, and they can now offer customers specific simulations for their ordered machines.

AMET – exposed to HPC and performed simulations in a matter of hours which would have taken years with their in-house facilities. They can now offer their customers improved competency, and they are continuing to work with their PRACE partner to further pursue the project.

Nexio – have now an HPC version of their program, the performance of which has assisted them in winning two new major contracts. They intend to commercialise the HPC version as they have observed a demand from customers for solving larger models.

Lapcos – their CFD simulation can now be run on HPC infrastructure, with an improved user interface. Already one customer is looking to adopt this new approach. In the future there is a huge potential market for the OpenPump application.

MONOTRICAT – HPC has enabled a reduction in costs for the SME allowing the possibility to exclude certain models and testing tank sessions.

So, to summarise, in many of the pilot projects there are already tangible measures of the return on investment for the SHAPE work – staff have been employed, contracts have been won, costs have been reduced. For those where there is not yet any measurable ROI, there is optimism that the improvement in the service or software solution that the companies offer will lead to an increase in customers, or that the companies research and development will be accelerated along with reduced costs as a direct consequence of adopting HPC. In addition there is a commitment to continue working with HPC in the future from all the projects, be that in-house, or via further access to PRACE resources.

3 SHAPE Second Call for Applications

After the successful conclusion of the SHAPE Pilot, the PRACE aisbl decided to implement the SHAPE programme on a permanent basis with the support of adequate resources from the Project. The PRACE aisbl will organise the calls, their management, including the related review process, and the Project will perform the support of the selected proposals. In October 2014, the PRACE aisbl decided to launch the PRACE second call in November 2014 (the first call has been identified with the SHAPE Pilot).

This section describes the activity done by PRACE-3IP WP5 during the extension period to assist the aisbl in launching the SHAPE second call. The cooperation involved, from one side, the organisation of the call including the publicity and, from the other, a direct dissemination activity with the SMEs to specifically publicise this opportunity.

3.1 The Launch of the Call

Starting on October 2014, the members of PRACE-3IP WP5 worked in close collaboration with the PRACE aisbl office to prepare the launch, on the basis of the PRACE aisbl mandate.

The call aims to work with selected SMEs and introduce HPC-based tools and techniques into their business, operational, or production environment. It is open to all European SMEs that have an interesting idea that can be implemented using HPC. The selected solutions should bring a potential tangible Return on Investment to their business. Following an open selection process based on business and technical criteria, the project work will involve the following:

- Defining an appropriate HPC model for the selected solution;
- Assessing the solution's business and technical viability;
- Possibility of using PRACE's resources in order to test the solution (through PRACE Preparatory Access in an open R&D model).

The call has been opened on **10 November, 2014** with a closing date of **15 January, 2015**.

The SHAPE section of the PRACE Web site has been re-organised to better evidence the activity and enlighten the call. See http://www.prace-ri.eu/SHAPE and the sub-sections:

- SHAPE Pilot Call
- SHAPE 2nd Call
- SHAPE Related News

The on-line project proposals submission form has been revised with respect to the one of the pilot and it is available at http://prace-ri.eu/shape-application-form

3.2 Publicity and Dissemination Activity

A wide publicity of the call started just after its launch. A Press release was issued on 10 November, 2014 (see http://www.prace-ri.eu/shape-secondcall-launch-pr/).

The notice of the call has been constantly highlighted on the PRACE web site by means of a scrolling banner reporting the following advertisement:

Second Call for Applications now open!

The text of the call has been widespread through the general PRACE Mailing list and the mailing lists of the PRACE Members. Furthermore some PRACE Members linked the notice on their own Web sites.

During Supercomputing 2014 (http://sc14.supercomputing.org New Orleans, LA, 16-21 November, 2014) the Press release and the information was disseminated at the PRACE booth.

The recipients of the mailing list shape@prace-ri.eu, which is used as contact address for SHAPE, has been updated with the names of the PRACE-3IP WP5 partners involved in the SHAPE activity and members of the PRACE office. In this way a good number of competent people are available to answer the questions and provide information to the potential SHAPE applicants.

Since the launch of the call, the members of PRACE-3IP WP5 activated specific contacts with different SMEs in order to explain them the opportunity of the SHAPE programme and assist in case they are willing to submit applications. This activity continued from November to the closing date of the call and was coordinated by means of biweekly teleconferences between the members of WP5.

On 18 November, 2014, at Supercomputing 2014, PRACE SHAPE has been awarded the *HPCwire Readers' Choice Award for the best HPC Collaboration between Government & Industry*. See: http://www.hpcwire.com/2014-hpcwire-readers-choice-awards/20/.

The motivation was: "**PRACE SHAPE helps European SMEs overcome barriers to using HPC**. *In order to draw more small- and medium-sized enterprises (SMEs) to HPC usage, PRACE initiated SHAPE: SME HPC Adoption Programme in Europe in September 2013. The project helps European SMEs to overcome barriers to using HPC, such as cost of operation, lack of knowledge and lack of resources. It facilitates the process of defining a workable solution based on HPC and defining an appropriate business model. So far, 10 SMEs from six different countries have successfully used SHAPE services and demonstrated tangible results and ROI in using HPC in their business models. Since the successful first pilot, SHAPE is now a permanent service of the PRACE Research Infrastructure and new calls for proposals are planned for the end of 2014."*

The HPCwire awards each year are determined by HPCwire's readers across the HPC community, to recognize the most outstanding individuals and organizations in the industry. The receipt of the award was the occasion to further publicise the second call for applications.

3.3 The Review Process

The PRACE aisbl defined the rules for the review process of the applications submitted to the second SHAPE call, based on recommendations draws from the experience from the SHAPE Pilot. See [2] and [3].

The two main criteria considered for the review of the applications are:

- Strength of the business case;
- Technical Adequacy.

Other aspects to consider in the evaluation are:

- The commitment of the SMEs to co-invest with PRACE in achieving the project goals;
- The innovative aspect of the proposed solution;
- The social and economic *impact on society as a whole*.

The Selection Committee will consist of two representatives each of the PRACE Industrial Advisory Committee (IAC), the PRACE Board of Directors (BoD) and the PRACE IP Project.

The two representatives proposed by the PRACE Project are:

- Marcin Ostasz (BSC, ES)
- Paul Graham (EPCC, UK)

These two names will be approved by the PRACE Management Board.

The two names designed by the IAC and the two designated by the BoD are expected to be nominated before the closing of the call on January 15th 2015.

In this way, the Review Panel, in charge of evaluating the applications, will immediately start the evaluation and will create a ranked shortlist no later than 15 February, 2015. Then, the PRACE Management Board will make the final decision on the successful proposals selection from the shortlist.

Successful applicants will have access to PRACE resources as of **1 March, 2015** and will complete their activity in no more than 12 months.

At the closing of the call 12 Applications have been submitted: four from France, four from Italy and one each from Finland, Germany, Spain, and Switzerland.

The accepted applications will run with the resources foreseen in PRACE-4IP WP7 – provided this project is granted under Horizon 2020. The PRACE experts will work with the selected SMEs in order to develop their solutions, providing the participating SMEs with knowledge that will allow them to make an informed decision on the selected HPC solution.

4 Conclusions

This Deliverable has described the work carried out by PRACE-3IP WP5 during the extension period (July 2014 – January 2015). This activity was twofold, from one side it acted as a follow-up action toward the SMEs involved in the SHAPE Pilot after its conclusion in May 2014 and, from the other, it assisted the PRACE aisbl to launch the second call for applications of the SHAPE Programme.

The follow-up actions were intended to understand if and how the participating SMEs intended to adopt HPC as part of their R&D and production process and, in case, to continue to assist them in their decision process.

The feedback obtained directly from the SMEs participating in the SHAPE pilot demonstrated in general a dynamic activity and many positive outcomes for the businesses involved have been presented. In many of the pilot projects there are already tangible measures of the return on investment for the work done, measured in terms of new staff employed, new contracts, reduction of costs, etc. In general a commitment to adopt HPC in the near future has been stated from all the SMEs involved in the SHAPE pilot. The access to HPC is envisaged via in-house solutions, or via further access to the PRACE resources.

PRACE aisbl decided to include the SHAPE programme in its offering of regular services and PRACE aisbl was assisted in the launch of the second call for applications for the SHAPE Programme. At the closing of the call 12 Applications have been submitted.

After the closing of the call, the supporting activity now continues with the task to assist the selection committee in the review process for selecting the applications submitted by the SMEs. The selected applications, once approved by the PRACE Management Board will run using resources that will be made available by PPRACE-4IP WP7.

The activity promoted by SHAPE toward industries and the SMEs in particular, has been recognised at international level with the granting of the IDC HPC Innovation Excellence Awards to two SMEs participating to the SHAPE Pilot (Thesan, June 2014 edition, and Nexio Simulation, November 2014 edition) and the assignment of the HPCwire Reader's Choice Award (November 2014) to SHAPE for the best HPC collaboration between Government and Industry.

The adoption of SHAPE activity among the standard PRACE aisbl actions is strongly encouraged by these awards that confirm the decision to improve the services towards all HPC users.