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Research Infrastructures

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Results of the Integrated Access Programme Pilots

Final

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List of Acronyms and Abbreviations

AISBL	Association Internationale Sans But Lucratif (legal form of the PRACE RI)
BSC	Barcelona Supercomputing Center (Spain)
BPI	Banque Publique d'Investissement
CEA	Commissariat à l'énergie atomique et aux énergies alternatives (France)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
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.
EC	European Community
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)
ESFRI	European Strategy Forum on Research Infrastructures; created roadmap for pan-European Research Infrastructure.
FZJ	Forschungszentrum Jülich (Germany)
GENCI	Grand Equipement National de Calcul Intensif (France)
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)
IAP	Integrated Access Programme
ICHEC	Irish Centre for High-End Computing (Ireland)
IPB	Institute of Physics Belgrade (Serbia)
IPR	Intellectual Property Rights
IT	Information Technology
IPR	intellectual property rights
ISV	Independent Software Vendors
JSC	Jülich Supercomputing Centre (FZJ, Germany)
KI	knowledge and innovation
KPI	Key Performance Indicators
MoU	Memorandum of Understanding.
NCF	Netherlands Computing Facilities (Netherlands)
NCSA	National Centre for Supercomputing Applications (Bulgaria)
NDA	Non-Disclosure Agreement. Typically signed between vendors and customers working together on products prior to their general availability or announcement.
OEM	Original Equipment Manufacturer
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
ROI	Return on Investment
R&D	Research and Development
SaaS	Software as a Service
SARA	Stichting Academisch Rekencentrum Amsterdam (Netherlands)

SHAPE	SME HPC Adoption Programme in Europe
SME	Small Medium Enterprises
SMM	Small and Medium sized Manufacturers
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
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 WP 5. The mission of the SHAPE programme is to help SMEs to demonstrate a tangible Return on Investment (ROI) by 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.

Before implementing the final structure of the programme, a SHAPE pilot was launched in June 2013. The Pilot was set up to test the idea of the programme and the readiness of the PRACE infrastructure and resources to run a permanent programme in this area, while helping a number of European SMEs to adopt HPC.

The pilot involved ten European SMEs from six countries and the related projects were completed in May 2014. The applications covered a wide range of topics demonstrating the interest in HPC of many industrial sectors and the vitality of different SMEs at European level.

The SHAPE Pilot has succeeded in raising interest from a significant number of SMEs in a limited amount of time. The infrastructure and resources of PRACE are well prepared to adopt such work as the projects have been running smoothly, with a number of them already achieving tangible benefits for the SMEs.

The SHAPE Pilot results, documented in this Deliverable have been fundamental in recommending the implementation of the full SHAPE programme by the PRACE AISBL on a permanent basis, as originally defined by PRACE-3IP WP5.

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, presented in the PRACE-3IP Deliverable 5.2 [2] aims to provide European SME the awareness and expertise necessary to take advantage of the innovation possibilities opened by HPC and to increase their competitiveness. The mission of the programme is to help European SMEs to demonstrate a tangible Return on Investment (ROI) by assessing and adopting solutions supported by HPC, thus facilitating innovation and/or increased operational efficiency in their businesses.

Before implementing the final structure of the programme, in order to assess and refine the SHAPE offering, a smaller-scale SHAPE Pilot programme was proposed [3] The SHAPE Pilot's Open Call for SMEs was launched in June 2013, after the approval of the PRACE-3IP Management Board, and closed on 15th September 2013.

The call had a very good response, involving fourteen SMEs, from seven different European countries.

The Review Panel in charge of evaluating the applications identified a group of ten applications for the Pilot activity, based on two main criteria: technical adequacy and strength of the business case.

After the approval of the PRACE-3IP Management Board, the experts, identified among the PRACE 3IP-WP5 partners, worked with the selected SMEs until May 2014 in order to run the pilot, to develop the solutions and to provide the participating SMEs with knowledge that will allow them to make an informed decision on the selected HPC solutions and to plan future actions.

This deliverable describes the results of the pilot, presents some lessons learned and collects feedback from the SMEs and the involved partners, which are useful in producing recommendations to PRACE AISBL for the full implementation of the SHAPE Programme.

Section 2 describes the management of the SHAPE pilot call and the implementation of the pilot itself. Section 3 presents a summary of each pilot project and the feedback from the ten SMEs involved. Section 4 gives a summary of the lessons learned. Finally Section 5 presents some recommendations and draws some conclusions.

The Deliverable is intended to support the PRACE AISBL in the 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. 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 synergic action with SHAPE and SMEs.

2 SHAPE Pilot: Call and Management

This section describes the SHAPE Pilot call and its management after the launch on June 2013.

2.1 The applications

On 15th September 2013, at the deadline of the SHAPE Pilot Call, 14 applications had been submitted from SMEs from seven different European countries (Bulgaria, France, Germany, Ireland, Italy, Spain and UK). The list of applications is reported in Table 1.

Company	Project Title
Albatern Ltd UK	Numerical Simulation of Extremely Large Interconnected WaveNET Arrays
AMET s.r.l. Italy	Robustness in safety performances analysis (ROSPA)
Audionamix France	Unmix Up
Biovet Bulgaria	Overcoming the resistance of the ribosome by new modification of the tiamulin
Do IT Systems s.r.l. Italy	Invisible Cloud
ENTARES Engineering France	CAPITOL-HPC+
INGELIANCE Technologies France	Computational activities development with HPC
Juan Yacht Design, SL Spain	Testing LES turbulence models in race boat sail
Lapcos Scrl Italy	Virtual Test Bench for Centrifugal Pump
MONOTRICAT S.r.l. Italy	CFD simulation of an innovative hull
NSilico Life Science Ltd Ireland	High Performance Computation for Short Read Alignment
OPTIMA pharma GmbH Germany	Enhanced airflow simulations around filling machines in clean rooms
Termo Fluids S.L. Spain	Development of a Multilevel Wind Farm Design Tool
THESAN S.p.A Italy.	Improvement of hydraulic turbine design through HPC

Table 1: ***SHAPE Pilot Application submitted***

2.2 The Review Process

The final proposals went through the following two-stage review process.

1. A Review Panel, issued by the PRACE 3IP Management Board, reviews the applications and creates a ranked shortlist.
2. The PRACE-3IP Management Board makes the final decision on the successful proposals selection from the shortlist.

2.3 The Review Panel

The Review Panel, in charge of evaluating the applications, was composed of the following members:

- 2 persons appointed from the PRACE-3IP Management Board:
  - Annaïg Le Guen (GENCI, FR)
  - Jozef Duhovnik (UL, SI)
- 2 persons appointed by the PRACE Board of Directors :
  - Jürgen Kohler (Chair of the IAC, Daimler, DE)
  - Anders Rhod Gregersen (Vice-chair of the IAC, Vestas, Sweden)
- 3 persons from the SHAPE team:
  - Giovanni Erbacci (CINECA, IT)
  - Marcin Ostasz (BSC, ES)
  - Paul Graham (EPCC, UK)

2.4 Selection criteria

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

- Strength of the business case

The expertise and resources provided during the SHAPE Pilot are expected to produce a significant Return on Investment for the company. In the mid-term, the SME should be able to build on the results to, for instance, increase its market share, renew its investment or recruit dedicated staff. One must also be careful that the solution implemented will fall into a business plan to further engage in HPC in the long term.

- Technical Adequacy

The applications were expected to fit the timeframe and resources available in the project. The pilot activity was scheduled from 15th October 2013 until 31st May 2014 and must only lean on expertise already available within PRACE partners. Access to PRACE systems was possible through Preparatory Access with the cut-off date of 1st December 2013.

Other aspects considered were:

- The commitment of the SMEs to co-invest with PRACE in achieving the project goals. The effort should at least be equally split between the company and PRACE;
- The innovative aspect of the proposed solution;
- The social and economic *impact on society as a whole*.

2.5 Evaluation Activity

The final version of the 14 applications and the guidelines for evaluating the applications were sent to the Review Panel on 1st October 2013 by the WP5-3IP leader, asking each reviewer to provide a ranked list with an overall comment for each application no later than

10th October. On 11th October the review panel members met via teleconference to agree on the final ranked short list, based on the ranks of each member of the panel.

The ranked short list finally was submitted for the final decision of the PRACE-3IP Management Board on 23rd October.

2.6 Ranked Short List

The following decisions were taken by the Review Panel:

1. Four applications did not meet the requirements for the SHAPE pilot: Biovet, Do iT, Ingeliance and Termo Fluids.
2. Six applications were strongly recommended for the SHAPE Pilot: THESAN, Albatern, NSilico, Audionamix, Juan Yacht Design and OPTIMA.
3. A further four applications (AMET, ENTARES, Lapcos and MONOTRICAT) should be further considered for the Pilot, if some additional effort was available for the SHAPE Pilot in the PRACE Project. The applications in this latter group were characterised by short effort requirements.

The ranked short list with the six applications strongly recommended is reported in

Table 2, whereas Table 3 reports the four further applications.

Company	Project Title
THESAN S.p.A Italy.	Improvement of hydraulic turbine design through HPC
Albatern Ltd UK	Numerical Simulation of Extremely Large Interconnected WaveNET Arrays
NSilico Life Science Ltd Ireland	High Performance Computation for Short Read Alignment
Audionamix France	Unmix Up
Juan Yacht Design, SL Spain	Testing LES turbulence models in race boat sail
OPTIMA pharma GmbH Germany	Enhanced airflow simulations around filling machines in clean rooms

Table 2: ***Ranked Short List***

Company	Project Title
AMET s.r.l. Italy	Robustness in safety performances analysis (ROSPA)
ENTARES Engineering France	CAPITOL-HPC+
Lapcos Scrl Italy	Virtual Test Bench for Centrifugal Pump
MONOTRICAT S.r.l. Italy	CFD simulation of an innovative hull

Table 3: ***Additional Applications List***

2.7 Effort Required and Availability

The PRACE 3IP-WP5 partners checked the resources available in WP5 (in terms of Person Months and available skills) to take care of the applications identified by the Review Panel.

After the evaluation of the resources, it was agreed that PRACE 3IP WP 5 had the skills and the resources necessary to successfully manage the six applications of the ranked short list. Furthermore some more resources were identified in PRACE 3IP WP5 to also take care of the four applications identified in the additional list prepared by the Review Panel. The estimated person months of effort and the SHAPE partner identified for each of the ten applications are presented in Table 4**.**

Company	Project Title	PM SHAPE	Work taken by
THESAN S.p.A Italy.	Improvement of hydraulic turbine design through HPC	6	CINECA
Albatern Ltd UK	Numerical Simulation of Extremely Large Interconnected WaveNET Arrays	6	EPCC
NSilico Life Science Ltd Ireland	High Performance Computation for Short Read Alignment	4-6	ICHEC+ GENCI
Audionamix France	Unmix Up	1	GENCI
Juan Yacht Design, SL Spain	Testing LES turbulence models in race boat sail	5	BSC
OPTIMA pharma GmbH Germany	Enhanced airflow simulations around filling machines in clean rooms	2	HLRS
AMET s.r.l. Italy	Robustness in safety performances analysis (ROSPA)	2	CINECA
ENTARES Engineering France	CAPITOL-HPC+	1	GENCI
Lapcos Scrl Italy	Virtual Test Bench for Centrifugal Pump	3	CINECA
MONOTRICAT S.r.l. Italy	CFD simulation of an innovative hull	3	CINECA + KTH

Table 4: ***Ranked List with estimated PM and responsibility***

This ranked list was submitted on 15th October 2013 by the WP5 PRACE-3IP leader to the PMO for the final decision of the PRACE-3IP Management Board. The list was approved on 23rd October 2013.

After the approval of the list of the ten applications, the PRACE experts started the work with the selected SMEs. Complete work-plans were agreed between the PRACE experts and the SMEs. Five of the ten SMEs asked for PRACE Tier-0 resources, submitting a preparatory access request (Type C) in time for the cut-off of 2nd December 2013. For the remaining five SMEs it was estimated that the use of Tier-1 resources, made available by the PRACE partners, was more appropriate.

The pilot ran until May 2014 when the activity completed successfully for all the projects presented by the ten SMEs involved.

The results obtained by six of these SMEs were presented during the PRACEdays14 meeting on 20th -22nd May, 2014 in Barcelona.

3 Pilot Project Summaries

This section provides summaries of the ten pilot projects undertaken in the first run of the SHAPE programme. For each project there is a brief overview describing the participants and problem to be solved, the activity done, how PRACE was involved, the benefits to the SMEs, and finally the lessons learned with reference to the SHAPE programme itself. The lessons learned are also discussed further in Section 4.

Note that each pilot project is also producing a technical white paper which will cover the activities and results of the projects in greater detail than presented here. The intention of this section is to give a flavour of the broad range of projects and the diversity of the subject areas, along with summarising the benefits of the SHAPE programme to the SMEs.

3.1 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)

3.1.1 *Overview*

This work deals with the optimization of a volumetric machine. The machine is under active development, and a prototype is already working and fully monitored in an experimental mock-loop setup. This prototype operates under controlled conditions on a workbench, giving as an output the efficiency of the machine itself. The main goal is to obtain an increased efficiency through the design and realization of the moving chambers in which fluid flows. To this end, an extensive CFD modelling and simulation is required to perform virtual tests on different design solutions to measure the physical quantities assessing the performance of a given geometry. The final goal is to design a better geometry of the different components, mainly the supply and exhaust chambers, cutting down time and resources needed to produce a physical prototype and to limit the physical design only on a single geometry of choice. The modelling should allow then, through an optimization strategy, to perform parametric studies of key parameters of the design of the moving chambers in which fluid flows, in order to identify the main geometrical parameters able to drive the optimal configuration. High Performance Computing facilities and Open-Source tools, such as OpenFOAM, are therefore crucial in handling the complex physical model under consideration and in performing a sufficient amount of design configuration analysis.

3.1.2 *Activity done*

In order to get a more detailed insight about the fluid dynamics pattern present into the prototype turbine the following activities were performed:

- Build a CFD rotating model using the OpenFOAM (OpenCFD Ltd.) toolbox starting from the CAD of the prototype device;
- Study four CFD rotating conditions fixing RPM and Mass Flow Rate at the inlet according to experimental measurements;
- Visualize flow patterns to get a better understanding of the fluid dynamics;
- Quantify meaningful fluid-dynamics indices.

More details are reported in the white paper [4].

3.1.3 *PRACE cooperation*

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

All simulations have been run on CINECA Tier-1 system PLX.

3.1.4 *Benefits for SME*

According to the economical information provided by the first physical prototype developed by Thesan and used in performing the experimental measurement campaign, the costs faced by Thesan were between 20 and 30 thousand of euros and involved Thesan qualified personnel for about eight months. On one hand, a novel physical prototype development is estimated to cost about eight thousand euros and it will involve personnel activity for about four months. On the other hand CFD-based prototyping using open-source tools on HPC systems will have a dramatic reduction in costs, about 15-20 thousand computer core hours and only one month for data accumulation (here data interpretation and decision making will be a bottleneck).

3.1.5 *Lessons learned*

In conclusion we can state that CFD tools can be very useful in getting a better understanding of industrially relevant problems when planning to define a new product prototype and when used together with experimental data. Moreover CFD tools are cost effective with the respect to more traditional experimental tools allowing for a dramatic time reduction in novel prototype design evaluation. Finally, thanks to CFD we were able to visualize flow patterns and quantify meaningful fluid-dynamics indices necessary to plan an improved prototype design of the proposed case. In the future the results obtained herein will be used by Thesan to design an improved version of the prototype device.

3.2 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)

3.2.1 *Overview*

Albatern develops 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.

The project was split into two concurrent activities with Albatern focusing of 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). The eventual goal is to integrate the two codes to provide a complex, parallel multibody physics simulation.

3.2.2 *Activity Completed*

Albatern created a prototype impulse based multibody dynamics simulator, following an approach suitable for parallelisation on DMP machines. The prototype solver was constructed with MATLAB as a technology demonstrator and proof of concept. The principle challenges in the development of the solver were maintaining numerical stability while managing error correction and managing computational effort.
More details are reported in the white paper [5].

3.2.3 *PRACE co-operation*

EPCC concentrated on creating a modelling parallel approach using the PETSc library. To this end, the simulation was a simplified rigid body simulation connected with a mooring system. The implementation took full advantage of the parallelised implicit solvers that PETSc provide.

3.2.4 *Benefits for Albatern*

The completion of the project leave Albatern with a path forward on how to continue developing their multibody dynamics solver in a scalable manner with a number of development options with which to determine the optimal solution.

The work that EPCC has performed serves as an excellent introduction and example of how to use complex HPC libraries to implement distributed memory processor (DMP) solvers.

3.2.5 *Lessons learned*

During the project period Albatern has learnt several different simulation approaches that appear suitable for both shared memory and distributed memory architecture systems. The most promising of these methods are sequential and simultaneous impulse methods. It is possible to parallelise both methods.

Albatern is now in a position to write a multibody dynamics code that will share common parts of the simulation procedure allowing interchange of either the simultaneous or sequential methods. The ability to write both shared memory and distributed memory versions of a parallel multibody dynamics code is also possible, maintaining the widest range of simulation options.

Albatern is now aware that PETSc is a powerful scientific computing library that is capable of forming the basis of the solution of a DMP solver for compatible with super computers. Potential areas of further development include using a range of implicit solvers that PETSc has available as well as manually writing the integration steps and relying on the PETSc functionality to solver the linear complimentary problem that forms the basis of the multibody dynamics problem.

3.3 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)

3.3.1 *Overview*

NSilico is an Irish based SME that develops software to 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, coordinated by the Irish Centre for High-End Computing (ICHEC), involves an initial identification of relevant bioinformatics codes used for analysing high-throughput genomic sequence data with the potential to be parallelised (if not already) and to be ported to run on many-core technology such as the Intel Xeon Phi co-processor. CINES in France was responsible for the parallelisation/porting work, while NSilico provided example datasets to test the development work. The project successfully applied for and made use of PRACE access to the Spanish Tier-0 system MareNostrum with support from BSC.

3.3.2 *Activity done*

After examining a number of bioinformatics codes, an implementation of the Smith-Waterman algorithm, in the form of a C/C++ library, was identified for further work. Benchmarking and profiling revealed parts of the code that are the best candidates to be ported onto many-core technologies, followed by the actual porting effort. While performance results are expectedly poor using current generation hardware, the code has been ported in a way to anticipate the next generation of many-core technology which should see a significant boost in performance results.
More details are reported in the white paper [6].

3.3.3 *PRACE cooperation*

The project involved extensive cooperation between NSilico and a number of PRACE partners: CINES, EPCC, GENCI and ICHEC. EPCC assisted with NSilico’s SHAPE application. ICHEC, based in the same country as NSilico, assumed the role of local coordinator to manage the project but also contributed in applying for machine access and the initial identification of the relevant bioinformatics code. GENCI provided advice and sought out personnel from CINES who carried out the parallelisation/porting work and generated the performance results. BSC provided support for working on the hybrid nodes of the MareNostrum system.

3.3.4 *Benefits for SME*

NSilico has gained valuable experience and knowledge on some of the steps involved in porting codes onto many-core architectures, aided by documentation produced during this project. While the code itself may still require more work and next-generation hardware to realise performance benefits, discussions on potential funding opportunities for follow-on work had taken place. NSilico is well positioned to be one of the early adopters of many-core technology in the bioinformatics domain.

3.3.5 *Lessons learned*

The cooperation between NSilico and the various PRACE partners has been an excellent demonstration of effective international collaboration. Each partner brought complementary skills into the project (e.g. bioinformatics and business insights from NSilico, bioinformatics domain expertise from ICHEC, many-core development expertise from CINES). NSilico has also gained access and experience working on the Spanish PRACE Tier-0 system (MareNostrum) as part of this project. The company has learnt both the limitation and the potential of many-core technology, including general challenges that one faces when porting codes onto specialised hardware.

3.4 Audionamix: Unmix Up

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

3.4.1 *Overview*

Audionamix is a technology company developing audio unmixing technologies, which rely on computationally intensive optimization algorithms. The low speed is an impediment to the application of the technology in a number of business cases. The *Unmix Up* software helps Audionamix explore the latest hardware and software solutions. First validations of the relevance of GPU-based computed will be confirmed on more recent hardware. The most recent solutions (OpenCL, Cuda, \MIC/MKL) are assessed with respect to the algorithm structure. The disruptive improvement in the technology speed is expected to unveil new business opportunities in licensing and for the processing of large audio material bases, and will accelerate R&D inside the company. Audionamix partnered with Thierry Gautier (team MOAIS at INRIA Grenoble) to get guidance about the solutions to accelerate its technology. The SHAPE contacts are Thomas Palychata and Nicolas Mignerey at GENCI.

3.4.2 *Activity done*

Audionamix first reviewed the state-of-the art of HPC technologies and investigated how they could be applied to the task at hand, advised by Thierry Gautier. The focus has been on GPU acceleration, with an emphasis on CUDA-based technology. Frameworks for linear algebra with matrix computations have been investigated too, since Audionamix's algorithms rely on that. Audionamix is now in the process of:

- coding its algorithms in C++ with the help of a high-level linear algebra library.
- connecting the aforementioned library to libraries that can leverage both CPU and GPU systems.

More details are reported in the white paper [6].

3.4.3 *PRACE cooperation*

PRACE has mainly been involved in the coaching process. They provided pointers to potential HPC solutions, after the algorithm structure was exposed to them. No access to machines has been used.

3.4.4 *Benefits for SME*

Audionamix is still in the process of porting its algorithms using GPU-accelerated libraries. The benchmarking of the solution showed a very good speed improvement potential, and there is no doubt it will drastically improve the company's technology speed. Overall, Audionamix's knowledge of the field has greatly improved, and the company is now able to make informed choices among the several HPC solutions. Future actions will focus on deploying the technology for production runs. Work on further parallelization will also be pursued.

3.4.5 *Lessons learned*

- The help of the academic expert was interesting to get a good overview of the field, and then to take the good technical decision about the HPC technology.
- Having one resource (an intern) working full time on the project has enabled the project to move forward.
- Once the implementation started, communication with the expert has been more scarce, as the R&D engineers gained autonomy and knowledge of the field
- The project took time to start because of the non-availability of Audionamix's internal resources until month 3. Therefore the project has been behind schedule, but this did not negatively affect the outcome in the end. It is important to synchronise the resources since the beginning of the project.

3.5 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)

3.5.1 *Overview*

The objective of this project is to implement LES (Large Eddy Simulation) turbulence models outside the academic world to simulate flow around sails to replace RANS (Reynolds-averaged Navier Stokes) models that are the standard in the industry. The implementation and testing in the finite code *Alya* is done by the Barcelona Supercomputing Center (the SHAPE contact) so that Juan Yacht Design SL (JYD) can appreciate the advantages of using an LES formulation for their problem. JYD is a Spanish company that specializes in the design of sail boats.

3.5.2 *Activity done*

An example case with strong flow separation where RANS models do not provide good results was selected by JYD based on their experience. The case to be studied included a certain wind and boat speed and geometry with three sails: main, genoa and jib. From this geometry a mesh was created with the commercial code ICEM. The case was then simulated using Alya with both the k-omega SST RANS turbulence model and two LES models: the WALE eddy viscosity LES model and an Implicit LES model known as VMS, Variational Multiscale Stabilization. The main quantity of interest is the force generated by the wind on the sails. Both LES models give very similar results but the WALE simulation is more robust. The force obtained with the RANS model is approximately 20% lower than the one obtained with LES indicating that the model used has a big influence on the results. Further details of the flow will be presented on a PRACE white paper [8].

3.5.3 *PRACE cooperation*

Barcelona Supercomputing Center, acting as the PRACE representative, was responsible for setting up the simulation and running the cases on four different European Supercomputers: Marenostrum, SuperMuc, JUQUEEN and Fermi.

3.5.4 *Benefits for SME*

JYD has been able to observe the differences that can be obtained with an LES model with respect to a RANS model. They can now use Alya to further test the model on their cluster. This could involve some further collaboration with BSC.

3.5.5 *Lessons learned*

As already mentioned, the significant difference on the forces on the sails indicates that LES could be an interesting alternative to RANS simulations for cases where such models do not provide accurate results. The results show that there are two vortices that are much better captured with LES than RANS. This surely affects the forces on the sails.

Converging the problem involved some work with the mesh. Some improvements in the boundary conditions at the outlet were also required.

Close to the end of the project JYD suggested that it would be good to include also the ship hull to better calculate the total aerodynamics forces. Obtaining a good mesh for this problem has been complicated. This has generated convergence problems in Alya that have not allowed us obtain a converged solution, so there is still work to be done on the mesh.

The SHAPE application process has been a bit complicated. Once the SHAPE project had been granted this did not directly include CPU time, this then had to be asked for through a Preparatory Access application. Time was requested on 4 supercomputers, but in retrospect it would have been better to have the total CPU time just on one machine, to remove the need to learn the basics of using each machine and transfer data among them.

On the other hand this had a positive side on the fact that the speed of Alya could be compared on the different machines for one same problem. Despite Alya being part of the PRACE benchmark suite, this comparison had not been performed before. It was confirmed that Alya works nearly at the same speed in Marenostrum and SuperMuc as one would expect since they are both Sandy Bridge machines. The Blue Gene machines, Fermi and JUQUEEN, initially gave speeds that were 8 times slower than the Sandy Bridge ones. This was a bit disappointing since only looking at the processor/core peak performance Blue Gene machines should only be approximately 40% slower than Sandy Bridge machines. Some effort was put into trying to solve this problem. The only solution found was to run 4 processes per core instead of just one as one would usually do in Marenostrum. This reduced the performance difference to only 3.6 times, which is better but still far from what one could expect from only looking at processor/core peak performance. Unfortunately due to the project ending this could not be investigated further.

3.6 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)

3.6.1 *Overview*

OPTIMA Pharma GmbH, located at Schwäbisch Hall, Germany, is a company operating worldwide with 600 employees, which develops and produces filling and packaging machines for pharmaceutical products. Sterile filling lines are enclosed in clean rooms, and a detailed and reliable knowledge of the airflow inside the clean rooms would enhance the design of the filling machines and support the CAE process. The goal of this project was to simulate the airflow using OpenFOAM, meeting the requirements of industrial production.

The team members were Ralph Eisenschmid (OPTIMA Pharma GmbH), Bärbel Große-Wöhrmann (HLRS, SHAPE coach) and Martin Winter (HLRS, CFD expert, internal consultant).

3.6.2 *Activity done*

Concerning mesh generation, OpenFOAM's snappyHexMesh's refinement parameters were varied to evaluate the final mesh sizes, the wall time and the memory used in order to set up the queue scripts for optimal utilization of resources and performance.

Resources required by other OpenFOAM tools and the solvers were evaluated in the same way. It was found that there was inadequate performance of the serial tools like decomposePar on large meshes with more than 40 M cells: memory consumption and wall time exceeded the resources of large memory compute nodes (64 GB) and the available queue lengths (24 hours). Scaling tests of stationary parallel solvers did not make sense, because stationary solver runs on meshes with 30 M cells take only some minutes on 64 cores anyway.

In addition, competing solvers and different turbulence models were analyzed by means of a 3D Karman-case with transient DNS solver as reference. Scaling tests of transient solvers will run until the end of July 2014.

More details are reported in the white paper [9].

3.6.3 *PRACE cooperation*

In close collaboration with the other two team members, the industrial partner Ralph Eisenschmid ran the OpenFOAM test cases on the machine Hermit within the granted PRACE preparatory access type C project 2010PA2080. There were frequent telephone calls, often daily, and weekly or bi-weekly meetings at the HLRS.

3.6.4 *Benefits for SME*

This SHAPE project enabled OPTIMA to utilize OpenFOAM on the Tier-0 system Hermit for their industrial development and design processes. With the findings summarized in section 3.6.2, it is now possible to set up a CFD case in considerably reduced time (about 80% savings). Prediction of mesh sizes, processor resources and wall time of all OpenFOAM processes helps to optimize the HPC case and to save much money and time. Therefore, full HPC capacity can be used with a minimal waste of resources and very reduced queuing times (jobs with runtimes predicted less than 4 hours). The final results will help to select the most appropriate solver for handling air flows in clean rooms at a maximum of accuracy and a minimum of resources.

3.6.5 *Lessons learned*

Generally speaking, the concept of the SHAPE pilot worked very well: supporting the industrial partner in writing the PRACE preparatory access application and in exploiting the possibilities provided by a Tier-0 system was sensible and successful. The industrial partner was so intent upon preparing the OpenFOAM cases for efficient, long-term usage that the time was quite short for this SHAPE project: there were only three months between the start of the preparatory access at the end of January and the writing of the final documents beginning in May. Therefore, a suggestion would be to better coordinate the SHAPE projects schedule with the allocation periods of the PRACE preparatory access projects. Furthermore, it cannot be assumed that the partners from industry have no other duties besides their SHAPE projects, and as such any impact of this should be considered early on in the project process.

3.7 AMET: HPC application to improve the comprehension of ballistic impacts behaviour on composite materials

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

3.7.1 *Overview*

The damage phenomenon occurring on composite materials when subjected to a ballistic impact is a complex problem. Therefore, the understanding of the influence of the parameters describing the material behaviour is not a straightforward task; moreover, due to the fact that these influences are mutually connected, the task of designing a new structure with improved characteristics in terms of resistance to ballistic impacts is a very hard one. Only resorting to a massive use of DOE (Design of Experiment) analyses, supported by suitable computing resources, may lead to a better understanding of the problem and to a definition of the parameters mostly influencing the physical phenomenon.

3.7.2 *Activity done*

In order to get a detailed insight into the problem the team had to perform a set of activity:

- Define hardware, software and computing requirements;
- Identify a case study sufficiently representative of a real business case, but sufficiently simple to remain within the boundaries of a pilot project;

- Implement an analysis framework on a HPC system integrating a suitable Finite Element solver with a DOE manager and the HPC system load and queue manager;
- Execute a massive numerical campaign on the case study to test the robustness of the framework and to investigate the mutual influence of the characteristics parameters of the material under examination;
- Compare the outcome of this approach with the standard experimental one;
- Analyse technical and business requirements of bringing this methodology to production.

Further details are presented on the PRACE white paper [8].

3.7.3 *PRACE cooperation*

In order to complete the activity, a strong cooperation between the technical teams of AMET and CINECA has been necessary. Technical personnel at AMET were able to describe the physical problem at hand, to define relevant material parameters and to interpret results, while CINECA personnel dealt with requirements analysis, implementation and test of the workflow.

All simulations have been run on CINECA Tier-1 system PLX.

3.7.4 *Benefits for SME*

AMET is hampered in the attempt of moving from the experimental approach to the simulation of composite materials in product design to a statistical approach, by the lack of both sufficient computing power and adequate competences to implement the approach in a HPC environment.

Even if advisable, a statistical approach has been up to now considered not affordable due to both cost and time (since AMET doesn't have the resources to develop such an approach offline, the only way to develop it could be by linking it to a real development project, but this is not acceptable in terms of project time delay: usual time to market makes it difficult for SMEs, even with the help of a HPC services provider, to dedicate effort to develop a lean statistical approach able to fit in the process). The help provided by the SHAPE pilot project was therefore crucial in providing the right jumpstart necessary to define and implement this approach.

The competitive advantage offered by this approach allows AMET to greatly increase its value proposition on the market and grant a first choice position within OEMs suppliers when developing projects involving the use of composite materials.

When making a business plan to define the advantages coming from this development, it is difficult now to define the fallout of such a disruptive approach: right now, to the best knowledge of AMET, none of their SME competitors has the capability to propose itself as able to run a product development project with a statistical approach. Being the first one in the market is therefore expected to give an impressive advantage.

It's clear to every OEM that a more robust process, while not compacting the time needed for the numerical simulations (where just the smart use of HPC will allow to make a statistical approach comparable to a deterministic one in terms of time), will dramatically shrink (up to two orders of magnitude) time and costs for a complete project, since the experimental tests will be definitely reduced from development tests to verification tests.

Being able to present to the market this approach will not only give AMET a sound competitive advantage, but it will also drive more resources to HPC: it's clear that, once the statistical approach becomes the standard one, computing power demand will drive to outsource analysis plans to supercomputing centres, not only for SMEs, but even for OEMs on the long run.

3.7.5 *Lessons learned*

Interaction between the domain specialist from AMET and HPC specialists from CINECA was particularly fruitful, after a series of initial discussions where a common vocabulary was defined and expectations were clearly defined.

The major issue encountered was in the involvement of ISVs. Since the choice of solver and DOE manager fell on commercial software, due to both market requests and the lack of a robust enough open-source alternative, licence costs become a major issue in defining the business value of the tool. An ISV was initially involved in the development and testing phase, but withdrew their support during the course of the experiment. Therefore a suitable new one had to be found and the toolbox newly customized. On one side this highlights the necessity of identifying ISV licensing models more suitable for SMEs needs, but on the other side in this project it allowed the construction of a more flexible tool.

3.8 ENTARES: *Electromagnetic simulation for large model using HPC*

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

3.8.1 *Overview*

ENTARES Engineering is a French SME, subsidiary of Nexio Group, developing electromagnetic simulation software to study the electromagnetic behaviour of any product during the design process, before the manufacturing phase.

Among the different applications of the software, the solver can be used to design an antenna and study its performances. Furthermore, it can help to optimize the placement of an antenna on its supporting structure (such a car, an airplane, a ship, etc.).

This project is in the framework of the SHAPE pilot programme for which ENTARES Engineering is supported by GENCI. The project aims to improve the parallel efficiency of an electromagnetic solver based on the concept of compressed “low-rank” matrix.

3.8.2 *Activity done*

A new version of the MSCBD algorithm has been implemented in which all the work is subdivided into asynchronous tasks. These asynchronous tasks have certain dependencies between them which need to be treated carefully. This approach will allow the use of a runtime parallelisation such as StarPU developed in INRIA. It is expected that good scalability will be possible with this new technique.

Furthermore, a scalability test has been performed at Marenostrum III for the two previously developed algorithms, the old version of MSCBD and the MLACA. The factorisation step of the MSCBD shows poor scalability which will be presumably improved with the new implementation. The MLACA presents very good performance with a hybrid MPI-OpenMP implementation. However, there is also room for improvement.

For further details, see the associated white paper [10] where explanations of the different methods as well as several numerical results are shown.

3.8.3 *PRACE cooperation*

- 200.000 core-hours on MARENOSTRUM at BSC, SPAIN
- One PRACE support expert, Nicolas Mignerey, GENCI, France
- Support of HPC Experts of INRIA Bordeaux, France

3.8.4 *Benefits for SME*

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

The SME had some interesting discussions with research teams from different laboratories specializing in HPC, (IRIT, INRIA, CALMIP) and this was considered very useful for them. The SME used different libraries (like PT-SCOTCH, MUMPS, STAR-PU) already optimized for HPC machines which reduced the development time and improved performance.

The machine access was also very important, especially for an SME developing an HPC program, because it was necessary to run a lot of tests and it is challenging for an SME to buy a server at the beginning of such a project given the uncertainties involved.

The expected business impact is to commercialize the HPC version of CAPITOLE software for global distribution.

It is expected that half of the sales of CAPITOLE in the future will be the HPC version because it has been observed that the demand to solve bigger models is increasing and also the operating frequency of telecommunication devices is increasing.

3.8.5 *Lessons learned*

At first, the CURIE machine of the TGCC was selected for this project because the characteristics were suitable to the application, but the access at TGCC was impossible due to security policies.

TGCC authorize only connection from enterprise networks, and not from internet access provider which is usually the case for an SME. A connection to a special network (like RENATER in France) is prohibitively expensive for an SME.

For this reason, during the project, usage was switched to MARENOSTRUM at BSC and this was a very good resource.

There is a limitation because of the memory available on each node: the application is very demanding in terms of memory. The SME planned to bypass this limitation and to use hard disk instead of RAM memory.

There was a meeting at Bordeaux with INRIA at the beginning of the project to discuss using the STAR-PU runtime in the SMEs program. Unfortunately the STAR-PU had no Fortran interface, thus making it not straightforward to use directly with the application, and there was not enough time to develop a Fortran interface during the project.

3.9 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)

3.9.1 *Overview*

The aim is the implementation on a HPC platform of one of Lapcos's software developed for the automation of CFD calculations based on the OpenFOAM CFD toolbox. This software is able to calculate the performance curve for a centrifugal water pump head (meters) vs. flow rate (liters/min). This tool is very useful for a rapid virtual testing of the performance for novel pump designs before manufacturing a real prototype. The HPC platform and the good scalability of the OpenFOAM software can improve the time to market of new design.

3.9.2 *Activity done*

The proposed HPC solution is based on software for CFD analysis for centrifugal water pump originally developed by Lapcos. This software is developed using the open source code OpenFOAM, improved for a better and faster convergence rate. The interface software is able to automate the job boundary condition, the multi-point analysis, and to extrapolate the main output information in simple graph output. In particular the software can predict the performance curve pump head vs. flow rate.

The main tasks involved the following activities:

- Compilation and porting of the source code on the CINECA system
- Integration with the HPC scheduler
- Testing and scalability analysis.

The software is made of two main components, a batch custom flow solver linked to the OpenFOAM CFD library, and a graphical user interface. Both were compiled and ported to the Tier-1 CINECA PLX cluster and tested. On the basis of the available solver and Lapcos's data, scalability tests were conducted in order to identify the best configuration for a typical case. Scalability analysis results are shown in Figure 1 below. Further details are presented on the PRACE white paper [12].

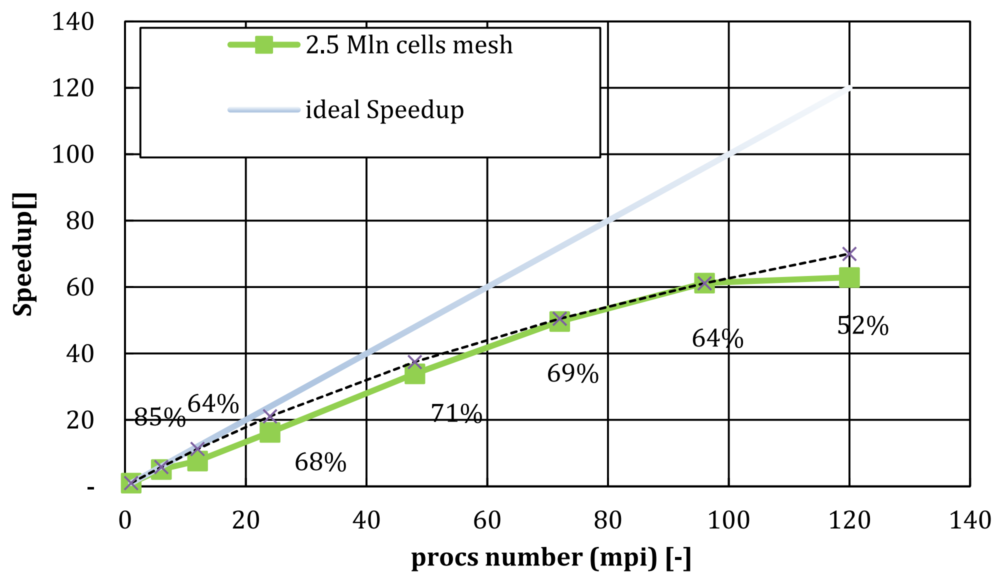

Figure 1: ***Scalability of the Lapcos solver***

3.9.3 *PRACE cooperation*

CINECA granted the use of the PLX cluster, a Tier-1 system with a pool of resources available by remote SSH console and a batch jobs scheduling system (PBS Pro, Altair Inc.). CINECA supported the porting tasks by providing a C++ development environment, both for the batch component of the system (GNU gcc and Open MPI) and for the GUI component (Codeblocks, a C++ OSS IDE specific for the WxWidgets framework). The GUI is provided by a remote visualization service based on Nice DCV® protocol.

Experts on HPC technical computing and in parallel architecture were involved to speed up the integration of the existing software with the CINECA platform.

3.9.4 *Benefits for SME*

Lapcos, exploiting CINECA as a technological partner, might start to propose this new service to centrifugal pump manufacturers. On this activity, a pre-marketing activity as email campaign/questionnaire was carried out (as a side activity). Some potential users of such this service were identified and contacted. The advantages for those customers are:

- they can easily access CAE sophisticated tools thanks to their deployment on a HPC services with a SaaS (Software as a Service) distribution model;
- The cost model fits their needs better, being charged only for their “consumption” of the service;
- They can smoothly scale up their problem through the HPC infrastructure, without worrying about IT fixed costs or additional licensing costs. Scalability analysis reported that a speed-up by a 3-4x in the time-to-market is feasible.

3.9.5 *Lessons learned*

- Porting and compilation of GUI components might be a tricky operation in heterogeneous cluster that have both computing and visualization nodes on the same environment. The use of GUI based components is, however, necessary when you “replicate” a typical CAE workflow on a remote HPC cluster.
- Response times as a key performance index for industrial usage can be vital and should be carefully considered with regards to queue setup in a shared resource scenartio. During the tests excessively long queue times were reported. This should be factored in for consideration when the decisions on resource selection are being made.
- A massively (compared to medium size industry systems) large cluster can improve time-to-market for the design of a product; this might increase the quality and the ROI of final users.

3.10 Monotricat: CFD simulation of 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)

3.10.1 *Overview*

Monotricat S.r.l. (Italy) is a company that designs an innovative ship hull, which is characterized by its hydrodynamic efficiency. However, the current R&D process relies heavily on field tests, which are conducted in a suitable infrastructure called a naval basin, and access costs are usually high. The goal of the proposed project is to develop a solution based on computer simulations run on a HPC facility that can be used by a Monotricat designer as an alternative R&D tool.

The project is implemented by two PRACE partners CINECA – acting as a contact point for PI and SNIC-KTH implementing the project.

3.10.2 *Activity done*

The work on the project has been planned in the following way:

1. Creation of a mesh from the CAD model that will be used as an input for the simulations
2. Development of the Open Foam set up, development of the turbulence model that best fits the experimental results.
3. Initial scalability analysis
4. Deliverable: SHAPE Project final report and the white-paper

In the project the whole hull simulation for Monotricat has been developed, based on the OpenFOAM open source package. The mesh has been generated from the CAD model and simulations have been run. The numerical hull resistances with various velocities agree well with the experimental data. We have also presented the scalability results on a Cray XE6 system. The pilot project verifies that OpenFOAM is valid tool for HPC enabled simulation for the hull product. Further details are presented on the PRACE white paper [8]

3.10.3 *PRACE cooperation*

The project is implemented by the PRACE expert at PRACE SNIC-KTH HPC centre PDC and the simulations have been run on the PRACE Tier-1 Machine called Lindgren at the same centre.

3.10.4 *Benefits for SME*

In this PRACE SHAPE project, for Monotricat not only the performance analysis but also whole hull simulation processing has been conducted, that is, mesh generation of complex geometries, efficient solvers with various turbulent modelling and optimized parameters as well as visualization. This project helped Monotricat to take advantage of HPC enabled simulation tools and potentially replace the traditional experiments. It has also drastically saved costs for Monotricat.

3.10.5 *Lessons learned*

A difficulty faced during this project is that there were language differences between the participants, and thus there were difficulties in communicating the specific details of the model between partners. Another aspect was the chosen tool, that is, OpenFOAM. In the first stages of implementation it was clear that another software product would have been more suitable although OpenFOAM worked fine. However, the wish to use OpenFOAM was one of the PI’s requirements. For similar situations, a suggestion arising from this would be, where possible, to have a face-to-face meeting with the PI and partners to discuss all project aspects in more detail.

4 SHAPE Pilot: Summary of Lessons Learned

Considering the pilot summaries in the previous section, there are some pertinent lessons to be learned and acted upon in any future SHAPE or SHAPE-like programme:

- The use of coaches to assist the SMEs in formulating their applications was invaluable.
- There were some challenges in applying for time on the PRACE machines via the preparatory access programme. The process for SHAPE projects needs to be considered and clarified: as it stands, the application system is geared more towards users perhaps already familiar with the machines or who have clearer requirements, whereas many of the SHAPE applicants and codes were using or being run for the first time in an HPC environment.
- Timescales – there was a discrepancy between the time of applying for preparatory access and the timescale of the projects, this needs to be considered in any future programme.
- SME engagement - all the SMEs were very engaged with the programme, but it must be kept in mind that their ability to commit time and resources is strictly limited (if this was not the case, they probably would not need SHAPE!), which means that upfront the responsibilities, interactions and plans must be discussed and agreed. Also, some flexibility in scheduling of resources from the technical partners would assist with this.
- Industry users have different expectations of machine usage – many are used to almost instant response times to, say, job submission, not waiting in queues. This should be either highlighted upfront to the SMEs as a limitation, or it should be ensured that the resources requested have appropriate queues to deal with this access model.
- Third party software – Licence agreements and such-like with ISVs need to be considered early on as they may cause restrictions to which (if any) PRACE machines can be used.
- IPR – When dealing with industrial partners, the management of IPR in the framework of SHAPE activities should receive great attention, that could require the definition of a general conditions agreement to be signed by the selected industry.

5 Recommendations and Conclusions

The SHAPE programme will allow SMEs to access high-value expertise in order to identify their needs, to design an industrial project and to try out a proof-of-concept model by using the PRACE HPC facilities, thus facilitating innovation and/or increased operational efficiency in their businesses.

The SHAPE Programme foundations and the framework have been thoroughly designed in Deliverable 5.2 [2] and Deliverable 5.3.1 [3]. SHAPE builds on the success of past PRACE initiatives such as the Open R&D Access Programme and the work of the industrial Work Packages of the PRACE Project as well as the experience of PRACE partners accumulated through national SME initiatives.

A SHAPE pilot was launched in June 2013 to refine the main assumptions of the programme. The pilot involved ten SMEs until May 2014 and the results have been presented in this Deliverable. The SHAPE Pilot has been a success and demonstrated the feasibility of the programme as originally designed. The SHAPE process defined in [3] and presented in Figure 2 has been evaluated positively and should be implemented in the SHAPE programme as initially designed.

SHAPE should offer SMEs an integrated service that includes information and networking, coaching, access to expertise in different HPC and computational sciences domains as well as access to HPC resources within an Open R&D model. SHAPE should focus on working on a one-to-one basis with SMEs willing to adopt a new HPC-supported solution.

Some recommendations for the final implementation of the SHAPE programme, suggested by the pilot results, are presented below:

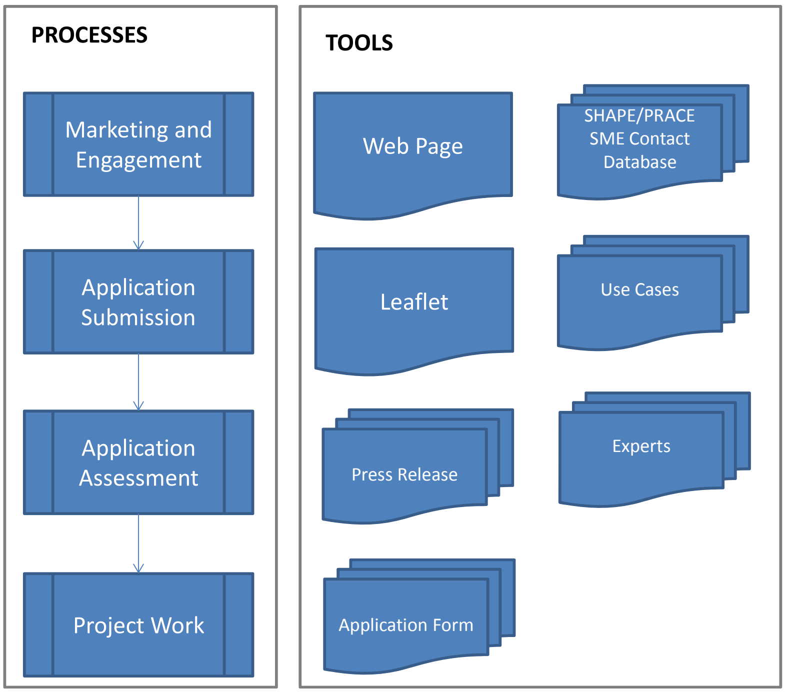

Figure 2: ***The SHAPE Process Map and supporting tools***

- The Marketing and Recruitment phase is of great importance for reaching awareness about the programme and involve SMEs. From the experience of the Pilot appears that often SMEs do not know the presence of PRACE and do not perceive the importance of HPC and computational services for their business. It is important to push for a continuous dissemination action at pan-European level and support the SHAPE logo and brand. Specific training actions for SMEs within the PATC activities, need also be intensified, linked to SHAPE activities. The outcome of SHAPE projects must produce a well visible database of use cases and success stories to be used to reinforce the Marketing and Recruitment phase.

- The application submission phase as described in [3] is effective. The application form appears complete and well balanced in terms of information presented for the project review activity.
- The review process is important but at the same time it must be dynamic and effective. The pilot review panel was composed by two members appointed from the PRACE-3IP Management Board, two appointed by the PRACE BoD and three from the SHAPE Team. For the programme implementation it is suggested to adopt a more simple composition for the review panel, involving members from the SHAPE team involved in local programmes with SMEs and delegated by the Industry Advisory Committee (IAC) and PRACE BoD.
  It is important to underline here that the proposals coming from SMEs often are quite simple in terms of HPC needs and requests, usually more oriented toward Tier-1 resources than Tier-0, in fact these SMEs in general approach HPC for the first time.
- The 1:1 coaching has resulted of fundamental importance and effectiveness for the success of the activity with the SMEs. It is important to assist the SMEs in the whole activity from the business project proposal submission to the completion of the whole activity with the evaluation of the final results and the feedback on the overall process.
- The HPC resources for the pilot had been granted via PRACE type C preparatory access projects or local Tier-1 resources. The mechanism is still recommended for the SHAPE programme implementation, especially considering that SMEs often are not ready to exploit a wide use of Tier-0 resources. To avoid confusion a new type of PRACE preparatory access (type D) should be implemented and reserved to SHAPE. In this way the SMEs can apply directly to this resources best tailored for the need of SMEs and also the review process can immediately identify and manage the SHAPE applications among all the preparatory access applications submitted from the scientific communities.
- The SHAPE projects should be better synchronized with the allocation periods of the PRACE preparatory access projects (6 months). As writing the proposal for the PRACE preparatory access project is usually one of the first tasks during a SHAPE project, the overall run-time of a SHAPE project should be definitely more than 7 months (we recommend 9 months) in order to be able to exploit the whole allocation period.
- There might be SHAPE projects that require less than 9 months and/or do not apply for preparatory access resources (they require e.g. training, general information on the possibilities offered by HPC, access to local HPC resources, etc.). Therefore, it could be worthwhile to consider two different run-times of SHAPE projects (similar to type A and type B/C PRACE preparatory access projects): 9 month if SMEs require Tier-0 preparatory access and 6 month for the other cases. In this way, the SME itself could choose the most appropriate run-time for its SHAPE project.
- The involvement of the Tier-1 Centres, relying on existing national initiatives towards SMEs, as one of the key importance for the success of the programme should be considered in the final SHAPE implementation.
- We recommend at least 2 calls per year, because the waiting time for the SMEs will be too long if there is only one call per year. We recommend a running-call (which is

always open so that proposals can be submitted at any time) with at least 2 deadlines per year.

- All SMEs having taken part in the SHAPE pilot were known to the HPC centres before the SHAPE pilot started, and they were easily persuaded to apply for a SHAPE pilot project. In our opinion, the difficulties of finding new SMEs willing to try SHAPE should not be underestimated. PRACE needs an elaborated marketing strategy. Just announcing the next SHAPE call will not be sufficient.
- To help SMEs it is important to make available a HPC use cases Database with outlines of actual HPC projects that SHAPE partners have undertaken with industrial and commercial SMEs and larger organisations. Furthermore it is important to implement a database of experts with skills that may be relevant to the potential SME applicants to the programme. The final report should contain recommendation sections written from SHAPE experts outlining both the possible steps further for the involved company and a list of resources or experts from SHAPE database that could support the industry in their implementation.
- The implementation of the SHAPE Programme will complement other European initiatives for SMEs, as well as the national initiatives and will act as a co-ordinated and single PRACE interface to the expected Network of SMEs.
- SHAPE acknowledges the existence of independent HPC Service Providers that offer HPC consulting services to SMEs. The Programme is not in a position to involve such companies directly in any part of the process. SHAPE does not pose any threat to the market position of such businesses. On the contrary, SHAPE should contribute to the strength of the ecosystem consisting of the SME which will adopt HPC, which in turn will benefit all HPC service providers and vendors. The aim of the SHAPE programme is not to establish a commercial offer and to compete with other service providers, but to inform the SMEs of the potentialities of HPC adoption.

  The SHAPE Programme provides one to one coaching from PRACE experts to SMEs. The notion of coaching in SHAPE is new but involves activities which PRACE is already doing for industry within its open R&D Programme, enabling of open source codes, and training roll-out. The Programme aims at help SMEs to understand the value of a HPC-based solution and it does not participate in the building of any commercial model.

  The SHAPE activity is a one-shot proof-of-concept and after the SHAPE demonstration, the companies will have a clear view about potential of HPC, investments to perform, skills to hire, software or methodologies to develop, etc.

  Once the SME has understood what HPC can bring, it is out of the programme and is ripe to identify a proper HPC adoption strategy, i.e. buying their own HPC facilities, access PRACE services for Open R&D services, access remote HPC services on commercial HPC or cloud platforms, perhaps working with independent service providers. In this way a synergic activity should be established between SHAPE and the service providers, benefiting all the HPC eco-system.

In the end, it is recommended that the SHAPE programme is implemented by PRACE AISBL on a permanent basis with the support of adequate resources of the Project involving PRACE members with SME-related expertise. In particular, PRACE AISBL should organise the calls and the review process, and the Project (or members) should perform the actual support of the selected proposals. A special emphasis should be placed on SME market development, which is in line with the objectives set by the EC in its HPC Infrastructures Work Programme.