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PRACE-5IP

PRACE Fifth Implementation Phase Project

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Periodic Report on Applications Enabling Services
Final

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List of Acronyms and Abbreviations

aisbl	Association International Sans But Lucratif (legal form of the PRACE-RI)
BCO	Benchmark Code Owner
BG	BlueGene
CoE	Centre of Excellence
CPU	Central Processing Unit
CUDA	Compute Unified Device Architecture (NVIDIA)
DARPA	Defense Advanced Research Projects Agency
DEISA	Distributed European Infrastructure for Supercomputing Applications EU project by leading national HPC centres
DoA	Description of Action (formerly known as DoW)
EC	European Commission
EESI	European Exascale Software Initiative
EoI	Expression of Interest
ESFRI	European Strategy Forum on Research Infrastructures
GB	Giga (= 2^{30} ~ 10^9) Bytes (= 8 bits), also GByte
Gb/s	Giga (= 10^9) bits per second, also Gbit/s
GB/s	Giga (= 10^9) Bytes (= 8 bits) per second, also GByte/s
GÉANT	Collaboration between National Research and Education Networks to build a multi-gigabit pan-European network. The current EC-funded project as of 2015 is GN4.
GFlop/s	Giga (= 10^9) Floating point operations (usually in 64-bit, i.e. DP) per second, also GF/s
GHz	Giga (= 10^9) Hertz, frequency =10^9 periods or clock cycles per second
GPU	Graphic Processing Unit
HET	High Performance Computing in Europe Taskforce. Taskforce by representatives from European HPC community to shape the European HPC Research Infrastructure. Produced the scientific case and valuable groundwork for the PRACE project.
HMM	Hidden Markov Model
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HPL	High Performance LINPACK
IAC	Industrial Advisory Committee
ISC	International Supercomputing Conference; European equivalent to the US based SCxx conference. Held annually in Germany.
KB	Kilo (= 2^{10} ~10^3) Bytes (= 8 bits), also KByte
LINPACK	Software library for Linear Algebra
MB	Management Board (highest decision making body of the project)
MB	Mega (= 2^{20} ~ 10^6) Bytes (= 8 bits), also MByte
MB/s	Mega (= 10^6) Bytes (= 8 bits) per second, also MByte/s
MFlop/s	Mega (= 10^6) Floating point operations (usually in 64-bit, i.e. DP) per second, also MF/s
MOOC	Massively open online Course
MoU	Memorandum of Understanding.
MPI	Message Passing Interface

NDA	Non-Disclosure Agreement. Typically signed between vendors and customers working together on products prior to their general availability or announcement.
PA	Preparatory Access (to PRACE resources)
PATC	PRACE Advanced Training Centres
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE 2	The upcoming next phase of the PRACE Research Infrastructure following the initial five year period.
PRIDE	Project Information and Dissemination Event
RI	Research Infrastructure
TB	Technical Board (group of Work Package leaders)
TB	Tera (= $2^{40} \sim 10^{12}$) Bytes (= 8 bits), also TByte
TCO	Total Cost of Ownership. Includes recurring costs (e.g. personnel, power, cooling and maintenance) in addition to the purchase cost.
TDP	Thermal Design Power
TFlop/s	Tera (= 10^{12}) Floating-point operations (usually in 64-bit, i.e. DP) per second, also TF/s
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
UNICORE	Uniform Interface to Computing Resources. Grid software for seamless access to distributed resources.

List of Project Partner Acronyms

BADW-LRZ	Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Germany (3rd Party to GCS)
BILKENT	Bilkent University, Turkey (3rd Party to UYBHM)
BSC	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion, Spain
CaSToRC	Computation-based Science and Technology Research Center, Cyprus
CCSAS	Computing Centre of the Slovak Academy of Sciences, Slovakia
CEA	Commissariat à l’Energie Atomique et aux Energies Alternatives, France (3rd Party to GENCI)
CESGA	Fundacion Publica Gallega Centro Tecnológico de Supercomputación de Galicia, Spain, (3rd Party to BSC)
CINECA	CINECA Consorzio Interuniversitario, Italy
CINES	Centre Informatique National de l’Enseignement Supérieur, France (3rd Party to GENCI)
CNRS	Centre National de la Recherche Scientifique, France (3rd Party to GENCI)
CSC	CSC Scientific Computing Ltd., Finland
CSIC	Spanish Council for Scientific Research (3rd Party to BSC)
CYFRONET	Academic Computing Centre CYFRONET AGH, Poland (3rd party to PNSC)
EPCC	EPCC at The University of Edinburgh, UK
ETHZurich (CSCS)	Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland
FIS	FACULTY OF INFORMATION STUDIES, Slovenia (3rd Party to ULFME)

GCS	Gauss Centre for Supercomputing e.V., Germany
GENCI	Grand Equipement National de Calcul Intensiv, France
GRNET	Greek Research and Technology Network, Greece
INRIA	Institut National de Recherche en Informatique et Automatique, France (3rd Party to GENCI)
IST	Instituto Superior Técnico, Portugal (3rd Party to UC-LCA)
IT4Innovations	IT4Innovations National supercomputing centre at VŠB-Technical University of Ostrava, Czech Republic
IUCC	INTER UNIVERSITY COMPUTATION CENTRE, Israel
JUELICH	Forschungszentrum Juelich GmbH, Germany
KIFÜ (NIIFI)	Governmental Information Technology Development Agency, Hungary
KTH	Royal Institute of Technology, Sweden (3rd Party to SNIC)
LiU	Linkoping University, Sweden (3rd Party to SNIC)
NCSA	NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS, Bulgaria
NTNU	The Norwegian University of Science and Technology, Norway (3rd Party to SIGMA)
NUI-Galway	National University of Ireland Galway, Ireland
PRACE	Partnership for Advanced Computing in Europe aisbl, Belgium
PSNC	Poznan Supercomputing and Networking Center, Poland
RISCSW	RISC Software GmbH
RZG	Max Planck Gesellschaft zur Förderung der Wissenschaften e.V., Germany (3 rd Party to GCS)
SIGMA2	UNINETT Sigma2 AS, Norway
SNIC	Swedish National Infrastructure for Computing (within the Swedish Science Council), Sweden
STFC	Science and Technology Facilities Council, UK (3rd Party to EPSRC)
SURFsara	Dutch national high-performance computing and e-Science support centre, part of the SURF cooperative, Netherlands
UC-LCA	Universidade de Coimbra, Labotatório de Computação Avançada, Portugal
UCPH	Københavns Universitet, Denmark
UHEM	Istanbul Technical University, Ayazaga Campus, Turkey
UiO	University of Oslo, Norway (3rd Party to SIGMA)
ULFME	UNIVERZA V LJUBLJANI, Slovenia
UmU	Umea University, Sweden (3rd Party to SNIC)
UnivEvora	Universidade de Évora, Portugal (3rd Party to UC-LCA)
UPC	Universitat Politècnica de Catalunya, Spain (3rd Party to BSC)
UPM/CeSViMa	Madrid Supercomputing and Visualization Center, Spain (3rd Party to BSC)
USTUTT-HLRS	Universitaet Stuttgart – HLRS, Germany (3rd Party to GCS)
WCNS	Politechnika Wroclawska, Poland (3rd Party to PNSC)

Executive Summary

Task T7.1 "Applications Enabling Services on PRACE Systems" in Work Package 7 (WP7) of PRACE-5IP aims to provide HPC enabling support for the applications of European researchers and small and medium enterprises to ensure the applications can effectively exploit the various PRACE HPC systems. Task T7.1 within PRACE-5IP is an ongoing activity which was already established and described in deliverables of former PRACE-IP projects. There were two activities in T7.1:

T7.1.A Preparatory Access:

This activity provides code enabling and optimisation to European researchers as well as industrial projects to make their applications ready for Tier-0 systems. Projects can continuously apply for such services via the Preparatory Access Calls Type C (PA Type C) and Type D (PA Type D) with a cut-off every three months for evaluation of the proposals. PA Type C provides support and access to a PRACE Tier-0 system while PA Type D provides support and access to a PRACE Tier-1 system to finally reach Tier-0 scalability. Five Preparatory Access cut-offs have been carried out in PRACE-5IP so far and eleven projects received support within the context of the project.

Beside the statistical overview about the cut-offs and all supported PRACE PA Type C and Type D projects, the report focuses on the optimisation work and results gained by the completed projects in PRACE-5IP. In total four PA Type C projects have finished their work since the last deliverable D7.2 in PRACE-4IP [2].

T7.1.B SHAPE:

This activity continued the support for SHAPE (the SME HPC Adoption Programme in Europe). SHAPE aims to raise awareness and provide European SMEs with the expertise necessary to take advantage of the innovation possibilities created by High-Performance Computing (HPC), thus increasing their competitiveness. It holds regular calls, and successful applicants to the SHAPE programme get support effort from a PRACE HPC expert and access to machine time at a PRACE centre. In collaboration with the SME, the PRACE partner helps them try out their ideas for utilising HPC to enhance their business.

This document reports on the status of the SHAPE projects: status reports for the currently active and recently finished projects from the 4th, 5th and 6th calls; and follow-up reports from the SME projects completed last year, in order to evaluate the effectiveness of the SHAPE programme in terms of the SMEs' ongoing engagement with HPC, including measurements against key performance indicators.

SHAPE participants have reported many positive outcomes following taking part in the programme, including tangible measurements of the Return on Investment: new staff hired, increasing sales and new business, lower costs, continued HPC Access, in-house HPC systems deployment, integration into the HPC ecosystem and engagement with other national and European industry programmes.

1 Introduction

Computational simulations have proved to be a promising way of finding answers to research problems from a wide range of scientific fields. However, such complex problems often have so high demands regarding the needed computation time that these cannot be met by conventional computer systems. Instead, supercomputers are the method of choice in today's simulations.

PRACE offers a wide range of different Tier-0 and Tier-1 HPC architectures to the scientific community as well as to industrial innovative projects. The efficient usage of such systems places high demands on the used software packages and in many cases advanced optimisation work has to be applied to the code to make efficient use of the provided supercomputers. The complexity of supercomputers requires a high level of experience and advanced knowledge of different concepts regarding programming techniques, parallelization strategies, etc. Such demands often cannot be met by the applicants themselves and thus special assistance by supercomputing experts is essential.

PRACE offers such a service through the Preparatory Access Calls. PA Type C and PA Type D are managed by Task 7.1.A. This includes the evaluation of the PA proposals as well as the assignment of PRACE experts to these proposals. Furthermore, the support itself is provided and monitored within this task. Section 2 gives a more detailed description of PA and some facts on the usage of PA Type C and PA Type D in PRACE-5IP are listed in 2.1. The review process, the assignment of PRACE experts to the projects and the monitoring of the support work are detailed in Section 2.2, Section 2.3 and Section 2.4 respectively. The contents of Sections 2.2 - 2.4 can already be found in deliverable D7.2 of PRACE-4IP [2]. They are repeated here for completeness and the benefit of the reader. Section 2.5 describes the relation and hand over between the PRACE-4IP and PRACE-5IP project regarding PA. Section 2.6 gives an overview about the Preparatory Access projects covered in PRACE-4IP and PRACE-5IP, which were not reported in former deliverables. The announcement of the call is described in Section 2.7. Finally, the work done within the projects along with the outcome of the optimisation work is presented in Sections 2.8 - 2.10.

The second part of this deliverable is the report on the SME HPC Adoption Programme in Europe (SHAPE), which is a pan-European programme to support the adoption of High Performance Computing (HPC) by European small to medium-size enterprises (SMEs). It was developed by PRACE under its PRACE-3IP European Union funded project and has continued under PRACE-4IP and PRACE-5IP.

The SHAPE programme, presented in the PRACE-3IP Deliverable 5.2 [3] aims to equip European SMEs with the awareness and expertise necessary to take advantage of the innovation possibilities opened by HPC, increasing their competitiveness. The mission of the Programme is to help European 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.

It can be challenging for SMEs to adopt HPC. They may have no in-house expertise, no access to hardware, or may be unable to commit resources to a potentially risky endeavour. This is where SHAPE comes in, by making it easier for SMEs to make use of high performance computing in their business - be it to improve product quality, reduce time to delivery or provide innovative new services to their customers. Successful applicants to the SHAPE programme get support effort from a PRACE HPC expert and access to machine time at a PRACE centre. In collaboration with the SME, the PRACE partner helps them try out their ideas for utilising HPC to enhance their business.

The initial SHAPE pilot [4] [5] was launched in 2013 and helped 10 SMEs adopt HPC, with a follow-up exercise to gauge the business impact for the SMEs showing in almost all the cases that the pilot had been of real value to the SMEs, with tangible measures of the ROI for the SHAPE work [6]. Following this pilot, the PRACE Council decided to operate the SHAPE programme as a permanent service. An overview of the SHAPE programme is provided in section 3.1, and a summary of the status of the current projects is in section 3.2.

The SHAPE second call was launched November 2014 and closed in January 2015, and 11 SMEs were approved to receive assistance from SHAPE; the third call for SHAPE was launched in November 2015, closing in January 2016, with eight projects eventually approved. Then the calls moved to shorter intervals, with the 4th, 5th and 6th calls running June-September 2016 (4 applications approved), April-June 2017 (6 approved), and October-December 2017 (2 approved) respectively. The 7th call is due to open in April 2018 running to June 2018.

In the previous deliverable (PRACE-4IP D7.2 [2]), follow-up reports were introduced to measure the impact of working with SHAPE for the SMEs once some time (typically a year) had passed since the project had concluded. At the time, this covered eight of the second call projects (the other three second call projects finished too late to be considered). In this deliverable follow-up reports have been requested from those remaining second call projects, and all the third call projects – these are reported in section 3.3.

Summaries of the progress of the other ongoing projects are in section 3.4 (fourth and fifth call). The sixth call projects have just started and are briefly discussed in section 3.5. Finally, section 3.6 looks at the plans and recommendations for SHAPE going forward.

The deliverable closes with a summary in section 4 highlighting the outcomes of Task 7.1.A and Task 7.1.B.

2 T7.1.A Preparatory Access

Access to PRACE Tier-0 systems is managed through PRACE regular calls, which are issued twice a year. To apply for Tier-0 resources the application must meet technical criteria concerning scaling capability, memory requirements, and runtime set up. There are many important scientific and commercial applications that do not meet these criteria today. To support researchers PRACE offers the opportunity to test and optimise their applications on the envisaged Tier-0 system prior to applying for a regular production project. This is the purpose of the Preparatory Access (PA) Call. The PA Call allows for submission of proposals at any time. Depending on the PA scheme, the review of these proposals takes place directly after the submission of the proposal (Type A and B) or at a fixed date every three months (Type C and D). This procedure is also referred to as cut-off. It is possible to choose between four different types of access:

- Type A is meant for code scalability tests, the outcome of which is to be included in the proposal in a future PRACE Regular Call. Users receive a limited number of core hours; the allocation period is two months.
- Type B is intended for code development and optimisation by the user. Users get also a small number of core hours; the allocation period is 6 months.
- Type C is also designed for code development and optimisation with the core hours and the allocation period being the same as for Type B. The important difference is that Type C projects receive special assistance by PRACE experts to support the optimisation. As well as access to the Tier-0 systems, the applicants also apply for 1 to 6 PMs of supporting work to be performed by PRACE experts.
- Type D allows PRACE users to start a code adaption and optimisation process on a PRACE Tier-1 system. PRACE experts help in the system selection process. In addition to Tier-1 computing time, the PRACE user will also receive Tier-0 computing time towards the end of the project in the form of a PA Type A project to test the scalability improvements. The work is supported by PRACE experts similar to Type C. The maximum duration of Type D projects is 12 months.

The following Tier-0 systems were available for PA during the reporting period:

- CURIE, BULL Bullx cluster at GENCI-CEA, France
- HAZEL HEN, Cray XC40 at GCS-HLRS, Germany
- MARCONI, Lenovo NextScale at CINECA, Italy
- MARENOSTRUM, IBM System X iDataplex at BSC, Spain
- PIZ DAINT, Cray XC30 System at CSCS, Switzerland
- SUPERMUC, IBM System X iDataplex at GCS-LRZ, Germany

For the Type D access scheme the following Tier-1 systems were available during the reporting period:

- ABEL, MEGWARE MiriQuid at UiO, Norway
- ARCHER, Cray XC30 at EPCC, United Kingdom
- ARIS, IBM NextScale at GRNET, Greece
- BEM, Haswell based Cluster at WCSS, Poland
- CARTESIUS, Bull Bullx B720/B710 at SURFsara, Netherlands
- CY-TERA, IBM System X iDataplex at CaSToRC, Cyprus
- EAGLE, Haswell based Cluster at PSNC, Poland
- GALILEO, Lenovo NextScale , at CINECA, Italy
- SALOMON, SGI ICE-X at VSB-TUO at IT4I, Czech Republic
- SISU, Cray XC40 at CSC, Finland

2.1 Cut-off statistics

In PRACE-5IP between January 2017 and April 2018, five cut-offs for PA took place resulting in nine new projects so far. Two projects, which started in March 2017 from the December 2016 cut-off of PRACE-4IP were taken over by PRACE-5IP, as written in D7.2 [2]. In total, eleven projects were supported by PRACE-5IP T7.1.A. Three projects were already finalised during the reporting phase. The other projects are ongoing. In addition, one project of PRACE-4IP was finalized in April 2017 and will be reported in this deliverable.

In the March 2017 cut-off, four new PA Type D and one PA Type C project were accepted. This was the first cut-off for PA Type D. In June 2017, one PA Type D was accepted and one PA Type C was rejected as the planned project mostly focused implementation instead of optimisation work. In September 2017, one Type D and one Type C project were accepted and another Type C project was accepted in the December 2017 cut-off. In March 2018, one PA Type D project was rejected which didn't fit into the scope of the preparatory access call.

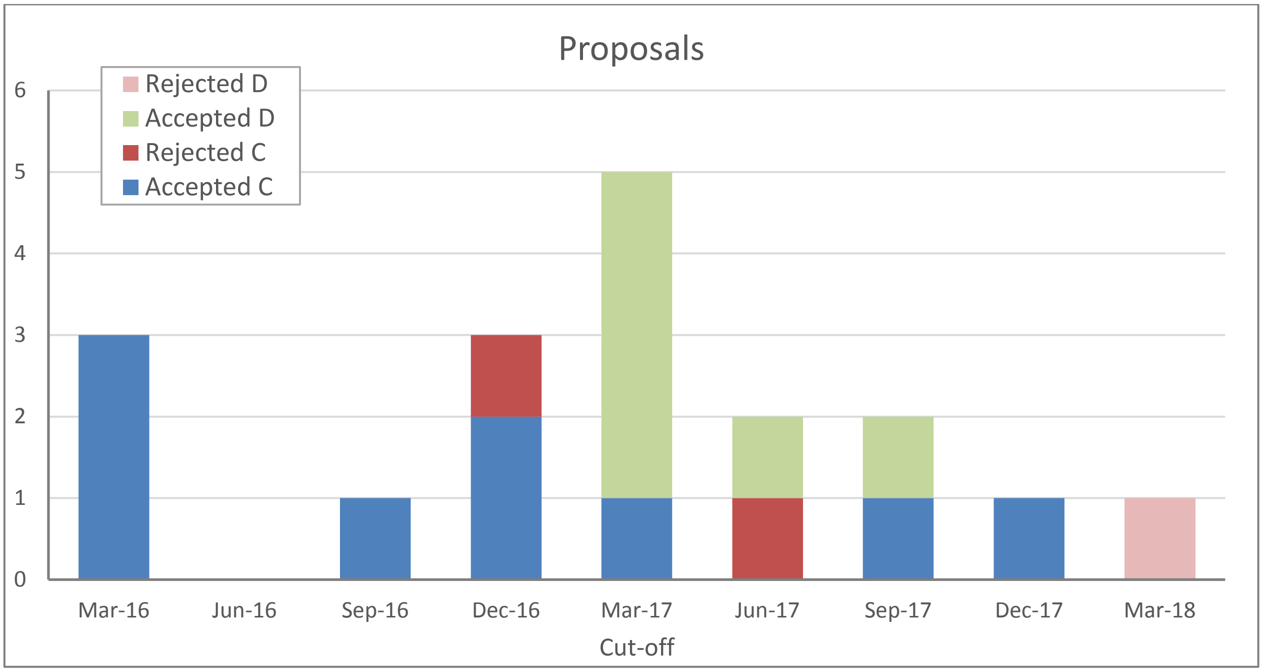

Figure 1: Number of proposals for PA type C and type D per cut-off.

Figure 1 presents the number of proposals that have been accepted or rejected respectively for each cut-off. In total, nine out of eleven proposals were accepted during the reporting period of the PRACE-5IP cut-off phase beginning in March 2017 until the cut-off in March 2018.

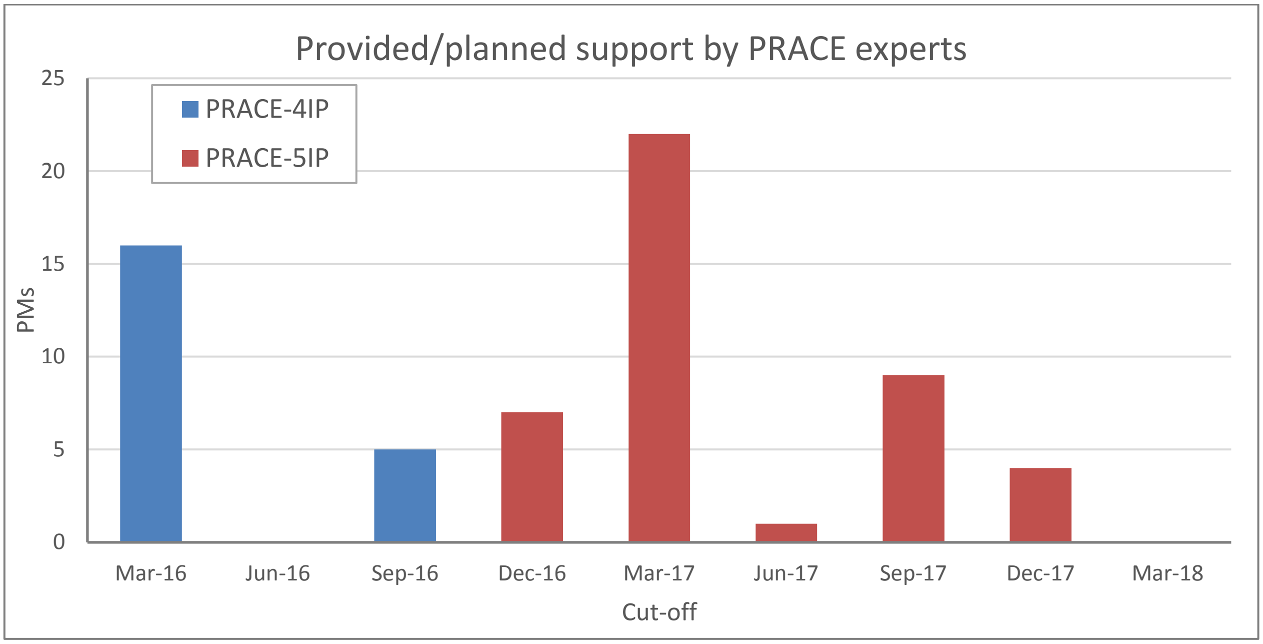

Figure 2: Amount of PMs assigned to PA projects per cut-off

Figure 2 gives an overview of the number of PMs from the PRACE project assigned to the projects per cut-off. In total 43 PMs were made available to these projects within PRACE-5IP.

Finally, Figure 3 provides an overview of the scientific fields, which are covered by the supported projects in PRACE-5IP.

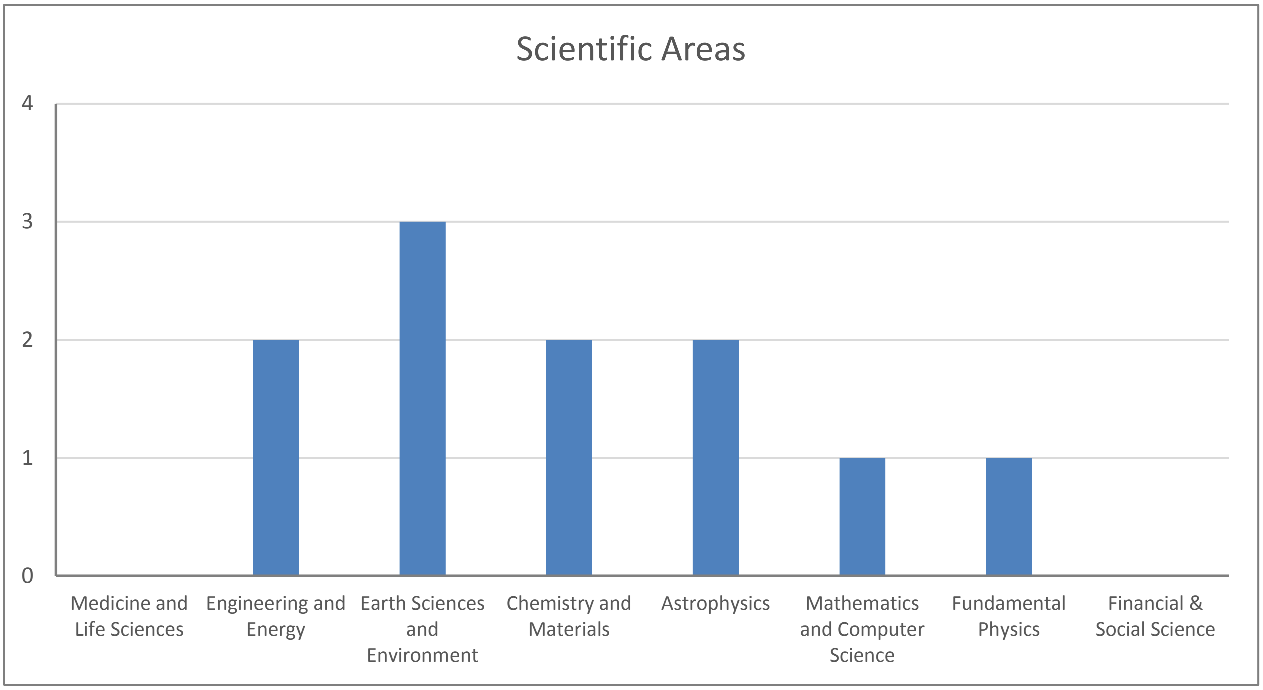

Figure 3: Number of projects per scientific field.

2.2 Review Process

The organisation of the review procedure, the assignment of PRACE collaborators and the supervision of the PA C projects are managed by task 7.1.A. In this section, the review process for the preparatory access proposals of Type C and Type D is explained.

All preparatory access proposals undergo a technical review performed by technical staff of the hosting sites to ensure that the underlying codes are in principle able to run on the requested system. For PA C projects, the technical review starts directly after the cut-off. For PA D projects, the technical review is done after the Tier-1 system is finally selected.

In parallel, all projects are additionally reviewed by WP7 staff in order to assess their optimisation requests. Each proposal is assigned to two WP7 reviewers. The review is performed by PRACE partners who all have a strong background in supercomputing. The task leader has the responsibility to contact them to launch the review process. As the procedure of reviewing proposals and establishing the collaboration of submitted projects and PRACE experts takes place only four times a year, it is necessary to keep the review process swift and efficient. A close collaboration between PRACE aisbl, T7.1.A and the hosting sites is important in this context. The process for both the technical and the WP7 review is limited to four weeks. In close collaboration with PRACE aisbl and the hosting sites, the whole procedure from PA cut-off to project start on PRACE supercomputing systems is completed in less than six weeks.

Based on the proposals the Type C and Type D reviewers need to focus on the following aspects:

- Does the project require support for achieving production runs on the chosen architecture?
- Are the performance problems and their underlying reasons well understood by the applicant?
- Is the amount of support requested reasonable for the proposed goals?
- Will the code optimisation be useful to a broader community, and is it possible to integrate the achieved results during the project in the main release of the code(s)?
- Will there be restrictions in disseminating the results achieved during the project?

For Type D, the reviewer should also make suggestions for the Tier-1 selection process. The 7.1.A task leader finally selects the Type D Tier-1 computing site based on the suggestions of the PI, the potential PRACE collaborator, the reviewers and the computing site availability.

In addition to the WP7 reviews, the task leader evaluates whether the level and type of support requested is still available within PRACE. Finally, the recommendation from WP7 to accept or reject the proposal is made.

Based on the provided information from the reviewers the PRACE Board of Directors has the final decision on whether proposals are approved or rejected. The outcome is communicated to the applicant through PRACE aisbl. Approved proposals receive the contact data of the assigned PRACE collaborators, rejected projects are provided with further advice on how to address the shortcomings.

2.3 Assigning of PRACE collaborators

To ensure the success of the projects it is essential to assign suitable experts from the PRACE project. Based on the described optimization issues and support requests from the proposal experts are thus chosen who are most familiar with the subject matter.

This is done in two steps: first, summaries of the proposals describing the main optimization issues are distributed via corresponding mailing lists. Here, personal data is explicitly removed from the reports to maintain the anonymity of the applicants. Interested experts can get in touch with the task leader offering to work on one or more projects.

Should the response not be sufficient to cover the support requirements of the projects, the task leader contacts the experts directly and asks them to contribute.

There is one exception to the procedure when a proposal has a close connection to a PRACE site which has already worked on the code: in this case this site is asked first if they are able to extend the collaboration in the context of the new PA Type C or PA Type D project.

The assignment of PRACE experts takes place concurrently to the review process so that the entire review can be completed within six weeks. This has proven itself to be a suitable approach, as the resulting overhead is negligible.

As soon as the review process is finished, the support experts are introduced to the PIs and can start the work on the projects. The role of the PRACE collaborator includes the following tasks:

- Formulating a detailed work plan together with the applicant,
- Participating in the optimization work,
- Reporting the status in the task 7.1A phone conference every second month,
- Participating in the writing of the final report together with the PI (the PI has the main responsibility for this report), due at project end and requested by the PRACE office,
- Writing a white paper containing the results, which is published on the PRACE website [1].

2.4 Monitoring of projects

Task 7.1.A includes the supervision of the Type C and Type D projects. This is challenging as the projects' durations (six months for PA Type C and twelve months for PA Type D) and the intervals of the cut-offs (3 months) are not synchronised. Due to this, projects do not necessarily start and end at the same time but overlap, i.e. at each point in time different projects might be in different phases. To solve this problem, a phone conference takes place in task 7.1.A every two months to discuss the status of running projects, to advice on how to proceed with new projects and to manage the finalization and reporting of finished projects.

In addition, the T7.1.A task leader gives a status overview in a monthly WP7 conference call to address all PRACE collaborators who are involved in these projects.

The T7.1.A task leader is also available to address urgent problems and additional phone conferences are held in such cases.

Twice a year, a WP7 face-to-face meeting is scheduled. This meeting gives all involved collaborators the opportunity to discuss the status of the projects and to exchange their experience.

2.5 Hand-over between the different PRACE IP projects

The support for Preparatory Access projects has been and is part of all PRACE projects (PRACE-1IP, -2IP, -3IP, -4IP, -5IP). For the hand-over between the PRACE-4IP and PRACE-5IP projects, the tasks decided to treat the regarding projects in the following way:

The two projects out of the PRACE-4IP December 2016 cut-off started in March 2017 were completely taken over by PRACE-5IP. No other project has to be moved or handed-over.

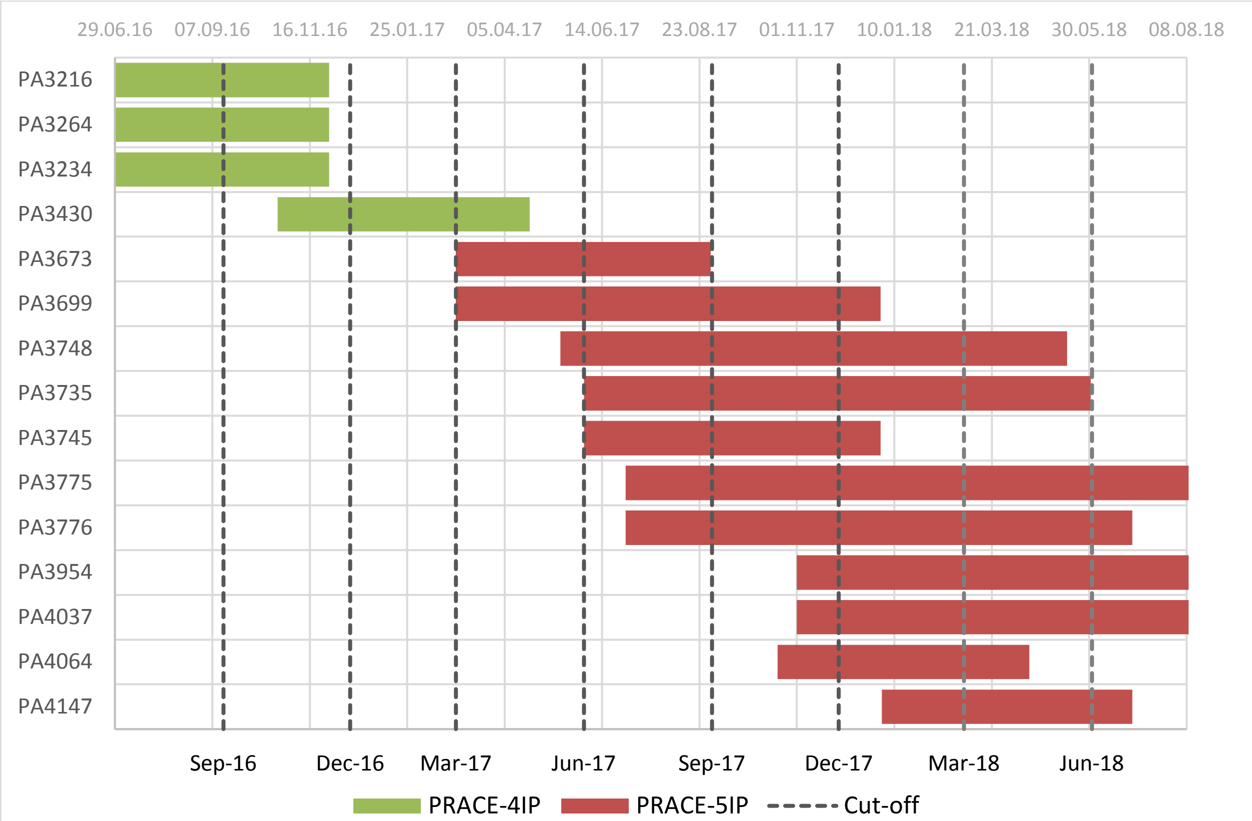

Figure 4: Timeline of the PA projects.

The timeline of these projects is shown in the chart in Figure 4. The chart shows the time span of each project. Projects, which were supported by PRACE-4IP are shown in green. The projects which received supported by PRACE-5IP are shown in red.

The slightly different starting dates of the projects per cut-off are the result from the decisions made by the hosting members, which determine the exact start of the projects at their local site. Additionally, PIs can set the starting date of their projects within a limited time frame.

If necessary, due to unexpected problems or organizational issues, projects can apply for an extension of their project duration. No additional support PMs or computing time are granted in such a case. The extension should stay within a limited time frame.

2.6 PRACE Preparatory Access projects covered by this report

Projects completed before March 2017 were already reported in deliverable D7.2 of PRACE-4IP [2]. One project of PRACE-4IP was finalised in April 2017 and is finally reported within this deliverable. Beside this project, two PA Type C projects from the December 2016 and one PA Type C project from the March 2017 will be presented. All other projects of PRACE-5IP, especially all running PA Type D projects, are still ongoing and will be reported in the upcoming deliverable. In total four projects are reported in the current deliverable. Table 1 lists the corresponding projects.

Table 1: Projects, which are reported in this deliverable.

Cut-off September 2016	
Title	**Optimization of REDItools package for investigating RNA editing in thousands of human deep sequencing experiments.**
Type	C
Project leader	Ernesto Picardi
PRACE expert	Andrew Emerson, Tiziana Castrignanò
PRACE facility	MARCONI
PA number	2010PA3430
Project's start	24-Oct-2016
Project's end	23-Apr-2017

Cut-off December 2016	
Title	**OPtimized mulTI-fluid plasMA Solver (OPTIMAS)**
Type	C
Project leader	Andrea Lani
PRACE expert	Chandan Basu, Thomas Boenisch
PRACE facility	HAZELHEN, JUQUEEN
PA number	2010PA3673
Project's start	01-Mar-2017
Project's end	31-Aug-2017
Title	**Water droplets and turbulence interaction inside warm cloud -- clear air interface**
Type	C
Project leader	Daniela Tordella
PRACE expert	Andrew Emerson, Vittorio Ruggiero
PRACE facility	MARCONI, SUPERMUC

Cut-off December 2016	
PA number	2010PA3699
Project's start	01-Mar-2017
Project's end	31-Dec-2017

Cut-off March 2017	
Title	**Quasi-particle self-consistent GW approximation: avoiding the I/O bottleneck**
Type	C
Project leader	Mark van Schilfgaarde
PRACE expert	Wei Zhang
PRACE facility	MARCONI, HAZELHEN, SUPERMUC
PA number	2010PA3745
Project's start	01-Jun-2017
Project's end	31-Dec-2017

All remaining projects have to be reported in the next deliverable, as those projects are still ongoing or were not completely finalized. Table 2 lists the corresponding projects.

Table 2: Currently running PA projects.

Cut-off March 2017	
Title	**Extending the scalability and parallelization of SEDITRANS code**
Type	D
Project leader	Guillermo Oyarzun
PRACE expert	Ricard Borrell
PRACE facility	CARTESIUS
PA number	2010PA3748
Project's start	15-May-2017
Project's end	14-May-2018
Title	**Automation of high fidelity CFD analysis for aircraft design and optimization**
Type	D
Project leader	Mengmeng Zhang
PRACE expert	Lilit Axner

Cut-off March 2017	
PRACE facility	ARCHER
PA number	2010PA3735
Project's start	01-Jun-2017
Project's end	31-May-2018
Title	**Scalable Delft3D FM for efficient modelling of shallow water and transport processes**
Type	D
Project leader	Menno Genseberger
PRACE expert	Wim Rijks, Martijn Russcher
PRACE facility	CARTESIUS
PA number	2010PA3775
Project's start	01-Jul-2017
Project's end	30-Sep-2018
Title	**Radiative Transfer Forward Modelling of Solar Observations with ALMA**
Type	D
Project leader	Sven Wedemeyer
PRACE expert	Wei Zhang
PRACE facility	ABEL
PA number	2010PA3776
Project's start	01-Jul-2017
Project's end	30-Jun-2018

Cut-off June 2017	
Title	**High-precision nonadiabatic rotational states of hydrogen molecule**
Type	D
Project leader	Jacek Komasa
PRACE expert	Piotr Kopta
PRACE facility	EAGLE
PA number	2010PA3954
Project's start	01-Nov-2017
Project's end	31-Oct-2018

Cut-off September 2017	
Title	**Automatic generation and optimization of meshes for industrial CFD**
Type	D
Project leader	Johan Hoffman
PRACE expert	Jing Gong
PRACE facility	ARCHER
PA number	2010PA4037
Project's start	01-Nov-2017
Project's end	31-Oct-2018
Title	**Optimisation of EC-Earth 3.2 model**
Type	C
Project leader	Virginie Guemas
PRACE expert	Kim Serradell
PRACE facility	MARENOSTRUM
PA number	2010PA4064
Project's start	18-Oct-2017
Project's end	17-Apr-2018

Cut-off December 2017	
Title	**Optimization and scalability of the tmLQCD package for production of gauge configurations at the physical pion point**
Type	C
Project leader	Silvano Simula
PRACE expert	Giorgio Amati
PRACE facility	MARCONI
PA number	2010PA4147
Project's start	01-Jan-2018
Project's end	30-Jun-2018

2.7 Dissemination

New PA Cut-offs are normally announced on the PRACE website [1].

Sites are also asked to distribute an email to their users to advertise preparatory access and especially the possibility of the dedicated support.

Each successfully completed project should be made known to the public and therefore the PRACE collaborators are asked to write a white paper about the optimization work carried out. These white papers are published on the PRACE web page [1] and are also referenced by this deliverable.

2.8 Cut-off September 2016

This section and the following sub-sections describe the optimisations performed on the Preparatory Projects. The projects are listed in accordance with the cut-off dates in which they applied. General information regarding the optimisation work done as well as the achieved results are presented here.

2.8.1 Optimization of REDItools package for investigating RNA editing in thousands of human deep sequencing experiments, 2010PA3430

Overview:
RNA editing by A-to-I deamination is the prominent co-/post-transcriptional modification in humans. It is carried out by ADAR enzymes and contributes to both transcriptomic and proteomic expansion. RNA editing has pivotal cellular effects and its deregulation has been linked to a variety of human disorders including neurological and neurodegenerative diseases and cancer. The advent of high-throughput sequencing technologies has largely improved the computational detection of RNA editing events at genomic scale, revealing its pervasive nature in the human transcriptome. Recently, the first computational tool, called REDItools, was developed to identify A-to-I events in large transcriptome sequencing experiments (RNAseq) by traversing individual genomic positions of multiple read alignments. Despite these findings, many functional aspects of RNA editing are yet unknown and further investigations are needed to elucidate the dynamic regulation of editing sites. Handling huge amount of RNAseq data, however, is quite computationally intensive. Each RNAseq experiment includes at least 50 million reads and REDItools take on average from 10 to 24 hours for time-to-solution to provide a complete RNA editing profile, precluding such kind of analyses on standard servers. Although High Performance Computing (HPC) could drastically reduce computational times, REDItools require software modifications to run on HPC systems. Here it was proposed to optimize and redesign the main REDItools algorithm in order to efficiently scale on large HPC systems. Optimisation steps will include the development of a novel algorithm supporting parallelisation and the inclusion of dedicated functions in order to strongly decrease computational times. The optimisation will make REDItools ready for HPC systems and able to handle really huge amount of RNAseq experiments without any precedent.

Scalability results:
To evaluate the scalability of the optimised REDItools version, it was extensively tested on the Marconi HPC infrastructure at CINECA by using tens to hundreds of cores. In particular, scalability tests have been performed by running the parallel algorithm using 36, 72, 144 and 288 Intel Broadwell cores.

The project calculated computing time for each configuration and plotted the data on the chart depicted in Figure 5, showing the strong-scaling behaviour of the algorithm running on multiple cores. The tests prove that the algorithm scales, but also shows a performance degradation when more than 200 cores are taken in to account. This behaviour may be due to the serial overhead of the code especially in the start-up phase of the execution.

In addition, the project checked the relationship between the elapsed time and the number of input genomic intervals. Such analysis progress is depicted in Figure 6. First 3-6 minutes are required to dynamically calculate genomic regions with approximately equal read density. Then, selected threads start analysing each individual assigned interval. As shown in Figure 6, the curve steepness of the completed intervals increases with the increase of the number of cores.

In conclusion, the results demonstrate that the speed up scales almost linearly with the number of used cores. Therefore, the novel and parallel REDItools code is ready to profile RNA editing in single large-scale experiments in just a few minutes.

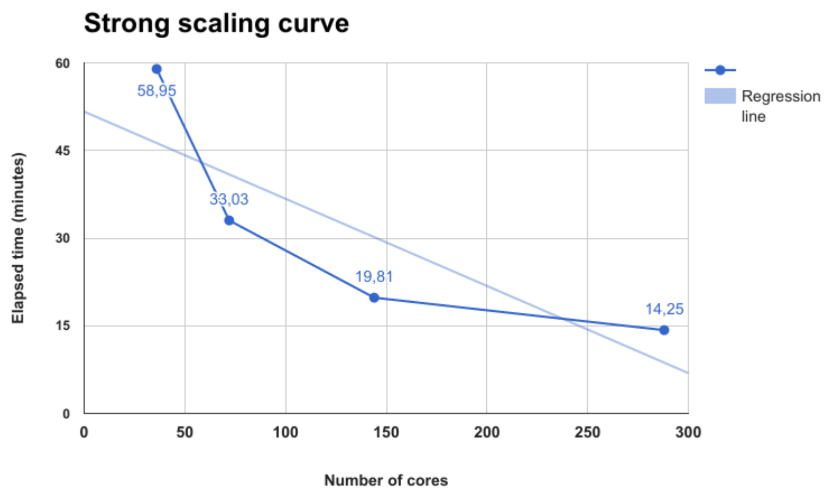

Figure 5: Strong scaling curve for REDItools.

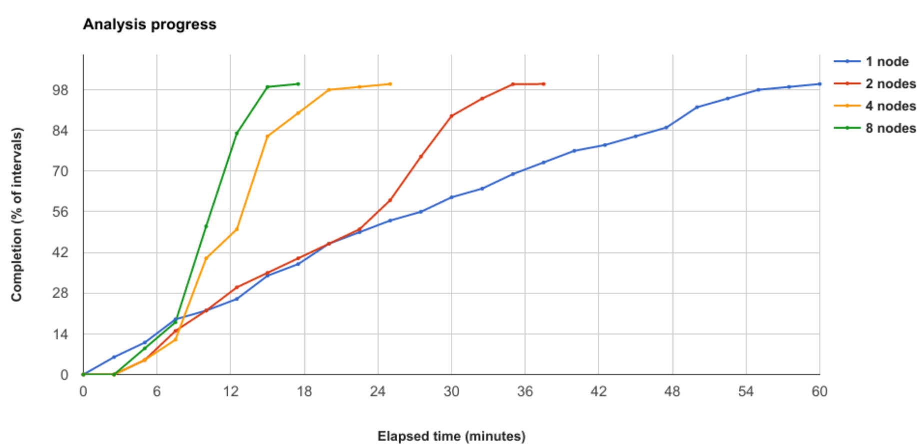

Figure 6: Analysis progress test with REDItools using 36 cores per node.

Accomplished work:

REDItools have been designed to handle massive sequencing data. However, they require a lot of computational time in standard non-HPC infrastructures. In a sample of 2600 public RNAseq experiments, REDItools took, in many cases, from 100 to 300 hours to complete a single experiment using only a core and 2GB of RAM (tests performed at INFN infrastructure in Bari-Italy comprising a server farm with 150 nodes and 4000 cores).

The optimisation process started with the redesign of the main REDItools algorithm in order to employ the parallel computation. In particular, an ad-hoc pre-processing step has been implemented, consisting in finding optimal genomic intervals to reduce computational peaks. Once such intervals are identified, the REDItools software runs on each chromosomal region in parallel and depending on available cores.

The parallel implementation of REDItools is based on a central MPI dispatcher which iteratively assigns subtasks (intervals) to MPI slave processes, then waits for their completion and finally collects the output into a single textual file.

To this end the main algorithm implemented in REDItools was redesigned in order to run the code in HPC infrastructures. The core of REDItools is written in Python and the traversing of multiple read alignments in BAM format is facilitated by ad-hoc routines which leverage on the latest Pysam module (v. 0.11), a wrapper of SAMtools. Before developing a novel parallel code, a first optimisation of the existing serial code has been applied. In the previous version of REDItools, for each genomic position analysed, all the aligned reads were loaded multiple times, considerably increasing the overall computing time. In the novel version, reads are kept in memory until their final aligned nucleotide. In this way, only a small set of reads are kept in memory at a given time, avoiding the loading of the same read multiple times.

Then, a parallelised version of the optimized code, named REDItools2.0, has been implemented in order to perform all genomic intervals with size inversely proportional to their read density. Thanks to this optimisation the execution time decreases proportionally to the number of genomic intervals. The novel code, written in Python, is based on the MPI paradigm and achieves customisable parallelism by assigning the analysis of each interval to any given MPI process available, maximising the overall throughput. After all the intervals have been analysed, editing events detected by the algorithm are finally collected into a single text file by means of a centralised routine.

Results of the enabling process:

Thanks to the preparatory access project two main algorithmic results have been achieved:

1. The serial version of the previous REDItools has been considerably improved.
    a. The original code made use of the Pysam function called ‘mpileup’ which returns the set of reads aligned to a given genomic position. The mpileup function was naively invoked for each position during the traversal of the reference genome from the first position to the last, and it has probably not been optimized for a systematic traversal of genome but rather designed to work only on random positions. The repetitive invocation of the function on adjacent positions probably caused the same

read to be loaded from disk as many times as the length of the reads, making the I/O the true bottleneck of the analysis.

   b. To the end, the loading of the reads from disk was optimized, by requesting each read only once and keeping in memory as far as it mapped with any reference position (and discarding it as soon as the algorithm proceeds after the end of the read).

2. A parallel (multi-node) version of the first version of REDItools has been released [7].

Main results:
REDItools have already been extensively tested on Intel machines (HP Proliant systems) and results on a limited number of RNAseq experiments have already been reported in literature [9]. REDItools are currently used worldwide and some research groups have already employed REDItools capabilities to detect RNA editing in human diseased samples focusing on recoding changes potentially involved in tumour onset and progression [10] REDItools have also been used to profile RNA editing in single cells providing really exciting biological insights.

The novel version of REDItools is expected to be demanding by the scientific community since the detection of RNA editing sites in large-scale genomic experiments is yet a challenging task. In addition, an accurate identification of RNA editing sites is quite time-consuming. The tests prove that REDItools2.0 is on average ten times faster than the previous version and scalability results show that the speed up scales almost linearly with the number of cores involved in the experiment.

Relevance and future work: Having an optimized code to profile RNA editing in few minutes, made REDItools2.0 suitable for large scale transcriptome investigations, facilitating the discovery of RNA editing in large cohorts of RNAseq experiments (>10,000 samples) like those produced in GTEx or TCGA projects. In addition, the optimized version of REDItools will be useful to explore RNA editing in non-human organisms. The parallel implementation of REDItools2.0 will also facilitate the use of the software in different scientific contexts helping to decipher the real biological role of RNA editing in human and facilitating the medical research in finding new prognostic targets or in developing novel and innovative drugs for the incoming “genomic surgery”.

The project also published a white paper, which can be found online under [8].

It is planned to apply for PRACE Project Access since the optimized software is now ready to work on thousands of real experiments in order to profile the RNA editing in a variety of physiological and pathological conditions.

2.9 Cut-off December 2016

2.9.1 OPtimized mulTI-fluid plasMA Solver (OPTIMAS), 2010PA3673

Overview:
A massively parallel numerical solver for simulating multi-fluid, chemically reacting and radiative magnetised plasmas on unstructured grids is being developed since 2013 within the open source COOLFluiD platform. The C++ code, which is truly unique in its kind and results from the collaboration among VKI, KU Leuven and NASA researchers, is unsteady, time-implicit and its

main target applications include computationally intensive 3D simulations of crucial phenomena such as magnetic reconnection, wave propagation through the solar atmosphere and solar wind/earth magnetosphere interactions. Before moving towards more realistic, scale-resolving 3D simulations, requiring prohibitively large meshes in order to fully capture the physics of the phenomena it was wanted to investigate, if a careful performance assessment and optimisation is needed on Tier-0 systems. The usage of the latter is mandatory for fulfilling the memory and run-time requirements of the target 3D test cases. During this project the MPI-based parallel algorithms (i.e. parallel mesh extrusion from 2D to 3D), including I/O (i.e. parallel reading of input mesh data files, parallel writing of solution files in different formats), for realistic 3D setups (<=1 billion mesh points, 18 PDEs) were tested and optimised to be run on up to 100,000 CPU cores. The two different architectures (IBM BlueGene/ Q and CRAY XC40) allowed the project to:

- improve portability of the code, which requires tuning of the CMake-based configuration system and implement compilation-related fixes;
- compare simulation and I/O performances on those systems; identify and tackle pitfalls (especially in I/O) by upgrading existing parallel algorithms;
- maximise memory scalability which, if not optimal, could be an issue especially on BlueGene/Q systems which have very limited memory per core.

Scalability results:

All granted CPU-time has been consumed to port, debug and test the code on up to 16,000 cores on JUQUEEN and up to 60,000 cores on Hazel Hen, leaving no time remaining for running scalability tests.

Moreover, due to the impossibility of compiling with full optimization enabled using the IBM compiler on JUQUEEN, the code was running about 5X slower than on other systems (given the LINPACK performance per core, a factor of 3X in relation to HAZEL HEN would have been expected), which would have also increase the complexity of scalability tests. It is expected to perform the scalability tests on Hazel Hen within a follow-up PRACE preparatory access B project and test up to 100,000 cores.

Accomplished work:

The first goal of the project has been to be able to compile the code using static linking and the native compiler (IBM and CRAY) on the system. This has required a few fixes in the CMake-based configuration system which had been only tested with dynamic linking up to now and never with IBM compilers. Some difficulties have arisen from the particular versions of some dependency packages (PETSc, Boost, ParMETIS) which were available on the systems and different from the one initially supported by COOLFluiD, but minor fixes were implemented to ensure compatibility.

The second goal has been to run the code. This unfortunately has turned out to be the most time-consuming activity of the whole project, especially for JUQUEEN, requiring almost 3-months of debugging, code modifications and heavy interaction with JUQUEEN support team. Herein, O2 was the maximum allowable compiler optimization level for the IBM C++ compiler on JUQUEEN not to have issues at the end (i.e. after including all other fixes), which unfortunately caused the code to run ~5X slower than on the Hazel Hen system. In order to circumvent the problem, more and more intrusive solutions have been implemented, ending up with implementing a new mechanism that was bypassing the self-registration of objects.

The end goal has been to improve the parallel writing algorithm by integrating a portable core-to-node algorithm which was developed by NSC experts. This modification allowed for ensuring a better memory balancing amongst processes since the existing algorithm was blindly assigning aggregating cores on the base of the rank, which can easily lead to overload only a few nodes with I/O. Such a modification to the parallel writing which was successfully tested on both systems, has been favourable for both the COOLFluiD mesh extruder and the plasma solver which share the same algorithm.

The next goal has been to generate a set of computational meshes, which allowed for debugging the parallel mesh extruder and testing it on both systems.

Once meshes were ready, testing of the plasma solver started on both systems. Problems with the parallel reading phase forced the project to first fix the existing code by preventing more than one process reading the same portion of data (boundary data) concurrently.

Another issue was related with the existing algorithm to create some parallel data structure for keeping track of ghost points for parallel synchronization. The code was segfaulting and since the algorithm was old, overly complex and not easily understandable, it was decided to just re-implement it from scratch.

Results of the enabling process:

The CMake-based configuration system of COOLFluiD has been adapted to compile/ run using static linking on the JUQUEEN and Hazel Hen system using the native IBM and CRAY compiler.

A mechanism to completely bypass the self-registration technique, by introducing more dependencies into the code and getting rid of any use of static data (inside abstract object Factories), has been implemented. This could be useful in the future with other compilers as well besides IBM.

The plasma solver has been successfully run on up to 16,000 cores on JUQUEEN and 60,000 cores on Hazel Hen, including I/O (both reading and writing) but no scalability data are available since all CPU-time was consumed before.

The existing parallel mesh generation tool, able to extrude from 2D to 3D meshes, has been debugged and made fully memory scalable by removing some global-size arrays. It has been tested to generate meshes up to 1.3 billion points on JUQUEEN using up to 240 cores and 2.7 billion points on Hazel Hen using 4,000 cores.

A portable mapping core-to-node algorithm developed by NSC experts has been integrated into the writing algorithm, making the memory distribution more balanced (allowing to select the same number of aggregating cores per node on both systems). This algorithm is used by both the COOLFluiD solver and the mesh extruder so this development has been extremely useful to improve both.

The parallel reading algorithm has been modified to avoid having all processes reading a part of the mesh data at a particular point (boundary data) which was originally causing the reading to fail on both systems; in the modified version, data are only read by the master process and then broadcast to the others.

The existing parallel algorithm to build the ghost point mapping in each partition has been totally re-implemented by reusing data collected during partitioning (previously re-built on-the-fly) and optimized to get past this simulation phase on more than 10,000 cores.

All mentioned algorithms were written in C++ and rely on MPI for communication.

Main results:
Overall, the project was quite successful, also considering that it took about three months before being actually able to run something on JUQUEEN or Hazel Hen. The code has been made more portable by upgrading the CMake-based build system and enabling the static linking on BlueGene/Q and XC40 systems.

The parallel I/O has been strengthened, made more robust and tested on up to 60,000 cores.

No time was left to implement a two-step partitioning based on ParMETIS, but this feature is desirable since ParMETIS is known to fail on ~100,000 cores.

Originally, it was expected that the PRACE expert would have implemented a binary version of the parallel TECPLOT format file writer, but this was not achieved, due to time constrains.

Unfortunately, most of the CPU-time was consumed for debugging purposes leaving no allocation left for actual scalability tests which are planned within a follow-up Preparatory access.

The target application in its full setup takes a lot of memory and still remains challenging to fit it on PRACE systems. However, some ways to save memory have been identified (use of cheaper PETSc preconditioner: PCBJACOBI instead of PCASM) and already partially implemented (ghost point algorithm).

The target remains to be able to apply for a PRACE project. In order to reduce the needed computational resources, a reduced setup will be proposed in that case.

2.9.2 Water droplets and turbulence interaction inside warm cloud -- clear air interface, 2010PA3699

Overview:
The project was born and written within the group of H2020 MSCA ITN COMPLETE, which is a research/training network for the study of microphysics, turbulence and telemetry of warm clouds, (see [14] and [15]).

Hitherto, simulations of lukewarm clouds assumed static and homogeneous conditions on average. However, the project was interested in the unsteady dynamics of the transport through the interface between cloud and the clear air surrounding it.

In the simulation, cloud interfaces are modelled through two interacting regions at different turbulent intensity. Different initial conditions reproduce local stable or unstable stratification in density and temperature. The droplet model includes evaporation, condensation, collision and coalescence. The typical water content inside the cloud parcel simulated (about 500 m^3), associated to an initial condition where drops are 30 microns in diameter, leads to an initial number of drops of 10^{11}. A grid up to 4092x2048x2048 points is seek, which leads to a Taylor's microscale Reynolds number of 500. The governing equations are Navier-Stokes equations in Boussinesq‘s approximation coupled to equations describing the evolution of water drops seen as inertia particles, transported by background turbulence and gravity.

Aims of the project:

- Code organization/optimization with respect to the inherent difficulty of the physics which leads to a highly discrete, uneven, unsteady distribution of the drops as seen by each core;
- Code scalability to a few thousands of cores.

Scalability results:

The following Table 3 show the data test cases: the first one is for a grid of 256X256x512 points, while the second one, Table 4, shows data for a bigger grid of 1024x1024x2048 points. The speed-up of the first table has been computed taking as reference time the value of time obtained using one core, while in the second case the reference time is the value obtained using 256 cores. The wall clock time refers to the mean time step.

Table 3: Data obtained running a simulation on a grid 256x256x512.

Number of cores	Wall clock time	Parallel Efficiency	Number of Nodes	Number of process
1	190	1	1	1
4	34,8	1,36	1	4
8	16,8	1,415	1	8
16	8,3	1,43	1	16
32	4,7	1,27	1	32
64	2,9	1,02	1	64
128	1,8	0,83	2	128
256	1,2	0,6	4	256

Table 4: Data obtained running a simulation on a grid 1024x1024x2048.

Number of cores	Wall clock time	Parallel Efficiency	Number of Nodes	Number of process
256	57,2	1	4	256
512	27,9	1,03	8	512
1024	15	0,96	16	1024

Accomplished work:

Both versions of the code with slab parallelization, the one without water droplet and that with water droplets, have been analysed by means of a careful profiling with Vtune [11], Scalasca [12] and Advisor [13].

Both code versions have been modified by reversing the order in some loops to improve memory access performance and vectorization. This last has been improved by adding compiler directives: Forcing vectorization where this was efficient and enforcing it where the automatic vectorization was not efficient.

Bottlenecks where identified by using Scalasca. In the pencil parallelized version without particles, the bottleneck was the MPI barrier calls due to the load unbalancing among processors. In the slab parallelized version with particles the bottleneck was the increase of the communications among processors (in the `MPI_Send_receive_replace` call) which was directly associated to the increase in the number of processors.

A pencil parallelization was also developed for the code version without droplets. However, given the related high increase in core communications, this code structure is not considered suitable for the highly uneven workload associated with the presence of the droplets and their turbulent transport.

Results of the enabling process:
The algorithm for the initial generation of the population of water droplet has been improved. The initial conditions have now been obtained from a linear matching of the two initially homogeneous and isotropic fields over a narrow region - as large as the flow integral scale - by means of a weighting function. For the stable stratification simulations it is foreseen to vary over about two orders of magnitude relevant parameter ($0.1 < Fr < 10$). The NAG library has been substituted with the FFTW library in order to optimize the code. Another modification of the code concerns the I/O subroutines, in fact the old version of the code did not include the possibility to have a restart.

Main results:
The activity carried within this preparatory grant was very useful:

- To optimize some numerical features already present in the code;
- to learn how to profile the code source and to exploit the potentiality of advanced Fortran compiling programs;
- to reason with the help of PRACE system administrators on good strategies to obtain the best computational performance of the code, which is in continuous evolution to follow new ideas and necessity of the research team, in relation to the current state and feasible improvement of the model used to represent the physical system under study;

It is planned to apply for one of the next Tier-0 regular PRACE calls, to extend the previous investigations and to enhance the interdisciplinary applications of this research in geophysical sciences.

2.10 Cut-off March 2017

2.10.1 Quasi-particle self-consistent GW approximation: avoiding the I/O bottleneck, 2010PA3745

Overview:
The Questaal Code is a novel, highly accurate, electronic structure code which allows to go beyond the standard density functional theory level as it implements the quasi-particle self-consistent GW method. This method has the capability to set a new standard in accuracy, and forms a natural basis for further methodological improvements, such as an extension to dynamical mean field theory.

However, the calculations are, computationally extremely demanding. In previous UK based ARCHER dCSE and eCSE projects, the code has been parallelized, introducing several layers of MPI parallelism, including a distributed memory version using PBLAS/ScaLAPACK.

Despite the implementation of parallel I/O using HDF5, the nature of the loop structure required independent file access of the different processors. This caused a major bottleneck for large physical systems (more than 50 atoms) as the size of output files could reach several 100 GBytes.

The main purpose of the PRACE PA project was to change the code in order to allow collective IO.

Scalability results:
The original code showed very bad scaling, which was partially due to the I/O bottleneck, and partially due to a load balancing problem. Table 5 shows a direct strong scaling comparison of the old and new I/O approach.

Table 5: Comparison of strong scaling for the old and new I/O approach

	Old (non-collective I/O)		New (collective I/O)	
# of cores	Wall time	CPU time	Wall time	CPU time
16	125	108	122	108
64	174	74	87	75
256	133	50	62	50

Accomplished work:
The main action has been to fully implement and fix the padding of parallelized loops, which then allowed the use of collective parallel I/O using HDF5. The forced individual access which was used before in order to prevent deadlocks had an impact on the I/O performance. This issue has now been resolved.

Results of the enabling process:
For a typical example, a 16 atom supercell of Silicon, which is still at the small end of the scale, running on 256 cores, the I/O bottleneck was already substantial, and enabling collective I/O reduced the wall-clock time by a factor of 2. For larger systems, even better speed-ups are expected.

Main results:
The main result of the project was that the non-collective I/O, indeed, posed a large bottleneck and for the system of consideration increased the CPU time by a factor of 2. The changes, implemented, now allow to enable collective I/O and removed that bottleneck.

The main results of the project revealed further optimization needs, which go far beyond the current work. There are plans to restructure the code in a way to avoid much of the expensive I/O in the first place.

3 T7.1.B SHAPE

In this section, the progress in task 7.1B SHAPE will be discussed. Section 3.1 gives an overview of the SHAPE process and related statistics. Section 3.2 gives a high-level view of the current status of the SHAPE projects.

In the period since the previous deliverable (PRACE-4IP D7.2 [2]), the three unfinished second call projects have concluded, along with all the third call projects. Follow-up requests have been sent to those projects, to see how the work performed with the assistance of SHAPE has affected the SMEs' business – these are reported in section 3.3. Summary reports for the ongoing fourth and fifth call projects are reported in section 3.4, along with an overview of the lessons learned with regards to the implementation of the SHAPE programme. In addition, following the recently concluded 6th SHAPE call, the successful projects have now begun and are discussed in section 3.5. Finally, the future of SHAPE is discussed in section 3.6.

3.1 SHAPE Overview

SHAPE (SME HPC Adoption Programme in Europe) is a pan-European initiative supported by the PRACE project. The Programme aims to raise awareness and provide European SMEs with the expertise necessary to take advantage of the innovation possibilities created by High-Performance Computing (HPC), thus increasing their competitiveness. The programme allows SMEs to benefit from the expertise and knowledge developed within the top-class PRACE Research Infrastructure.

It can be challenging for SMEs to adopt HPC. They may have no in-house expertise, no access to hardware, or be unable to commit resources to a potentially risky endeavour. This is where SHAPE comes in, by making it easier for SMEs to make use of high-performance computing in their business - be it to improve product quality, reduce time to delivery or provide innovative new services to their customers.

Successful applicants to the SHAPE programme get effort from a PRACE HPC expert and access to machine time at a PRACE centre. In return the SME commits a comparable amount of effort and provides their domain expertise. In collaboration with the SME, the PRACE partner helps them try out their ideas for utilising HPC to enhance their business. So far, SHAPE has assisted 41 SMEs (see the project website http://www.prace-ri.eu/hpc-access/shape-programme/ for examples), and the 7th call for applications will open in April 2018 so there will be more SMEs introduced to the benefits of SHAPE participation.

Table 6 shows the calls, applications, approved projects and person months committed from PRACE so far in SHAPE.

Table 6: SHAPE call statistics

Call	Call open	Applications	Approved	PMs
Pilot	June 2013	14	10	35
2	Nov ’14 – Jan ‘15	12	11	45.25
3	Nov ’15 – Jan ‘16	8	8	30.75
4	Jun ’16 – Sep ‘16	8	4	17
5	Mar ’17 – Jun ‘17	7	6	20.75
6	Oct ’17 – Dec ‘17	5	2	9.5
7	Apr ’18 – Jun ‘18	-	-	-
	Totals	54	41	158.25

Figure 7 shows the broad range of industry domains that have been represented in SHAPE so far, and Figure 8 the countries from which the participating SMEs originate.

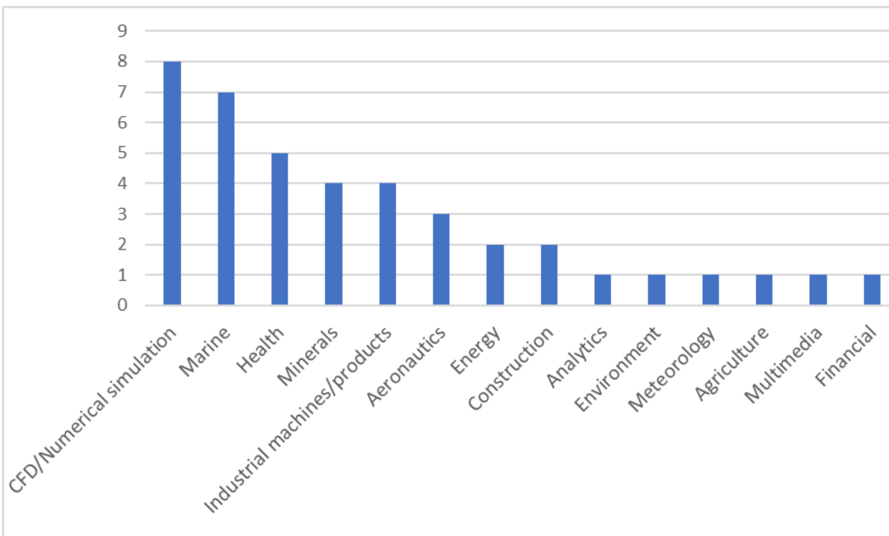

Figure 7: SHAPE: SME industrial domains

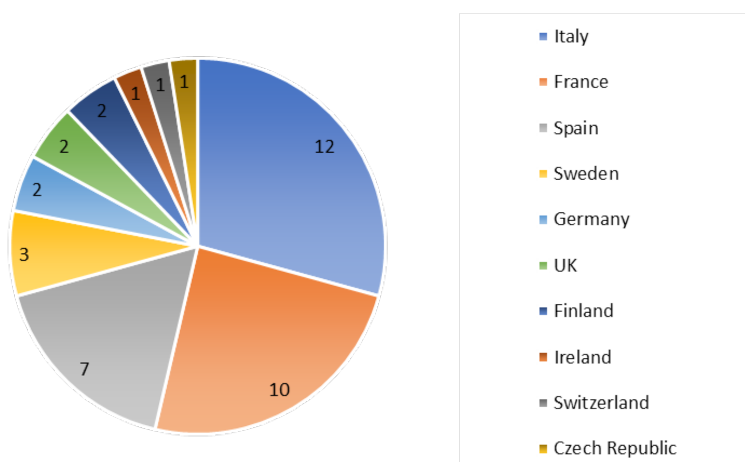

Figure 8: SHAPE: SME country of origin

3.1.1 SHAPE Process

The process for SHAPE is as follows:

- SHAPE Call is launched. There is a form to be filled in (by the SME, although assistance from PRACE is available if required) which can be completed online or downloaded and submitted via email – the form contains suggestions and information on how to complete it.
- The Call closes: The applications are reviewed by the SHAPE review panel (see below).
- Recommendations: The review panel makes their recommendations on which projects to approve, and the PRACE MB/TB ratifies this.
- Pairing: the successful projects are matched to PRACE partners who have effort available and relevant expertise.
- Machine time: with help from the PRACE partner the SME applies for machine time on an appropriate system – this is usually via Preparatory Access type D, but other arrangements are possible where agreements can be reached between the PRACE partner and the SME.
- Coordination: The SME and PRACE partner do the project work, and the SHAPE coordinator monitors progress.
- Deliverables and output: During the project the SME is expected to publicise their interaction with PRACE and SHAPE. This can be via their own website, press releases, publications in their field, and so on. In addition, they are expected to contribute to providing information for PRACE deliverables (such as this document) on the status of the project, in collaboration with their PRACE partner.
- Conclusion: At the end of the project, it is expected that a white paper will be produced detailing the technical work and results, which will be made publicly available on the PRACE website following internal review. In addition, approximately 12 months after the completion of the work, a follow-up report will be requested from the SME to try and evaluate the Return on Investment of the SHAPE work.

3.1.2 Review of Applications

The composition of the review panel changes slightly with each call mainly due to availability, but typically it is:

- Two members from the PRACE Board of Directors,
- One member from the Industry Advisory Committee,
- One member from the PRACE Peer Review Team,
- Two members representing 5IP-WP7,
- One member representing the preparatory access team.

Given the current two-stage process of applying for SHAPE (apply to SHAPE, then if successful apply for machine time, usually via Preparatory Access), this final panel member is included to give a preliminary opinion on the technical suitability of the application from the PA point of view. It should be noted that this two-stage process has been streamlined for the most recent call to minimise the burden on the SME.

The criteria used in the review were:

- ***Fit with the goals of SHAPE***
  - The aim of SHAPE is to assist SMEs in overcoming the barriers to adopting HPC, such as risk, initial cost, lack of in-house expertise and lack of access to resources.
  - The target audience for SHAPE is SMEs with *no* or *little* experience of HPC, who can be assisted with *both* expertise from PRACE, *and* time on a PRACE machine.
  - It is *not* a way of getting processor cycles for production runs for existing codes – there are other avenues for this via PRACE such as the project access calls.
- ***Strength of the business case***
  - The expertise and resources provided through the SHAPE programme 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, offer new products or services, or recruit dedicated staff. The solution implemented should be part of a business plan to further engage in HPC in the long term.
- ***Technical Achievability***
  - The proposals are expected to be realistically achievable in the timescales described and with the resources made available.
- ***Other aspects considered***
  - The commitment of the SMEs to co-invest with PRACE in achieving the project goals. The effort for the project should be at least approximately equally split between the SME and PRACE.
  - the innovative aspects of the proposal.
  - the social and economic impact on society as a whole.

The applications are reviewed and ranked according to these criteria, then the final recommendations are put forward to the PRACE Board of Directors for approval.

3.2 SHAPE Project status

Here, an overview of the status of the SHAPE projects is reported. As mentioned earlier, where it has been a year since the conclusion of a project, the participating SMEs have been asked to provide a follow-up report to assess the impact of the SHAPE work on their business. For the remaining ongoing projects, each were asked to provide a summary of their project for this document. The details of these are provided in the following sections. On conclusion of the work, each project is expected to produce a white paper for review and publication on the PRACE website.

As of March 2018, the status of the remaining second and third call projects is as described in Table 7, and the fourth, fifth and sixth call projects in Table 8.

Table 7: SHAPE status - second and third call project follow-ups

Call	SME	PRACE	White Paper	Follow-up Report
2	WB-Sails	CSC	Published	Section 3.3.1
2	Principia	CINES	Internal technical report	Not provided, see Section 3.3.2 for details
2	Algo'tech	INRIA	Published	Not provided, see Section 3.3.3 for details
3	ACOBIOM	CINES	Published	Section 3.3.4
3	Airinnova AB	KTH	Published	Section 3.3.5
3	Creo Dynamics AB	KTH	Published	Section 3.3.6
3	AmpliSIM	IDRIS	Published	Section 3.3.7
3	ANEMOS SRL	CINECA	Published	Section 3.3.8
3	BAC Engineering Consultancy Group	BSC	Published	Section 3.3.9
3	FDD Engitec SL	BSC	Published	Section 3.3.10
3	Pharmacelera	RISC	Published	Section 3.3.11

Table 8: SHAPE status – fourth, fifth and sixth call projects

Call	SME	PRACE	White Paper	Status Report
4	Artelnics	BSC	Delivered, under review	Section 3.4.1
4	Milano Multiphysics	CINECA	Expected April 2018	Section 3.4.2
4	Renuda UK Ltd	EPCC	Accepted, due to be published	Section 3.4.3
4	Scienomics	IDRIS	Accepted, due to be published	Section 3.4.4
5	Disior Ltd	CSC	Tech work still ongoing	Section 3.4.5
5	Invent Medical Group, s.r.o.	IT4Innovations	Expected April 2018	Section 3.4.6
5	AxesSim	CINES	Tech work still ongoing	Section 3.4.7
5	E&M Combustion S.L.	BSC	Tech work still ongoing	Section 3.4.8
5	Svenska Flygtekniska Institutet AB	KTH	Tech work still ongoing	Section 3.4.9
5	Brabant Alucast International	CINECA	Tech work still ongoing	Section 3.4.10
6	Axyon AI SRL	CINECA	Project started Feb 2018	Section 3.5
6	Vision-e S.r.l.	CINECA	Project started Feb 2018	Section 3.5

3.3 SHAPE Second and Third call: Follow up for completed projects

This section presents the follow up reports from the SMEs which concluded their SHAPE work in 2016-2017. The key aim of this exercise is to ascertain how taking part in the programme has affected the SMEs: what are they now doing with HPC following the SHAPE activity, what is their return on investment, and so on.

A report template was distributed to the SMEs and PRACE partners, and included the following Key Performance Indicators (KPIs) affected by the SHAPE work to be considered (but not limited to):

- New customer acquisition,
- Turnover,
- Return on Investment (RoI),
- New product offers,
- New service offers,
- Access to new markets,
- Enhanced software features,
- Staff recruitment.

The full responses are presented below, and summarised in section 3.3.12

3.3.1 WB-Sails (Finland): Simulation of sails and sailboat performance

Project details	
Project Start – End Dates	1st April 2015 – 1st April 2017
PRACE Partner	CSC
PRACE effort (Person Months)	3
PRACE machine time	-

Project overview

WB-Sails designs and manufactures sails, specialising in top-end racing products. From the beginning WB-Sails has relied on technology, research and development to become one of the very few sailmakers in the world present at the Olympic level. In London 2012 their sails, designed and manufactured in Finland, won a gold and a bronze medal in two different disciplines (boat classes). In Rio 2016, a silver medal was won.

WB-Sails has a long tradition in CAD and CAM, with computer based design since 1979 and manufacturing (automated laser cutter) since 1988.

In this project WB-Sails wished to utilize HPC resources to perform simulations of sailboats using XFlow software. In addition to simulating airflow around sails, two phase studies with free surfaces and realistic motion of the hull in seaway were planned. Ultimately, the goal was to combine CFD with structural analysis of sails (FSI).

Unfortunately, due to a number of reasons (see D7.2 [2] for further information), not all the goals could be achieved and the obtained results were mostly qualitative. However, important experience in using HPC resources was gained which may prove valuable in future work.

HPC Usage

WB-Sails has not had access to HPC resources after the project. However, the necessary skills for a future HPC project in-house were acquired. WB-Sails will possibly have access to a commercial HPC provider during 2018.

Business impact of the SHAPE project

As the project was mostly about developing and testing methods for R&D use, it is difficult to assess the business impact. No increase in turnover or no new products or services can be attributed to the project. Also, the return of investment was negative considering the time that was spent without tangible results. No new staff members were recruited.

However, the XFlow software was deployed successfully at CSC and WB-Sails learned how to use CSC's HPC environment, which makes it easier to utilise similar resources in the future. Considering the acquired new skills and experience the project can still be viewed as successful.

3.3.2 Principia (France): HPC for Hydrodynamics database creation

Project details	
Project Start – End Dates	January 2016 – April 2017
PRACE Partner	CINES
PRACE effort (Person Months)	2
PRACE machine time	0 (local machines were used)

No report, as the company have not responded to requests for feedback. It should be noted that this is not surprising - the original work with SHAPE was not deemed a success (see D7.2 [2]), so at that time an internal technical report was produced rather than a white paper.

3.3.3 Algo'tech (France): High Performance to Simulate Electromagnetic Disruption Effects in Embedded Wiring

Project details	
Project Start – End Dates	Jun 2015 – April 2017
PRACE Partner	INRIA
PRACE effort (Person Months)	6
PRACE machine time	0 (time was arranged on a Bull machine in a separate agreement)

No report. The company have been recently taken over and did not respond to requests for feedback.

3.3.4 ACOBIOM (France): MARS (MAtrix of RNA-Seq)

Project details	
Project Start – End Dates	11th April 2016 – 20th April 2017
PRACE Partner	CINES
PRACE effort (Person Months)	4.25
PRACE machine time	0 (amount of core-hours requested was too large for the preparatory access calls, so a direct agreement was arranged between CINES and Acobiom allowing the use of 1.2 million core-hours on Occigen)

Project Overview

Acobiom is a French biotechnology company specialized in the discovery and the validation of new biomarkers for diagnostic and therapeutic purposes. The Acobiom business model is based on two main business lines:

- In-house innovative diagnostics for personalized medicine applications in oncology, neurodegenerative diseases;
- Services for discovering genomic/pharmacogenomic/transcriptomic biomarkers dedicated to research and diagnosis applications, as well as for helping to develop new drugs.

The RNA-Seq approach is used in a wide variety of applications. Since RNA-Seq provides absolute values and does not require any calibration with arbitrary standards, results can be compared at any time with other data, even that raised by independent laboratories. Once collected, these data can be digitalised and then easily and reliably compared in silico with the growing library of RNA-Seq databases generated for normal and pathological situations in other laboratories around the world (Human: ~27000 libraries and Mouse: ~42000 libraries). This project aimed at comparing and searching the specificity of our blood gene expression signatures (e.g. the *masitinib* in pancreas) against already existing data in different tissues or pathologies, in Human and Mouse Omic data.

Eventually the expected matrix was produced using the Human-omic data only.

HPC Usage

After completion of the SHAPE project, Acobiom did not invest further in internal HPC hardware solution. Nevertheless, their extensive usage of the MaRS database led them to choose an external HPC solution in compliance with Health data specifics regulation (such as: management system accreditation, security, maintenance, upgrades), which motivates the reason why Acobiom chose to reinforce their internal competencies in the handling of such data.

Business impact of the SHAPE project

The customer adoption of "Big Data" is often discussed but the implementation in their internal workflow is hard. Pharmaceutical Companies are still waiting for a Proof of Concept. In this light the MaRS project did not comply directly for new customer acquisition.

In Acobiom, the MaRS project cannot describe a measurable return on investment. But, for staff training and external communication, this SHAPE experience has shaped them a lot. Currently the MaRS database is used as a leverage to demonstrate their know-how and has helped in maintaining Acobiom in their place at the cutting edge in the race for the treatment of Big Data.

In conclusion, through the SHAPE project Acobiom learned a lot and increased its scientific network, but they cannot yet measure the "financial impact" in terms of new services or new customers. Undeniably though, the SHAPE experience has reinforced Acobiom and they expect positive tangible outcomes from it in the future.

3.3.5 Airinnova AB (Sweden): High-level Optimisation in Aerodynamic Design

Project details	
Project Start – End Dates	1st April 2016 – 31st September 2016
PRACE Partner	SNIC-KTH
PRACE effort (Person Months)	3
PRACE machine time	MareNostrum 50 kCPU, Beskow 200 kCPU

Project overview

The company is developing computational solutions for aerodynamic shape optimization, which is an important task in aircraft design. The goal is to design a lighter, greener, and quieter airplane by reducing drag especially in high speed. Aerodynamic shape optimization for reduced drag requires a large number of CFD solutions, and computational power is a limiting factor. Current ideas for surrogate modelling are being developed to improve computational efficiency.

HPC usage
The SHAPE project gives the SMEs the opportunity to experiment with HPC resources, and especially useful is the technical support from application experts. Airinnova benefitted from SHAPE via carrying out the high fidelity CFD simulations and highly parallel design cycles for high fidelity aerodynamic optimization through the Open-Source CFD tool in HPC/KTH-PDC. Working with KTH-PDC experts, Airinnova has enhanced its expertise for consultancy and project investigation for high performance simulations.

Business impact of the SHAPE project
By working with SHAPE, Airinnova has increased its computational capabilities, as well as the expertise of solving the high performance related problems, this in turn helps them to attract new customers and to investigate new markets. Airinnova is currently considering opening up new services based on the Open Source CFD through HPC. A more automatic and remote workflow will be investigated within their project. They foresee a closer ongoing collaboration with KTH-PDC through the SHAPE project.

3.3.6 Creo Dynamics AB (Sweden):

Project details	
Project Start – End Dates	1st April 2016 – 31st September 2016
PRACE Partner	SNIC-KTH
PRACE effort (Person Months)	3 PMs
PRACE machine time	MareNostrum 100 kCPU, Beskow 50 kCPU

Project overview
The project aimed to demonstrate how aero-acoustics simulation processes, based entirely on open source CFD software, can be tailored and deployed in parallel at large scale to produce robust and efficient results for real life applications. The chosen test case should be of high industrial relevance; e.g. the prediction of the unsteady aerodynamics flow field (and acoustics) around a road car.

Results from the project have been made public to showcase the technology and encourage new users to adopt and invest in HPC and open source software.

The envisaged CFD methodology is expected to deliver simulation accuracy in-line with current industry best practices at a considerably lower cost.

HPC usage
Research programmes such as PRACE SHAPE, giving smaller companies and research teams access to large-scale compute infrastructures, are instrumental in the development and validation of numerical tools and methods capable of delivering cost-effective simulations based on open source software.

Creo Dynamics has gathered valuable information and experiences during this project that will help in building more efficient and competitive simulation processes tailored towards high fidelity analysis of coupled aerodynamics and acoustic problems in automotive applications.

They foresee a significant increase in their HPC usage over time and remote HPC solutions such as the one provided by PDC/KTH are becoming increasingly attractive.

Business impact of the SHAPE project
The SHAPE project has allowed Creo to develop and apply efficient simulation procedures running remotely on hosting HPC systems. This has already increased their capabilities and efficiency of their services.

In particular, the testing and validation of numerical methods and tools for large-scale application could not have been done without dedicated HPC access and the support from application experts.

Overall, the project has made Creo more prepared to take on new and challenging engineering problems and helped them in developing new numerical tools and procedures targeting the automotive and aerospace markets.

3.3.7 AmpliSIM (France): DemocraSIM (DEMOCRatic Air quality SIMulation)

Project details	
Project Start – End Dates	1st May 2016 – 1st June 2017
PRACE Partner	IDRIS
PRACE effort (Person Months)	6.5
PRACE machine time	ADA, 15000 core hours

Project overview
AmpliSIM is a Paris-based French start-up, created in 2015. AmpliSIM provides an on-demand browser-based Numerical Simulation Service for businesses and public authorities, enabling operational urgent-computing. Their market is impact assessment for Air Quality and management of industrial hazards. They provide private users or public authorities with the capability to perform seamless numerical simulations needed for air quality impact assessment of industrial plants. The DemocraSIM project aims to bring Air Quality simulation to the general public. When the Fukushima hazard occurred, it was possible to display crowd-sourced data of radioactivity measurements on a single web map. If people are able perform their own measurements of radioactivity, and share them, then it raises the question of are they able to simulate an event and get an idea of their own potential exposure, for instance.

The DemocraSIM SHAPE project aim was to allow AmpliSIM to tackle technological locks on the use of urgent-computing, advanced visualization and data-analytics with PRACE HPC experts, before being able to launch an industrial solution on a private HPC-cloud. Also it allows the PRACE HPC expert to address these issues on "real cases", with potential reuse on academic cases of urgent-computing.

HPC usage
The overall goals of the project were:

- Connect the AmpliSIM service to the IDRIS cluster;
- Develop the community framework needed to allow users to share, publish and rate their results;
- Develop the big data analytics and statistical predictors;

- Deploy and test the big data analytics and statistical predictors.

Thanks to the applied HPC improvements, parallelism is now available throughout the computing intensive steps. Migration and deployment to other high performance computing centres is now easier.

AmpliSIM plan now to connect their web service with an HPC supercomputer platform, and enable performing simulations from the AmpliSIM web service:

- Define the test case and prepare the necessary input files, including the submission scripts;
- Upload the files on the service;
- Run the calculation and post-process the output;
- Download the processed output.

Business impact of the SHAPE project
The workflow of the AmpliSIM service consists of several steps:

- Case setup for the numerical model;
- Uploading of input data on IDRIS cluster;
- Launching of simulation;
- Retrieval of post processed data from IDRIS cluster.

As part of the SHAPE project and in order to connect with the IDRIS infrastructure, AmpliSIM upgraded their connection backend. This backend now allows the web portal to drop input files on the cluster, launch the simulations and retrieve the outputs.

AmpliSIM connection backend (ACB) relies on SSH to connect to the supercomputer. Regarding modularity, they had to generalize ACB launching scripts and introduced IBM LoadLeveler (LL) process. On top of being able to hook launching steps thanks to LL steps properties, AmpliSIM is now able to connect to other LL type clusters. IDRIS security constraints enforced them to strengthen SSH options used by the ACB. This is particularly important for their business: data handled by the AmpliSIM web service remains the property of AmpliSIM customers, and are often regarded as sensitive: for instance, pollution levels of an industrial facility are considered to be very sensitive for the customer, and can lead to deleterious effect on the general public if they are communicated without the necessary context of the study performed. The ability to assure their customer with the highest level of security for their data even when moving them outside of their web servers to the calculation backend is mandatory for their business.

Participation in SHAPE has been of real value for AmpliSIM, they are now able to use the portal on a HPC supercomputer and they wish to participate in other PRACE calls like Preparatory Access type D in order to work on an optimizing phase, enabling access to new markets. They also have created a link with IDRIS.

3.3.8 ANEMOS SRL (Italy): SUNSTAR - Simulation of UNSteady Turbulent flows for the AeRospace industry

Project details	
Project Start – End Dates	1st May 2016 – 31st October 2016
PRACE Partner	CINECA
PRACE effort (Person Months)	3
PRACE machine time	Marconi, 1000000 core hours

Project Overview

The proposed project was aimed at improving the robustness and performance of ANEMOS' in-house software on the HPC systems provided by PRACE. This is used for the simulation and the analysis of complex turbulent flows of relevance to the aerospace industry. The kernel of this software is an immersed-boundary-based, compressible, massively parallel flow solver, incorporating state-of-the-art numerical methods and advanced features for the simulation of supersonic flows in complex configurations.

HPC Usage

The code was born as an academic code, developed for the IBM BlueGene architecture. The engineering of the code for industrial applications and the dismissal of the BG architecture by IBM required the investigation of how to port the code to a more modern architecture while at least maintaining (and possibly increasing) parallel efficiency, while conserving numerical consistency. To achieve this goal the support of PRACE experts through the SHAPE project has been fundamental.

Business Impact of the SHAPE project

From a scientific point of view the project was a success, enabling the code to be ported on to the Marconi supercomputer and preserving the computational efficiency. Unfortunately, in terms of impact on the business, the participation of ANEMOS srl in the SHAPE project did not provide a real value for the company, and it did not lead to a measurable return.

The company ceased the activity in 2017.

3.3.9 BAC Engineering Consultancy Group (Spain): Numerical simulation of accidental fires with a spillage of oil in large buildings

Project details	
Project Start – End Dates	1st May 2016 – 31st March 2017
PRACE Partner	BSC
PRACE effort (Person Months)	2
PRACE machine time	Mare Nostrum, 100000 core hours

Project Overview

BAC Engineering Consultancy Group (BAC) is an engineering consultancy SME. It has four main activities:

- Civil Engineering, which includes activities in road works, rail, airports, waterworks and river hydrology, drainage and water treatment, and environment;
- Structural engineering, focusing on the field of structures. Activities include new works, rehabilitation, large equipment, and building height ;
- Quality control, specializing in areas such as quality control in building and civil engineering, inspections and testing, such as non-destructive testing, auscultation and control, naval inspection (thickness measurement) and inspection of tanks (Oil & Gas);
- R&D on prefabrication of concrete and metal structures, software development, studies and research prototypes in Fire Engineering and Wind Engineering.

The objective of the project was to develop a fire engineering analysis (Performance-Based design) of a steel structure building that belongs to the ITER (International Thermonuclear Experimental

Reactor) industrial complex in Cadarache (France), which is devoted to research in the field of Nuclear Fusion.

The SME performed benchmarking and scalability tests of the Fire Dynamics Simulator (FDS) code in BSC's MareNostrum machine up to 2,048 cores and then the results were compared with its in-house cluster. The company verified that its infrastructure is not optimal with respect to node connectivity and system configuration that minimise the scalability of the code. The BSC team supported them to improve parts of the local installation helping to optimize their current infrastructure and detect the bottlenecks to tackle for future clusters and installations.

HPC Usage

The participation in the SHAPE Project has allowed BAC to gain a detailed knowledge of the performance of its cluster, in comparison to what is considered an optimal installation such as at BSC. First of all, based on the collaboration with BSC members, BAC has been able to improve its workstation infrastructure, accelerating calculation times.

It must be taken into account that one of BAC's business areas is fire engineering, developing computer models of fluid dynamics and combustion. The ability to improve the calculation network has meant substantial advantages in the company's business.

Unfortunately, participation in the SHAPE project did not allow BAC to achieve the correct parallelisation of the models, with significant losses in performance in clusters of more than 1 workstation. However, currently, it has been possible to optimize a small HPC cluster of 4 servers (8 processors) in which performance has been significantly improved. Previously, BAC did not have the necessary knowledge to know if the loss of performance was a consequence of the program used (Fire Dynamics Simulator) or of the BAC infrastructure.

BAC's Fire Engineering Department director has been able, based on their participation in SHAPE, to gain experience in HPC at a user level and to understand the advantages that it can bring in the field of fire engineering applied to building engineering. Presently the director gives much more importance to HPC in the business of the company. It is currently being evaluated whether to increase the company's HPC capacity or make use of large HPC centres for specific projects.

In addition, and based on the collaboration of the BSC staff in the project and its recommendations, increasing the company's HPC capacity is an option that is not ruled out, depending on how the market evolves during the next year. The project has enabled the Company to assess the impact that HPC has on the quality of fluid dynamics projects.

Business Impact of the SHAPE project

Since the completion of the SHAPE project, BAC has used the improvements and knowledge obtained directly in various fire engineering projects. A clear example of one application has been the study of fire engineering applied to the dome of Torre Glories in Barcelona. Several models of computational fluid dynamics and combustion have been developed to determine people's safety and the structure's integrity in the case of fire. The experience gained from the SHAPE project has allowed BAC to be much more competitive in the market, offering maximum quality service in a shorter time frame (time frames have been reduced by an approximate factor of 1.6), thus being able to comply with the client's strict requirements.

In addition, the optimisation of the cluster and a better knowledge of HPC technology (applied to BAC's workstations infrastructure) have also made it possible to carry out two projects simultaneously, when previously one of the two projects would have had to be discarded due to the strict deadlines of the clients. All this has been done while guaranteeing the quality of fluid dynamics and combustion models.

Although it is not currently planned to offer new products or services that make use of HPC, they are working to reach a wider market and better position in the field of fire simulations based on fluid dynamics, built on the optimization in the calculation times and the ample knowledge of these simulations running on large HPC infrastructures such as those at BSC.

All this should mean an increase in the department benefits, due to an improvement in the service (shortening in the deadlines of delivery of the works) that improves one of the negative aspects in this type of studies for the clients, the delivery terms.

Depending on how the market evolves in general, and the workload of the fire engineering department in particular, the acquisition of new equipment will be evaluated at the beginning of second quarter of 2018 to provide optimal service to customers.

3.3.10 FDD Engitec S.L. (Spain): Pressure drop simulation for a compressed gas closed system

Project details	
Project Start – End Dates	1st April 2016 – 31st March 2017
PRACE Partner	BSC
PRACE effort (Person Months)	4.5
PRACE machine time	Mare Nostrum, 100000 core hours

Project Overview

FDD Engitec is a Spanish SME which designs and manufactures firefighting components and systems. Its core expertise is focused in the development of gaseous clean agent extinguishing systems. Its activities cover from the design of components and systems, validation tests, manufacturing and certification. It is oriented to the global market, but mainly based in the European and North Africa markets.

The objective of the project was to calculate by simulation the pressure drop of a firefighting pressure regulated discharge valve for an inert gas agent. In order to do that, it was necessary to simulate the discharge of a pressurized closed canister through the valve under realistic conditions.

As the project was moving forward, it became apparent that the initial objective was too ambitious. The main reason was that to simulate the real configuration, which is a complex geometry with regions including very small elements and high speed compressible flows, required much more resources than those provided by SHAPE. In the current development status of BSC's code Alya, either a much larger amount of computational resources or a much larger programming and development effort were required. Therefore, the focus was on simulating the first expansion stages instead of the whole process, analysing especially the temperature distribution and the regime's oscillatory behaviour.

HPC Usage

The company uses commercial CFD software for basic flow simulations. However, these simulations do not represent the full physical phenomena studied in the SHAPE project. The company still relies on an experimental trial-and-error approach and has not yet incorporated HPC in its daily work. The SHAPE project has helped the company to realize the potential benefits of

HPC, but the HPC costs and the expertise required to perform their complex simulations are significant entry barriers.

Business impact of the SHAPE project
The SHAPE project has been useful for the company to realize the potential benefits of HPC. Unfortunately, the large amount of computational resources needed to simulate its problem and the high expertise level do not allow the company to adopt HPC. Therefore, the project has not affected the company's business process and has not leaded to a measurable Return of Investment yet.

3.3.11 Pharmacelera (Spain): HPC Methodologies for PharmScreen

Project details	
Project Start – End Dates	March 31st 2016 – Feb. 28th 2017
PRACE Partner	RISC Software GmbH
PRACE effort (Person Months)	4
PRACE machine time	Mare Nostrum, 100000 core hours

Project Overview
Pharmacelera is a company that applies High Performance Computing to rational drug design. PharmScreen is a proprietary tool for screening libraries of millions of compounds, based on molecular modelling algorithms derived from research at the University of Barcelona. These algorithms use semi-empirical Quantum-Mechanics (QM) computations to represent molecules entirely in 3D by their electrostatic, steric and hydrophobic interaction fields, as opposed to less accurate models used by competing tools, such as fingerprints, pharmacophores and other 2D and 3D simplifications. PharmScreen is able to find candidate molecules that have higher chances to become a drug.

However, they have not been able to fully explore the potential of PharmScreen due to its significant computing requirements and as such have started exploring mechanisms to reduce its execution time. Hence, the SHAPE project aimed at applying HPC methodologies to PharmScreen in order to improve its performance / accuracy.

HPC Usage
For the duration of the project Pharmacelera used BSC resources to perform benchmarking of PharmScreen with a few data sets accepted by the scientific community, to tune the software to achieve a good balance between performance and accuracy, and make it more robust on HPC systems. Following this project, Pharmacelera has kept working on HPC and is now using Amazon Web Services as its main HPC provider. The company has good expertise on HPC software development but additional employees / collaborators with these type of skills may be required in the future.

Business impact of the SHAPE project

Pharmacelera has been able to show how much chemical diversity PharmScreen encounters in the first positions of the ranking in a given virtual screening campaign. The company has used 11 datasets from the Directory of Useful Decoys (DUD) containing 60,000 molecules, deriving into more than 6M molecular structures once conformations are computed. PharmScreen is able to find 2.7X more chemical diversity than existing tools (see Figure 9 below) and it finds more active

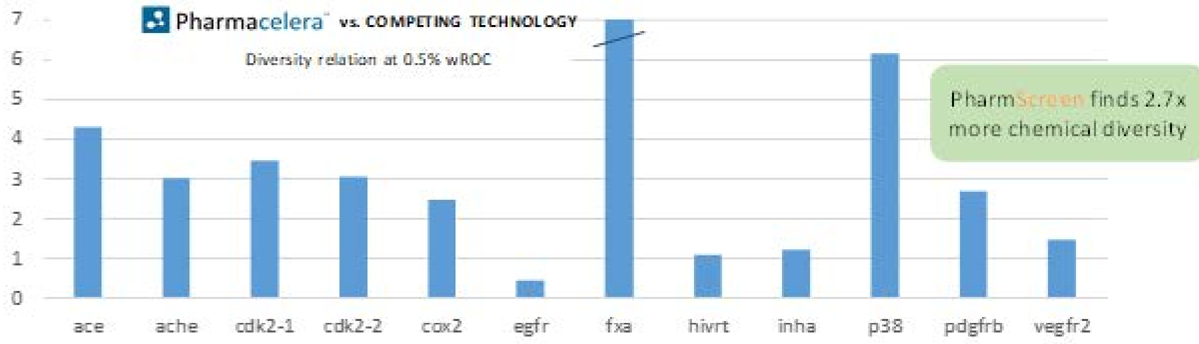

Figure 9: Chemical Diversity Comparison

molecules in the first positions of the ranking in 80% of the scenarios. This has been a strong commercial yet scientific message to our partners and customers. This has significantly increased the positioning of Pharmacelera in the pharmaceutical R&D ecosystem and the company has attracted new users and customers.

3.3.12 Summary of follow-up responses

The follow-up feedback from the SMEs has again generally been very positive with records to SHAPE. However, despite the template provided for response being more explicit in asking for quantitative measures against the key performance indicators, as for D7.2 the responses have been largely qualitative. This should be taken into account for future exercises and perhaps an alternative approach taken to gathering feedback.

Below the main points for each SME are summarised:

- WB Sails – gained in-house HPC skills.
- ACOBIOM – trained staff in HPC skills, improved external communications and leveraged their ability to demonstrate their knowledge in the area, expect positive tangible outcomes in the future.
- Airinnova – enhanced their expertise for high performance simulations, helped to attract new customers and investigate new markets – currently considering creating new services based on their experience of using HPC, and expect to continue working with KTH-PDC.
- Creo Dynamics – expect to significantly increase their HPC usage over the coming months, increased the capabilities and efficiencies of their services, made the company more prepared to tackle new and challenging engineering problems.
- AmpliSIM – their code is now enabled to make use of HPC resources, and the enhanced security introduced in the SHAPE project has provided the ability to reassure customers that their data is protected. They intend to continue working in HPC (possibly via PRACE and/or their link with IDRIS) and consider SHAPE to have been of real value to their business.
- BAC ECG – their SHAPE experience has highlighted the importance of HPC in their business and they are evaluating either increasing their in-house HPC capabilities or making

use of third-party providers for future projects. The SHAPE work has been used directly in various projects since its conclusion. The experience gained from SHAPE has allowed BAC to be more competitive in the market via improving the level of service they can offer to their customers.

- FDD Engitec S.L. – have not yet incorporated HPC into their daily work – SHAPE has made apparent the potential of using HPC for their business, but the scale of resources they would require has prevented them being able to adopt it yet.
- Pharmacelera – continue to use HPC via Amazon Web Services, and may employ staff skilled in HPC in the future. Their PharmScreen software was improved in terms of performance and accuracy via working with SHAPE, which has led to the company attracting new users and customers.

3.4 SHAPE fourth and fifth call Project Summaries

This section provides summaries of the projects still ongoing within the SHAPE programme, and those recently finished or just starting. For each of these there is a brief overview describing the problem to be solved, the activity undertaken, how PRACE was involved, the benefit to the SMEs, and finally the lessons learned for the further development of the SHAPE programme itself. The lessons learned are discussed further in Section 3.4.11.

Note that each SHAPE project is expected to produce a technical white paper that will cover the activities and results of the projects in greater detail than presented here (once published they can be found here [19]). The intention of the information presented in this document 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.

3.4.1 Artelnics (Spain): Adoption of High Performance Computing in Neural Designer

Overview

Project partners:

- Roberto Lopez, Artelnics S.L., robertolopez@artelnics.com
- Fernando Gómez, Artelnics S.L., fernandogomez@artelnics.com
- Judit Gimenez, BSC, judit.gimenez@bsc.es

Artelnics develops the professional predictive analytics solution called Neural Designer. It makes intelligent use of data by discovering complex relationships, recognizing unknown patterns, predicting actual trends or finding associations. Neural Designer stands out in terms of usability, functionality and performance.

Within the framework of the Performance Optimisation and Productivity Centre of Excellence (https://pop-coe.eu) BSC analysed the OpenNN (Open Neural Networks) code originally parallelised with OpenMP. As reported by the POP service, the parallel versions of OpenNN and Neural Designer are running more than five times faster than the serial versions in a desktop computer.

The objective is to further multiply the speed of OpenNN and Neural Designer by 10 or 100 when building predictive models. The next step to achieve this objective, which has been developed within the framework of POP and SHAPE, has been to implement shared and distributed memory parallelisation by means of OpenMP and MPI. The new version of the code allows Artelnics to build predictive models in computer instances with many virtual cores and in supercomputing clusters, respectively.

Activity Performed

The main incentive to introduce the MPI parallelization in the OpenNN library was to be able to load larger data sets and perform the required analysis of them. This objective has been successfully reached within this SHAPE project thanks to a close and iterative cooperation between Artelnics and BSC. The continuous feedback about the improvements implemented by the code owner guided the next optimizations and resulted in a very efficient parallel MPI plus OpenMP version with efficiencies around 90% in the scale under analysis.

The final evaluation was performed in the Marconi Broadwell partition and targeted both paradigms, to evaluate the combination of MPI and OpenMP and to study the scaling of the MPI implementation. A detailed description can be found in the white paper.

PRACE cooperation

This project used the Marconi-Broadwell system at CINECA.

Benefits for SME

The new version of the code allows Artelnics to build predictive models in computer instances with many virtual cores and in supercomputing clusters. Neural Designer is now capable of analysing larger data sets in shorter time scales, providing Artelnics customers with results in a way previously unachievable.

Lessons Learned

The SHAPE projects are a good opportunity for improving the SMEs situation, nevertheless it is difficult for an SME to respond to short time deadlines.

3.4.2 Milano Multiphysics (Italy): Use of CFD on new HPC accelerators for an accurate prediction of erosion and corrosion induced by flowing liquid metals

Overview

Partners:

- Milano Multiphysics, Carlo Fiorina
- CINECA, Vittorio Ruggiero, Claudio Arlandini

Milano Multiphysics is a small start-up company providing services in the field of numerical simulation of engineering systems. The main focus is on the simulation of systems involving complex, diverse and interconnected physical phenomena that can challenge the in-house competences of other companies and the capabilities of traditional numerical tools.

The project fits in the frame of the collaboration between Ansaldo Nucleare S.p.A and Milano Multiphysics s.r.l.s that aims at modelling, via an optimized version of OpenFOAM, the combined effects of corrosion and erosion of structural materials in flowing liquid metals, with a focus on nuclear applications. The performance of the structural materials envisioned to be used in GEN IV Heavy Liquid Metal-cooled fast nuclear reactors is limited a) by the degradation of physical and mechanical properties by long term exposures to neutron fluxes and b) by the chemical interactions with the flowing fluid. The computational power required for a high fidelity simulation is so demanding that it is really difficult for an SME to get access to the necessary resources. The new generation of Intel Xeon Phi processors, KNL, appears a very promising way to bridge this gap. PRACE provided a valuable contribution in supporting the company in the porting, optimisation and benchmarking process of selected OpenFOAM solvers which could be used for modelling corrosion and erosion processes in liquid metals.

Activity Performed

The activity was based on three pillars:

- Porting, deploying and running OpenFOAM on CINECA Marconi using the Intel Xeon Phi processors nodes;
- Enhancing the parallel performance of selected OpenFOAM solvers on Intel Xeon Phi by rewriting crucial blocks;
- Conducting a thorough performance analysis for a few test cases, including an industrial case provided by Ansaldo Nuclear S.P.A. and consisting of a fuel bundle of a lead fast reactor.

PRACE cooperation

CINECA, on behalf of PRACE, provided first of all machine access to the Marconi KNL partition (ca 300000 core hours) and coaching in use of the HPC system. The most effort was spent however in the joint analysis of the solver's behaviour, and the subsequent optimisation on the target architecture.

Benefits for SME

Currently, the modelling of the combined effects of corrosion and erosion of structural materials in flowing liquid metals mainly relies on experimental correlations. The expected engineering benefits related to the availability of a simulation tool for the prediction of the impact of such physical/chemical effects on structural materials are the possibility to detect via numerical simulations (i.e. without costly and lengthy experimental campaigns), and early in the design phase, any localized occurrence of the problem. Ansaldo Nucleare is following closely the outcome of the project, providing the geometrical models for the components and some experimental correlations to test the results of the model. If the outcome is considered interesting, Ansaldo Nucleare will likely finalise a consultancy contract with Milano Multiphysics to exploit the new knowledge.

In addition to the nuclear sector, the availability of a model for erosion, corrosion, wear-providing predictions in a reasonable engineering timeframe within OpenFOAM (an open software framework) to non-nuclear commercial industries enables:

- the creation of relevant reference data (as of now unavailable because of the impracticality of running models and simulations covering a wide range of flow regimes within the current limitations of commercial CFD codes);
- the opportunity to have access to a robust tool for optimising the design of a solid surface interacting with a fluid flow (e.g. coating industries, metal forming and forging, refineries and chemical manufacturing facilities);
- a more pragmatic, high fidelity approach for the expensive, and for significant industrial cases often not feasible, prediction of mechanical failures for all types of components, in a realistic range of flow regimes and for a large number of fluids.

These competences will allow Milano Multiphysics to gain visibility in the field of corrosion/erosion caused by liquid metals, with an ensuing possibility to strengthen its skills in the nuclear industry, and of gaining access to a vast pool of customers in the metallurgical industry.

Lessons learned

The project is being successfully completed.

Although the company made no official complaint, it expressed the request for a privileged access to the computing resources, with a higher priority with respect to academic users, in order to have a time-to-solution more compatible with an SME usual hectic pace.

3.4.3 Renuda UK Ltd (UK): Optimising 2D flow for faster, better steam turbine design

Overview

Partners:

- Renuda UK Ltd: Nicolas Tonello, Panos Asproulis
- EPCC: Kevin Stratford, Neelofer Banglawala, Paul Graham

This project was a collaboration between Renuda UK Ltd and EPCC, the High Performance Computing centre at the University of Edinburgh. The goal was to improve the performance of Renuda's industrial and power generation steam turbine modelling code, referenced as CodeX for this project.

Renuda offers several services, including consulting, software development and training and support. Renuda has recognised expertise in using and developing software for a large range of industrial thermal and fluid mechanics applications. Working mostly with *blue chips* clients in the UK and in Europe, such as Unilever and EDF, Renuda is involved in solving a wide range of problems: from how to simulate ventilation and contaminant dispersion in nuclear plants, the investigation and optimisation of mixing in chemical processing industries to improving the design of gear box oil cooling circuits and steam turbines. As part of the latter, Renuda, in a prior collaboration with EDF, has been developing CodeX, a throughflow steam turbine simulation code for fast optimisation of turbine designs and detailed investigations of turbine operation. Based on its core expertise in fluid mechanics, numerical methods, multi-language and multi-purpose software development of numerical solvers and Graphical User Interfaces (GUIs), as well as knowledge of the application markets, Renuda has been able to develop further capabilities into the software and is now looking to bring CodeX fully to market.

CodeX makes it possible to accurately model the performance of large industrial steam turbines with tens of stages. However, in its serial form, CodeX's marketability is restricted by its computing efficiency and unavailability on HPC systems. A parallelised and optimised version of CodeX, would transform the possibilities for the code, by opening market lines for Renuda as well as expanding the scope of application: from sale of software services, to consultancy and support for turbine design. Thus Renuda were interested in parallelising the code in order to speed up the calculations and make it possible to run on significantly denser computational meshes for increased accuracy, and to take advantage of different multi-core computer architectures.

Activity performed

The code was investigated, with initial benchmarks and analysis used to identify areas for improvement and to identify the most suitable optimisation approach to take. CodeX was then refactored and restructured to allow for the parallelisation of the code, but also to make improvements in the serial performance. The code has been parallelised using OpenMP directives, ensuring portability across platforms.

Benchmarks performed during the project indicate that for runs of typical operational models, the optimised serial code is over twice as fast as the original. For parallel runs this enhancement is reflected further, with a headline figure of over 27x faster than the original code on 16 cores - this equates to a reduction in runtime from over 1.5 days to less than 90 minutes. The technical work and results are described in more detail in the white paper for the project.

PRACE cooperation

EPCC represented PRACE in this collaboration with Renuda. EPCC performed the main performance analysis, optimisation strategy and development work on the code, with Renuda providing input and support via the industry test cases, validation and additional testing on alternative platforms. Regular meetings were held between Renuda and EPCC which greatly assisted in ensuring the success of the project, helping EPCC understand the code operation and impact of changes, and keeping Renuda appraised of and involved in the enhancements taking place on their code. It also allowed more involved technical discussions to take place which helped knowledge transfer in both directions, and should leave Renuda with a deeper understanding of the parallelisation process. As well as the white paper, an internal technical document was provided to Renuda describing the development work and results in further detail.

Benefits for SME

The final result of this project is an optimised, parallelised version of CodeX, which can be used to perform simulations in a significantly shorter timescale, thus enabling Renuda to offer enhanced services to their customers.

Lessons learned

Renuda think that the collaboration worked well and, most importantly, the project delivered. There was one moment of uncertainty when staff needed to be reshuffled but, to EPCC's credit, it was handled extremely well and did not adversely impact the project. All project members on EPCC's side were very competent, honest and open, which is essential to the success of such a high-tech project. An interesting observation for Renuda is the time to uptake the deliverables throughout and at the end of the project - an area which is often under-estimated in time planning, but which is of the utmost importance to ensure that the knowledge imparted and, here, the computer code developed, can be used effectively. Credit to the EPCC researcher the project was planned with, this was well sign-posted and it proved necessary. Ideally, this collaboration will continue both in an informal manner as it is important to keep the communication lines open for questions that might come up in the future but also for formal, future developments. One of the latter could be the possibility for using the results of the project remotely on EPCC's machines, and possibly also on other PRACE centres' systems.

3.4.4 Scienomics (France): Development of Chameleon Monte Carlo code for HPC: Toward Realistic Modelling of Complex Composite

Overview

Partners:

- Scienomics: Orestis Alexiadis, Xenophon Krokidis
- IDRIS: Isabelle Dupays, Sylvie Therond, Thibaut Very

Scienomics is a French IT company established in 2004 specialized in the development of Materials Modelling and Simulations Software. Scienomics' flagship "Materials Processes and Simulations platform (MAPS)" offers a unique combination of Modelling and Simulation Technology incorporating recent advances in theoretical and computational methods. Today scientists using MAPS worldwide are able to simulate the properties and the behaviour of several types of materials such as polymers, nanomaterials and composite and many others in order to achieve optimum design.

In order to perform de novo materials development and/or optimization, scientists need to work with reliable models at the atomistic level. Increasing complexity of modern materials make these models become excessively complex and large and subsequently exhibit characteristics that cannot be studied by standard techniques. In order to overcome this limitation Scienomics developed a piece of software, called Chameleon, which combines a Monte Carlo approach with modern algorithms for relaxing such materials, such as chain altering moves. Chameleon is now in its second phase of development and is currently able to simulate many different systems, however further code optimization and validations are still needed. The goal of this project is to improve Chameleon capabilities in several areas and test them on crucial industrial problems. Additionally this project will also leverage powerful machine memory capabilities to test the limitations of the MAPS platform ability to generate and visualize these very large systems (over 1 million atoms). Based on these tests, improvement of MAPS capabilities, such as porting MAPS to GPU/CPU architecture or improving MAPS code to speed up visualization of large system for example, will then be considered.

The overall goals of the project are

- Porting:
  - Deploy and run Chameleon on machine at IDRIS centre;
  - Deploy and run MAPS on IDRIS machine.
- Benchmarking:
  - Performance analysis for Chameleon sequential and OpenMP parallelization;
  - Performance analysis of MAPS over systems of increasing size
- Optimizing:
  - Enhance Chameleon parallel performances through improved OpenMP implementation.

Activity performed

Chameleon is a simulation tool based on the principles of the Markov Chain Monte-Carlo technique. As with any simulation method that aims to explore efficiently those regions of phase space (position-momentum space) that are most likely to physically occur, the Monte-Carlo (MC) method samples phase space by generating new configurations that satisfy some energetic criteria which ensure the states visited are indeed physically realizable states. New configurations are generated using a set of Monte-Carlo moves (in some cases MC moves are unphysical or even fictitious), which aim to equilibrate a set of desired characteristics of the system.

Most of the time is spent in the computation of non-bonded interactions, especially van der Waals type, for which the intensity decreases quickly with the distance between the particles. To reduce the number of interactions to compute, it is possible to define Verlet lists, which divide the system into smaller cells inside which the interactions are computed. The algorithm used to find particles was the naive O(N2) implementation. By using a hash table it was possible to reduce the timing by using an O(Nlog(N)) algorithm. This implementation explains the dramatic reduction of job duration with Chameleon.

One of the goals of this project was to port Chameleon on to HPC architectures. The use of processors with more cores and memory allows the code to run larger systems. Since the code is written with OpenMP support, the use of a complete node is possible. We compared the performances of two compilers:

On Ada, the code was built with:

- GNU g++ 4.4.7;
- Intel icpc 2017.1;

On Ouessant, the code was built with:

- PGI pgc++ (16.10, 17.01 and 17.05);
- LLVM xlc++_r;

Up to version 2.0 Chameleon depended on Qt for the management of arrays. A bug with the PGI compiler (versions prior to 17.05) prevented the code from compiling correctly. This bug was reported to the manufacturer and corrected in version 17.05.

Further details can be found in the white paper.

PRACE cooperation
PRACE was involved in the help to port the application on HPC, to optimize the code using OpenMP, to analyse with tools performances in order to find where the time is spent and advice to change in the application.

Benefits for SME
By accessing the computational resources provided within the project, Scienomics and IDRIS engineers were able to assess the performance of Chameleon in extreme system cases. Porting Chameleon on HPC architectures and using an increased number of processors with more cores and memory, allowed the execution of Chameleon using very large realistic systems and in the same time assess the full spectrum of non-bonded interactions (Van der Waals and Coulomb energies). This gave Scienomics the necessary feedback to identify the optimum number of cores above which the scalability of the OpenMP parallelization in Chameleon degrades. In addition, by applying powerful code profiling and analysis tools, they were able to assess the performance of Chameleon algorithms for both sequential and parallel execution and to identify major bottlenecks and hot spots of the code. They managed to achieve more than 10x speed-up for the sequential execution of the code with some fluctuations depending on the system size.

Lessons learned
In the collaboration with the SME, regular meetings helped management of the project. Scienomics also organized a training session about materials simulation methods available in MAPS, the Scienomics software, for IDRIS users. This project created links between the IDRIS) and the SME. The main problem resides in the fact that the SME is a small organisation with few people, so sometimes it is difficult to have quick answer because people are occupied working on other projects.

3.4.5 Disior Ltd (Finland): Performance optimization of structural simulation of bone fixation

Overview
Partners:

- Disior Ltd: Sakari Soini
- CSC: Peter Råback, Jussi Heikonen

Disior Ltd. [16] develops a treatment design tool for clinical use. The software tool works with CT (computed tomography) images of, for example, human bones, transforming them into a mathematical model capable of analysing bone fracture shape, measuring the key parameters and predicting the behaviour of the fracture area under loading thus giving an insight to the strength and life time of the fixation (implants).

The Disior medical device software system relies on an external library to compute the loading conditions from elasticity equation. These computations are used to optimise the implant configuration. A large number of different conditions needs to be computed. Even though a single solution of the elasticity problem is not massively parallel, the large number of the tasks makes it such. The optimisation process is time critical which means that the tasks cannot be solved sequentially.

The solution of the elasticity problem is carried out by the Elmer [17] open source finite element software which is mainly developed at CSC. The aim is to solve the different loading conditions as fast as possible. A typical task includes perhaps a few millions of tetrahedral elements in an unstructured mesh. Only the solution of the forward problem is considered. The finding of the optimal solution process is not part of the performance optimisation task.

Activity Performed

The Elmer finite element software already includes the basic models needed to model the bone fixation problem. The aim was to minimise the time needed for the solution of the problem. The time is roughly spent in two calculations: finite element assembly, and on the solution of the arising linear problems.

The starting point of the work was existing computations that had been run on commercial codes. The customer had initiated work using the Elmer open source library as the computational backend but satisfactory parallel strategies had not yet been obtained. Hence the baseline was the time spent on the commercial package with the optimal settings therein. To make the case even more challenging, the simulation must be very robust, i.e. divergence of iteration should not be an option. On the other hand, for a single case the parallelisation goal was rather modest. A large number of cases will run trivially in parallel.

A real meshed jawbone was used as a test case. It consisted of 1.67 million tetrahedral elements. When running the case in serial it consisted of 1.04 million unknowns. A large number of different strategies were tested including direct solvers and a large number of Krylov subspace methods (CG, BiCGStab, Idrs, Tfmqr, GCR, GMRes) with one level (ILUn) and multilevel (BoomerAMG) preconditioners. Typically the multigrid method fairs very well, but in this case the best performance considering robustness was obtained using MUMPS (and MKL Pardiso) direct solvers. With the method of choice (MUMPS), computation of one case took 29.5 seconds to compute using 24 cores of Intel Haswell E5-2690v3 2,6GHz processors. Of this 24.5 seconds was used for the linear system alone.

For optimal accuracy quadratic elements are desirable since linear elements suffer from numerical “locking”. Therefore limited effort was given to strive to optimise the linear performance. Any production runs will be run with quadratic elements that give superior estimates for the stress distribution. The quadratic case included 7.49 million degrees of freedom. Again, a large number of strategies was tested. The quadratic case is even more ill-conditioned than the serial case and thus the iterative methods were not really competitive.

Elmer has a hierarchical p-element implementation that allows to use the p-levels in a multigrid type of manner. The p2 elements preconditioned with the p1 solution using the MUMPS direct solver turned out to be the winning strategy. When using MUMPS as a preconditioner the factorisation may be reused. In this strategy, the time used for solving the linear system with 24 cores was just 32.2 seconds. This may be considered very economical since, compared to the linear case, the size of the problem is more than 7-fold, but the time consumption only rose around 28%. However, the assembly time was much more increased, mainly due to the more costly integration rules needed for quadratic elements. Hence, the spend for tasks other than the linear system solution rose from 4.1 to 26.6 seconds, an increase by a factor 6.5.

In order to optimise the performance, mainly the solver settings were updated. However, also some minor optimisation in code was performed, for example, in the optimisation of MPI barriers. The scaling tests for the quadratic case are shown in Table 9 below. It can be seen that the scaling of the linear system quickly fades whereas the total time still decreases as the assembly of the linear system scales almost trivially.

Table 9: Scaling tests for the quadratic case

#np	T_{tot}(s)	T_{linsys}(s)
4	284.1	115.5
8	146.9	70.7
16	84.0	45.0
24	58.8	32.2
32	49.7	29.4
64	37.0	25.5
128	28.2	20.2

The time consumption in the baseline solution using well-known commercial software were 575 seconds for the full solution, and 275 seconds for the linear system. Hence, the speedup compared to the reference solution was nearly tenfold. However, the CPUs were unfortunately not comparable so this speedup should be taken as a combined effect of faster CPUs and faster code.

Currently the platform for running the software in the university hospital is Microsoft Azure cloud computing environment. The testing was performed on the Taito cluster at CSC.

PRACE cooperation

The PRACE SHAPE project has provided the manpower for the performance improvements and the computational capacity to run the test runs.

Benefits for SME

The ultimate outcome of the work when embedded in the simulation software will be optimized data for diagnosis, better surgery planning and streamlined treatment processes resulting in 25% faster surgeries and 50% less complications. Disior software tools also offer novel methodology for research.

The work is still ongoing. Disior is performing further test to locate possible further performance bottlenecks. For example, there may be I/O bottlenecks when performing large number of tasks in short periods of time. These will be addressed if necessary.

Lessons learned

The application process for SMEs is conveniently lightweight, making it realistic also for quite busy companies to apply. For SMEs without special know-how on parallel computing the expertise provided by PRACE SHAPE may be very valuable.

One challenge in working with real data is the privacy requirements of the hospitals. These make it difficult to utilise standard supercomputing services. Therefore, the testing and development environment may not be the final production environment. However, when using similar kind of CPUs the performance optimisation is still relevant.

3.4.6 Invent Medical Group, s.r.o. (Czech Republic): Numerical Modelling of 3D Printed Cranial Orthoses

Overview

Project partners:

- Invent Medical Group:
    - Jiri Rosicky, CEO, jiri@ingcorporation.cz
    - Aleš Grygar, Chief designer, ales@inventmedical.com
- IT4Innovations:
    - Tomáš Karásek, Senior researcher, tomas.karasek@vsb.cz

IMG is a high-tech medical start-up company focused on research & development, advanced technologies and clinical application. They focus deeply on the synergy of cutting-edge technology with the human touch to produce the most personal wearables ever. The company cooperates with medical partners in 10 countries, and their ambition is to reinvent the application of cutting-edge technology in the medical field worldwide. |The main goal is an implementation of Direct Digital Manufacturing technology (3D scanning, computational modelling, 3D printing) in the field of custom-made orthotics and prosthetics to achieve product innovation, process innovation and business model innovation.

The objective of this project is to replace physical testing of cranial orthosis design by virtual prototyping using numerical modelling and simulation technologies. Because IMG has no prior experience with numerical modelling, the implementation of virtual prototyping technique into their design cycle will be done in several stages. In this project, focus will be put on the pre-processing stage of the numerical modelling. A semi-automatic system of mesh generation from a CAD model will be developed employing the open source software Netgen Mesh Generator [18]. Because cranial orthosis model is very complex and a volume mesh must be created, this semi-automatic mesh generation must be done in parallel. Output from this project will be a software tool which will take a CAD model as an input and will produce a finite element mesh with all the boundary conditions as an output. This produced mesh will be used for calculation of cranial orthosis stiffness using open source code ESPRESO.

Activity performed

Project activities consist of the following phases:

- Deployment of the Netgen mesh generator on a supercomputer architecture;
- The data format for data exchange between the CAD system used on the company's side and Netgen was specified;
- Modification of Netgen software to create a workflow for automated mesh generation by Netgen;
- Development and validation of numerical model of the inner part of the printed cranial orthosis;
- Verification of the workflow for automated mesh generation;

- Solution of the numerical model of the inner part of the printed cranial orthosis using open source code ESPRESO, and validation of the results by commercial code ANSYS.

PRACE cooperation
Project partners from IT4Innovations deployed requested open source software Netgen mesh generator on IT4Innovations supercomputing infrastructure and modified it in turn to create the workflow for automated mesh generation. Researchers from IT4Innovations also developed and validated a numerical model of the inner part of the printed cranial orthosis. All numerical simulations were performed using IT4Innovations infrastructure and the results of numerical simulations were compared with those obtained by physical experiment performed by Invent Medical Group. Findings of the project will be summarised in the imminent white paper being prepared jointly by both parties.

Benefits for SME
The Invent Medical Group (IMG) is designing and manufacturing cranial orthosis using 3D printing technology. Design of those orthoses is geometrically very complex and it is very difficult to ensure that they have the required properties and will work properly. The main goal that must be met is the stiffness of a cranial orthosis that is currently tested on a testing stand developed for this purpose. This physical testing must be done for each new design of orthosis. IMG will benefit by adopting and implementing virtual testing, instead of physical, into the design cycle of cranial orthosis in several ways. Firstly, this will help to reduce the time necessary to bring a new design of orthosis to the market. This alone is a huge benefit for the company which is motivated to produce a cutting-edge technology worldwide. A second benefit is that this step will increase the quality of their products for their customers.

Lessons learned
In terms of the SHAPE project and its administrative process everything has run very smoothly and project partners Invent Medical Group and IT4Innovations were very satisfied with all aspects. The company considers this project as a success and very beneficial. Obtaining an option to replace physical tests of their product by virtual ones brings a huge benefit to the company in terms of shortening the design cycle. It also allows them to create new products with higher added value for their customers.

3.4.7 AxesSim (France): HPC for connected objects

Overview
Project partners:

- AxesSim: Bruno Weber, Christophe Girard
- CINES: Bertrand Cirou, Victor Cameo Ponz

CINES is helping the SME AxesSim in gaining access to HPC resources and porting their scientific codes.

AxesSim was founded in 2007 in Alsace close to Strasbourg (Illkirch-Graffenstaden), resulting from a related activity initiated by Thales Group. AxesSim designs and develops software targeting the scientific community. Specialized in the field of electromagnetic simulation, it offers a consistent range of professional applications which can simulate the performance of products and systems in a realistic way, starting from their conception to their qualifications, and to evaluate the impact of electromagnetic environments when the products are used. Since its creation, AxesSim offers the following activities and services to its clients: engineered and customized solutions and functions that need specific functionalities from their software. This type of service includes conception, development and maintenance. Realization of studies are based on simulation tools developed by AxesSim with data coming from the client.

The objective of this project is to propose to vendors of connected objects measures and simulation tools for optimizing the design. This requires the simulation of electromagnetic waves produced by small antennas and their interaction with biological tissues. Such simulations are complex and expensive. They require to take into account complex geometries. In order to provide an answer to the client in a reasonable time, it is necessary to use highly optimized software, parallel computations and GPUs.

Activity performed
CINES made two tentative attempts at porting the parallel software stack with respectively GNU and CRAY compiler toolchains.

The software stack is composed by Metis, Boost, HDF5, Amelet, Axessign and Teta. The parallelism is expressed through C++ OpenCL and the usage of the MPI messaging library.

Unfortunately, both the produced parallel executables and libraries failed to exploit parallelism as there was an error with OpenCL. As an alternative, CINES recompiled a sequential version that subsequently give improved results.

PRACE cooperation
PRACE provided support from CSCS on the PizDaint machine, with access granted through PRACE peer review Preparatory Access.

Benefits for SME
The case under consideration is the simulation of a smartphone antenna next to a meshed human head. Wearable devices vendors would be interested in actual measurements, but also in precise prediction tools to evaluate the effects of small changes in the design. Thanks to the developed software, vendors of connected objects can optimize the electromagnetic design of their products. This would allow the improvement of the life of the battery and/or reduce the Specific Absorption Rate (SAR).

Lessons learned
What worked is the process of selection, machine and code/data access and communication between partners.

What didn’t work is the gap between the 500000 core hours initially granted, and the 2000 node hours actually accessed on PizDaint (that ultimately was reduced to 1000 node hours). There were some challenges encountered during the development work which caused delays, but there is a policy (heterogeneous among PRACE sites) on this machine to remove hours when they are not used by the deadline. This is not helpful when justification was provided, in terms of the problems encountered, for not using the hours in the original timescale.

3.4.8 E&M Combustion S.L. (Spain): High-fidelity simulation of an industrial swirling combustor

Overview
Partners:

- E&M Combustion: Iñigo Bejar Gonzalez
- BSC: Ricard Borrell

E&M Combustion (EMC) is a Spanish SME that designs and manufactures combustion systems, such as burners and boilers, for the industry. Its mission is to provide customised solutions for industrial combustion systems, creating equipment and designs that meet the customers' requirements. It focuses mainly on the energy sector, oil and gas, steel and metal industries.

The objective of the project is to investigate the reacting flow field of an industrial swirling combustor designed and manufactured by E&M Combustion, in order to characterise its performance (thermal power, combustion efficiency, and global emissions), so that the SME can make decisions to optimise the system in the future. In particular, the JBM 4.500 G burner is being simulated using RANS and large-eddy simulations with a flamelet database.

This project has been done in collaboration with the Barcelona Supercomputing Center (BSC). The code used to perform the numerical simulations is Alya, a multi-physics code developed at BSC. The code has been adapted to solve this application problem.

Activity performed
The technical work has consisted in preparing the geometry used for manufacturing processes to conduct CFD numerical simulations. This includes the cleaning of the geometry and the elimination of components not related to the burner part. Once the geometry was ready, different meshes of the burner have been generated, going from coarse to fine grain. Numerical simulations have been run using RANS and LES at the selected operating point of the burner. The outcomes of the simulations have allowed the analysis of technological aspects of the system performance (such as thermal power, combustion efficiency, global emissions) as well as mean values and turbulent statistics of quantities of interest: velocities, temperatures and pollutants.

In parallel, experimental measurements of the system have been carried out during real operation for validation of the numerical simulations.

PRACE cooperation
PRACE provided the expert support to adapt the code for this application and the machine time needed to perform the simulations.

Benefits for SME
The fact of having more environment-friendly burners will simply determine whether EMC can compete in certain markets or not. It is possible that in few years, those burner manufacturers that do not reach certain levels in terms of emissions will have to cease their activity because they cannot sell their products anymore.

The use of advance numerical simulations as a tool for design of combustion systems permits the evaluation of the combustion performance of a given burner before the manufacturing process takes place. This strategy can save a substantial amount of resources in the design process and optimise existing designs at relatively low cost. Nowadays, the computing power availability has increased with important progress in supercomputing platforms for HPC and cloud computing. Therefore, the use of high-fidelity simulations based on large-eddy simulation (LES) is an advanced numerical approach that can be accessed by the industrial sector at the present time for design and optimisation purposes. The use of these techniques can provide an important contribution to increase the efficiency and competitiveness of the companies that adopt advanced modelling and simulation techniques in the design process.

Lessons learned
This project has progressed as scheduled so far. The fluency of the communication between the SME and the PRACE experts from BSC at the beginning of the projects has facilitated the setup

of a realistic work plan, with a clear definition of the contribution required by both parts during the project.

The R&D oriented business approach of the SME has facilitated the collaboration.

3.4.9 Svenska Flygtekniska Institutet AB (Sweden): AdaptiveRotor

Overview
Partners:

- SFI AB: Tomas Melin melin@sftiab.se (SME owner)
- KTH: Jing Gong gongjing@kth.se

The Swedish Aeronautical Institute was founded in February 2016, modelled after other international private research institutes. It is registered as a limited company (AB) under the Swedish limited companies act. Operations are focused on three areas: research, education, and consulting work in aeronautics. The main objective is to maintain and develop safety in the air transport system, while providing environmentally and economically sound solutions. The current focus of the research activities is on aircraft design methodology to cater for new applications and procedures in the air transport system. One current project is aimed at developing flight mechanics and procedures for formation flight in commercial aviation. The institute operates as a 'research hotel', providing base services to independent researchers.

Their analysis software utilises a newly developed fluid structure interaction code to evaluate the aerodynamic efficiency of a flexible propeller blade, while keeping the blade structure within design limits, both on-design and off-design points. The final result would be an internal structure with a prescribed stiffness together with outer mould line shapes for an optimally efficient propeller with good robustness at the design line.

Activity performed
The Swedish Aeronautical Institute has started the work with the UAV Propeller Optimization Project. Some delays have accrued due to insufficient funding for the necessary engineering hours within the institute. These delays should however be easily accommodated later on in the project. The initial phase of generating the geometrical parameters needed for CAD generation has finished, and the partners have moved on to the next phase with CAD file generation and meshing. Also the teams have created a surface from the airfoils in a STL file and an OpenFoam mesh for the wing that needs further improvements. Currently, the focus is on setting the proper boundary and initial conditions.

Benefits for SME
The envisioned product line is a series of customized propellers for small aircraft ranging from 1 kg remotely piloted aircraft systems to 6000kg regional transports. The advent of electric propulsion will generate a need for highly customized propellers in order to ensure an overall good aircraft system.

If the AdaptiveRotor project is successful, the SAI would open up a new production line of propellers generating 3-7 new jobs locally, and indeed more globally, due to the new product development our rotors would enable.

Lessons learned
It would be good to include a section in the application where the PI writes a clear step-by-step plan to follow on a weekly basis. Also, it would be good to give or ask the PI an indication of the

possible amount/frequency of meetings with the PRACE expert in the application, in order for PI to have a clear idea of the amount of time they need to dedicate to the project. These can help to foster the collaboration in a more regulated way and avoid potential delays.

3.4.10 Brabant Alucast International (Italy): Multiphasic simulation in high pressure die casting process in HPDC platforms using open-source CFD tools

Overview
Partners:

- Brabant Alucast International: Bernardo Puddu
- CINECA: Raffaele Ponzini, Claudio Arlandini

Brabant Alucast International is located in Turin. The company's main activity is the design and development of high-pressure die casting components made in lightweight alloys for body, structural, powertrain and suspension parts for premium OEMs. Product development uses the latest software and technologies including simulations to determine product configurations and optimization of new lightweight concepts.

The company suffers from huge quality issues related to air entrapments in the casted components. With the support of PRACE, the company aims are realising high-fidelity simulations of the multiphasic process, of an unprecedented quality in the history of the company, and obtaining crucial insights to improve products quality.

Activity performed
The ongoing activity is divided in four pillars:

- Air entrapments evaluation before the chamber filling. In the high-pressure die casting process, before the die filling, the liquid alloy is loaded into the shots sleeve, a cylindrical tube, and then moved into the die by a plunger. The study of the fluid dynamics of alloy and air inside the shot sleeve is important to control the impurity levels in the finished product.
- Air entrapment evaluation in the chamber filling. In the high-pressure die casting process, the presence of air entrapment in the process products, called cast part components, is a main cause of waste.
- Evaluation of the filling phase of the high-pressure die cast process simulation with OpenFOAM software (workflow implementation, time to results optimization, results validation).
- Market & Benchmark Analysis. The company uses a benchmarking analysis to support the selection, planning and delivery of the projects, typically measuring factors like production performances, production processes, quality level, time and costs.

PRACE cooperation
CINECA, on behalf of PRACE, provided first of all machine access to the MARCONI Broadwell partition (ca 100000 core hours spent up to now) and coaching in use of the HPC system. The most effort was spent however in the modelling and fine tuning of the die-cast processing.

Benefits for SME
The high-pressure die-casting process has a very high complexity level, due to the different technologies used, and to the very stringent requirements of the customer car-makers in their Material and Engineering standards. A positive outcome of this project could represent an

important step further to implement a strategy of quality improvement of the company products. A quantitative evaluation of the economic impact of the project will be done at the end of the project and reported in the final white paper.

Lessons learned

The collaboration between and the company is rich and fruitful, with a constant feedback loop in both directions. The most important factor was the strong commitment of the company management that allotted sufficient dedicated time of a competent team to work together with the PRACE support technicians.

The work is still ongoing and the company is positive about a positive outcome, although the simulations are more complex than expected. The first important lesson learnt is that a few engineering assumptions that were normally adopted by the company did not correspond to reality and more refined physics are necessary to obtain meaningful results.

3.4.11 Summary of lessons learned

This section summarises the “lessons learned” arising from the project reports and attempts to identify common themes. These will be fed back in to SHAPE and more generally PRACE to help improve existing programmes and identify if other programmes need to be created.

- Flexibility – it can be hard for SMEs to be responsive to short timescales – the SHAPE project, while important to the SME, may not be on their critical path and thus there may be delays in responding. Partners should be aware of this in advance and be prepared to accommodate/mitigate this via, for example, a workplan with clear staged tasks, or ensuring the PRACE partner has other work which can be done whilst waiting for a response.
- Expectation management – an SME’s experience with gaining access to compute resources pre-SHAPE may greatly differ from that of accessing an HPC centre. For instance, it is unlikely that jobs can be prioritised on a large shared HPC resource. Such limitations should be highlighted at the start of the project.
- Machine access – as noted earlier, it is easy for delays to happen in SHAPE projects due to the nature of working with small companies, issues arising etc. However, machine time is often granted within PRACE with a “use-by” date, which does not fit in well with being flexible – indeed, if the compute is not used within time, it may be withdrawn and cannot be rolled over (this policy varies across centres) which has caused difficulties for some of our SHAPE SMEs.
- Planning – having a clear plan at the start helps all those involved, including details of expectations on partners in terms of meetings, deliverables etc.
- Training – SMEs should be made aware of the training opportunities offered by PRACE and the partners which are often free for industry attendees.
- Application process – in comparison to previous years, the application process has been commended by some of the SMEs which suggests that recent changes (most notably the streamlining of any subsequent Preparatory Access application) have had a positive impact on the experience of applying for SHAPE.

3.5 SHAPE: Sixth call

In this section a brief overview of the two 6th call projects is given, as they have only recently started.

Axyon AI SRL (Italy): Axyon Platform Optimisation
This SME has a proprietary deep learning platform (Axyon Platform) targeted at financial problems, allowing the rapid development of highly-accurate predictive models. The aims of the project are to enhance their platform to enable them to offer solutions and services that involve very large datasets. They will be working with CINECA.

Vision-e S.r.l. (Italy): Deep Tile Inspection
The SME focusses on the study, design and development of computer vision systems and algorithms for customised industrial applications of quality inspection. They have developed software for a ceramic tile inspection system based on computer vision to detect surface defects of tiles on a production line. The goal of the project is to move to a deep learning approach in order to fully automate the process, which will enable the SME to offer a more effective service for their customers. They will be working with CINECA as the PRACE representative.

3.6 SHAPE: future

The SHAPE programme will continue under PRACE-5IP (the seventh call will launch in April 2018) and is included in the proposal for PRACE-6IP. As noted in previous reviews, whilst SHAPE is perceived as a positive programme there is still room for improvement, in particular in supporting SMEs beyond their experience with SHAPE. To this end, case studies from successful SHAPE projects are being gathered to provide promotional material, principally for inclusion on a dedicated SHAPE web resource. In addition to these "success stories", the resource will list national and international programmes where the SMEs can seek further support, and provide guidance on the opportunities available via PRACE and via third party providers.

The PRACE-6IP highlights stronger links between SHAPE and the Industry Advisory Committee (IAC) in order to ensure SHAPE is being promoted broadly in both geographical and business domains. Work has already begun to this end and communication channels will be broadened and maintained. In addition, SHAPE articles have appeared via several outlets over the previous period, and the programme has been represented at various conferences and workshops. This will continue over the coming year.

4 Summary

Two parallel sub-tasks on application enabling in Work Package 7 of PRACE-5IP have been described including final reports on the supported applications. These two activities have been organised into support projects formed on a basis of either scaling and optimisation support for Preparatory Access or SHAPE.

4.1 Preparatory Access

During PRACE-5IP Task 7.1.A successfully performed five cut-offs for preparatory access including the associated review process and support for the approved projects.

In total five Preparatory Access type C and six Preparatory Access type D projects have been supported or are currently supported by T7.1.A in PRACE-5IP. The projects try to produce white papers by the end of the project phase. Approved white papers are published online on the PRACE

RI web page [19]. Table 10 gives an overview of the status of the white papers for all finalized projects.

Table 10: White paper status of the finalized PA projects of this deliverable.

Project ID	White paper	White paper status
2010PA3430	**WP258**: Optimization of REDItools package for investigating RNA editing in thousands of human deep sequencing experiments	Published online [8]
2010PA3673		No white paper produced
2010PA3699		White paper currently under development.
2010PA3745		No white paper produced

4.2 SHAPE

Within PRACE-5IP, the SHAPE programme has continued to assist SMEs in starting to utilise HPC in their business. Several technical reports have been produced in the form of white papers, whilst more are expected over the coming months. Work on a dedicated SHAPE web resource is underway, and links between the PRACE IAC and SHAPE are improving to help ensure the programme reaches a broad range of SMEs across Europe.