Horizon 2020

Call: H2020-TWINN-2015

Topic: H2020-TWINN-2015

Type of action: CSA

Proposal number: 691974

Proposal acronym: CoSTAR

Table of contents

How to fill in the forms

The administrative forms must be filled in for each proposal using the templates available in the submission system. Some data fields in the administrative forms are pre-filled based on the previous steps in the submission wizard.

Proposal ID **691974** *Acronym* **CoSTAR**

1 - General information

Topic H2020-TWINN-2015 Type of action CSA

Call identifier H2020-TWINN-2015 Acronym CoSTAR

Proposal title* Computational Science Twinning for Advancing Research

Note that for technical reasons, the following characters are not accepted in the Proposal Title and will be removed: < > " &

Duration in months *36*

Fixed keyword 1 *Cluster dynamics* Add

Free keywords *Computational Science, Computational Physics, Scientific computing, High Performance computing , Lattice QCD*

Abstract

The Computational Science Twinning for Advancing Research (CoSTAR) project aims to strengthen and advance the research capacity of the newly established Computation-based Science and Technology Research Centre (CaSToRC) of the Cyprus Institute in the cross-disciplinary field of Computational Science. Computational Science is an emerging field of study that combines Information Technology and Mathematics with thematic areas in other scientific disciplines to advance discovery and innovation via computation. The proposed programme seeks to ensure that the scientists engaged, and being trained, in this field at CaSToRC, have access to the highest levels of expertise and guidance from two of Europe's leading computational science research centres, the Institute for Advanced Simulation of the Juelich Research Centre and the Barcelona Supercomputing Centre. The Twinning partners bring world-leading competencies and are at the forefront of computational science, covering the current thematic focus of CaSToRC, namely Future and Emerging Technologies, Atmospheric and Climate Modelling, Computational Physics and Chemistry, topics that align with the Smart Specialisation Strategy of Cyprus. The underlining vision of the proposal is to develop an innovative training and mentoring program for the junior faculty of CaSToRC, advancing their cross-disciplinary interaction and the research teams in their respective thematic areas. Simultaneously, it will expand the education, training and technical capacity of CaSToRC to evolve into a stimulating research environment of international calibre. Coupled with extensive dissemination and building of European networks for long-term research sustainability, the project will help bridge the gap between Cyprus and high performing countries in Europe, particularly as computational science moves towards the exascale era.

Remaining characters 122

Has this proposal (or a very similar one) been submitted in the past 2 years in response to a call for proposals under the 7th Framework Programme, Horizon 2020 or any other EU programme(s)? ○ Yes ◉ No

Proposal ID **691974** *Acronym* **CoSTAR**

Declarations

1) The coordinator declares to have the explicit consent of all applicants on their participation and on the content of this proposal.	☒
2) The information contained in this proposal is correct and complete.	☒
3) This proposal complies with ethical principles (including the highest standards of research integrity — as set out, for instance, in the European Code of Conduct for Research Integrity — and including, in particular, avoiding fabrication, falsification, plagiarism or other research misconduct).	☒

4) The coordinator confirms:

- to have carried out the self-check of the financial capacity of the organisation on https://ec.europa.eu/research/participants/portal/desktop/en/organisations/lfv.html or to be covered by a financial viability check in an EU project for the last closed financial year. Where the result was "weak" or "insufficient", the coordinator confirms being aware of the measures that may be imposed in accordance with the H2020 Grants Manual (Chapter on Financial capacity check); or	◉
- is exempt from the financial capacity check being a public body including international organisations, higher or secondary education establishment or a legal entity, whose viability is guaranteed by a Member State or associated country, as defined in the H2020 Grants Manual (Chapter on Financial capacity check); or	○
- as sole participant in the proposal is exempt from the financial capacity check.	○

5) The coordinator hereby declares that each applicant has confirmed:

- they are fully eligible in accordance with the criteria set out in the specific call for proposals; and	☒
- they have the financial and operational capacity to carry out the proposed action.	☒

The coordinator is only responsible for the correctness of the information relating to his/her own organisation. Each applicant remains responsible for the correctness of the information related to him and declared above. Where the proposal to be retained for EU funding, the coordinator and each beneficiary applicant will be required to present a formal declaration in this respect.

According to Article 131 of the Financial Regulation of 25 October 2012 on the financial rules applicable to the general budget of the Union (Official Journal L 298 of 26.10.2012, p. 1) and Article 145 of its Rules of Application (Official Journal L 362, 31.12.2012, p.1) applicants found guilty of misrepresentation may be subject to administrative and financial penalties under certain conditions.

Personal data protection

Your reply to the grant application will involve the recording and processing of personal data (such as your name, address and CV), which will be processed pursuant to Regulation (EC) No 45/2001 on the protection of individuals with regard to the processing of personal data by the Community institutions and bodies and on the free movement of such data. Unless indicated otherwise, your replies to the questions in this form and any personal data requested are required to assess your grant application in accordance with the specifications of the call for proposals and will be processed solely for that purpose. Details concerning the processing of your personal data are available on the privacy statement. Applicants may lodge a complaint about the processing of their personal data with the European Data Protection Supervisor at any time.

Your personal data may be registered in the Early Warning System (EWS) only or both in the EWS and Central Exclusion Database (CED) by the Accounting Officer of the Commission, should you be in one of the situations mentioned in:
-the Commission Decision 2008/969 of 16.12.2008 on the Early Warning System (for more information see the Privacy Statement), or
-the Commission Regulation 2008/1302 of 17.12.2008 on the Central Exclusion Database (for more information see the Privacy Statement) .

Proposal ID **691974** *Acronym* **CoSTAR**

List of participants

#	Participant Legal Name	Country
1	THE CYPRUS INSTITUTE LIMITED	Cyprus
2	FORSCHUNGSZENTRUM JULICH GMBH	Germany
3	BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION	Spain

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **CYI**

2 - Administrative data of participating organisations

PIC	***Legal name***
965934440	*THE CYPRUS INSTITUTE LIMITED*

Short name: CYI

Address of the organisation

Street CONSTANTINOU KAVAFI 20

Town LEFKOSIA

Postcode 2121

Country Cyprus

Webpage www.cyi.ac.cy

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2012 - no

SME self-assesment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE code 721 -

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **CYI**

Department(s) carrying out the proposed work

Department 1

Department name	Computation-based Science and Technology Research Center
	☒ Same as organisation address
Street	CONSTANTINOU KAVAFI 20
Town	LEFKOSIA
Postcode	2121
Country	Cyprus

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **CYI**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: ○ Male ◉ Female

First name: **Constantia** Last name: **Alexandrou**

E-Mail: **alexandrou@cyi.ac.cy**

Position in org.: Institute Professor

Department: CaSToRC

☒ Same as organisation address

Street: CONSTANTINOU KAVAFI 20

Town: LEFKOSIA Post code: 2121

Country: Cyprus

Website: www.cyi.ac.cy

Phone: +35722208647 Phone 2: +35722208629 Fax: +35722208625

Other contact persons

First Name	*Last Name*	*E-mail*	*Phone*
Marios	Demetriades	sponsored.research@cyi.ac.cy	
Giannis	Koutsou	g.koutsou@cyu.ac.cy	

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **FORSCHUNGSZENTRUM JULICH GMBH**

PIC	***Legal name***
999980470	*FORSCHUNGSZENTRUM JULICH GMBH*

Short name: FORSCHUNGSZENTRUM JULICH GMBH

Address of the organisation

Street WILHELM JOHNEN STRASSE

Town JULICH

Postcode 52428

Country Germany

Webpage www.fz-juelich.de

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2012 - no

SME self-assesment ..... unknown

SME validation sme ..... 2012 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE code 721 -

Proposal ID **691974**	*Acronym* **CoSTAR**	*Short name* **FORSCHUNGSZENTRUM JULICH GMBH**

Department(s) carrying out the proposed work

Department 1

Department name	Juelich Supercomputing Centre (JSC)
	☒ Same as organisation address
Street	WILHELM JOHNEN STRASSE
Town	JULICH
Postcode	52428
Country	Germany

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **FORSCHUNGSZENTRUM JULICH GMBH**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Alan** Last name: **O' Cais**

E-Mail: **a.ocais@fz-juelich.de**

Position in org.: Scientist in Charge

Department: Juelich Supercomputing Centre

☒ Same as organisation address

Street: WILHELM JOHNEN STRASSE

Town: JULICH Post code: 52428

Country: Germany

Website: www.fz-juelich.de

Phone: +492461615213 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Other contact persons

First Name	***Last Name***	***E-mail***	***Phone***
Volker	Marx	v.marx@fz-juelich.de	+492461615831

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **BSC**

PIC	***Legal name***
999655520	*BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION*

Short name: BSC

Address of the organisation

Street Calle Jordi Girona 31

Town BARCELONA

Postcode 08034

Country Spain

Webpage www.bsc.es

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2011 - no

SME self-assesment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE code 72 - Computer & related activities

Proposal ID **691974**	*Acronym* **CoSTAR**	*Short name* **BSC**

Department(s) carrying out the proposed work

Department 1

Department name	Earth Science
	☐ Same as organisation address
Street	29th Jordi Girona Street
Town	Barcelona
Postcode	08034
Country	Spain

Department 2

Department name	Education & Training
	☐ Same as organisation address
Street	29th Jordi Girona Street
Town	Barcelona
Postcode	08034
Country	Spain

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **691974** *Acronym* **CoSTAR** *Short name* **BSC**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Mrs

Sex: ○ Male ◉ Female

First name: **Marina** Last name: **Azor**

E-Mail: **marina.azor@bsc.es**

Position in org.: Project Manager

Department: Management

☐ Same as organisation address

Street: 29th Jordi Girona Street

Town: Barcelona Post code: 08034

Country: Spain

Website: www.bsc.es

Phone: +34934134082 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Proposal ID **691974** *Acronym* **CoSTAR**

3 - Budget for the proposal

No	Participant short name	Country	(A) Direct personnel costs/€	(B) Other direct costs/€	(C) Direct costs of sub-contracting/€	(D) Direct costs of providing financial support to third parties/€	(E) Costs of inkind contributions not used on the beneficiary's premises/€	(F) Indirect Costs / € (=0.25(A+B-E))	(G) Special unit costs covering direct & indirect costs / €	(H) Total estimated eligible costs / € (=A+B+C+D+F +G)	(I) Reimbursement rate (%)	(J) Max. grant / € (=H*I)	(K) Requested grant / €
1	Cyi	CY	216 000	217 932	0	0	0	108483,00	0	542415,00	100	542415,00	512414,38
2	Forschungsze	DE	226 765	0	0	0	0	56691,25	0	283456,25	100	283456,25	283456,25
3	Bsc	ES	161 200	0	0	0	0	40300,00	0	201500,00	100	201500,00	201500,00
	Total		603 965	217 932	0	0	0	205474,25	0	1027371,25		1027371,25	997370,63

Proposal ID **691974** *Acronym* **CoSTAR**

4 - Ethics issues table

1. HUMAN EMBRYOS/FOETUSES		Page
Does your research involve Human Embryonic Stem Cells (hESCs)?	○ Yes ◉ No	
Does your research involve the use of human embryos?	○ Yes ◉ No	
Does your research involve the use of human foetal tissues / cells?	○ Yes ◉ No	
2. HUMANS		**Page**
Does your research involve human participants?	○ Yes ◉ No	
Does your research involve physical interventions on the study participants?	○ Yes ◉ No	
3. HUMAN CELLS / TISSUES		**Page**
Does your research involve human cells or tissues (other than from Human Embryos/ Foetuses, i.e. section 1)?	○ Yes ◉ No	
4. PERSONAL DATA (ii)		**Page**
Does your research involve personal data collection and/or processing?	○ Yes ◉ No	
Does your research involve further processing of previously collected personal data (secondary use)?	○ Yes ◉ No	
5. ANIMALS (iii)		**Page**
Does your research involve animals?	○ Yes ◉ No	

Proposal ID **691974** *Acronym* **CoSTAR**

6. THIRD COUNTRIES		Page
Does your research involve non-EU countries?	○ Yes ◉ No	
Do you plan to use local resources (e.g. animal and/or human tissue samples, genetic material, live animals, human remains, materials of historical value, endangered fauna or flora samples, etc.)? (v)	○ Yes ◉ No	
Do you plan to import any material from non-EU countries into the EU? *For data imports, please fill in also section 4.* *For imports concerning human cells or tissues, fill in also section 3.*	○ Yes ◉ No	
Do you plan to export any material from the EU to non-EU countries? *For data exports, please fill in also section 4.* *For exports concerning human cells or tissues, fill in also section 3.*	○ Yes ◉ No	
If your research involves low and/or lower middle income countries, are benefits-sharing measures foreseen? (vii)	○ Yes ◉ No	
Could the situation in the country put the individuals taking part in the research at risk?	○ Yes ◉ No	
7. ENVIRONMENT & HEALTH and SAFETY See legal references at the end of the section. (vi)		Page
Does your research involve the use of elements that may cause harm to the environment, to animals or plants? *For research involving animal experiments, please fill in also section 5.*	○ Yes ◉ No	
Does your research deal with endangered fauna and/or flora and/or protected areas?	○ Yes ◉ No	
Does your research involve the use of elements that may cause harm to humans, including research staff? *For research involving human participants, please fill in also section 2.*	○ Yes ◉ No	
8. DUAL USE (vii)		Page
Does your research have the potential for military applications?	○ Yes ◉ No	
9. MISUSE		Page
Does your research have the potential for malevolent/criminal/terrorist abuse?	○ Yes ◉ No	
10. OTHER ETHICS ISSUES		Page
Are there any other ethics issues that should be taken into consideration? Please specify	○ Yes ◉ No	

Proposal ID **691974** *Acronym* **CoSTAR**

I confirm that I have taken into account all ethics issues described above and that, if any ethics issues apply, I will complete the ethics self-assessment and attach the required documents. ☒

How to Complete your Ethics Self-Assessment

Proposal ID **691974** *Acronym* **CoSTAR**

5 - Call specific questions

Open Research Data Pilot in Horizon 2020

If selected, all applicants have the possibility to participate in the Pilot on Open Research Data in Horizon 2020[1], which aims to improve and maximise access to and re-use of research data generated by actions. Participating in the Pilot does not necessarily mean opening up all research data. Actions participating in the Pilot will be invited to formulate a Data Management Plan in which they will determine and explain which of the research data they generate will be made open.

We wish to participate in the Pilot on Open Research Data in Horizon 2020 on a voluntary basis	○ Yes	◉ No

Participation in this Pilot does not constitute part of the evaluation process. Proposals will not be evaluated favourably because they are part of the Pilot and will not be penalised for not participating.

[1] *According to article 43.2 of Regulation (EU) No 1290/2013 of the European Parliament and of the Council, of 11 December 2013, laying down the rules for participation and dissemination in "Horizon 2020 - the Framework Programme for Research and Innovation (2014-2020)" and repealing Regulation (EC) No 1906/2006.*

Data management activities

The use of a Data Management Plan (DMP) is required for projects participating in the Open Research Data Pilot in Horizon 2020, in the form of a deliverable in the first 6 months of the project.

All other projects may deliver a DMP on a voluntary basis, if relevant for their research.

Are data management activities relevant for your proposed project?	○ Yes	◉ No

COVER PAGE

Title of Proposal

Computational Science Twinning for Advancing Research (CoSTAR)

List of participants

Participant No *	Participant organisation name	Country
1 (Coordinator)	Computation-based Science and Technology Research Centre (CaSToRC)/The Cyprus Institute	Cyprus
2	Forschungszentrum Jülich GmbH	Germany
3	Barcelona Supercomputing Centre	Spain

1 Excellence

Introduction

Simulation has become an important pillar of scientific discovery, alongside theory and experiment, playing a fundamental role in our efforts to understand natural phenomena and to address challenges such as climate change, health hazards, design of drugs and biofuels, and the ever-increasing availability of information in our society. Computational Science is an emerging field of study in the science of simulation that combines Information Technology and Mathematics with thematic areas in other scientific disciplines to advance discovery and innovation via computation. The Cyprus Institute, recognizing the importance of scientific computing, established as one of its three centres the Computation-based Science and Technology Research Centre (CaSToRC) that provided the first large scale computational facility in Cyprus and initiated a research and educational programme in computational science. Despite these initial forward looking steps taken by CaSToRC, Cyprus lags behind other European countries in terms of High Performance Computing (HPC) expertise and output in Computational Science research.

This proposal seeks to **strengthen and expand the research agenda of CaSToRC**[1], whose founding objective was to establish the cross-disciplinary field of **Computational Science** as a coherent field of study. It recognises the fact that computational training is still largely absent from traditional science curricula, especially in countries in the Eastern Mediterranean (EM) region like Cyprus. The proposed programme seeks to ensure that the scientists engaged, and being trained, in this field at CaSToRC, have access to the highest levels of expertise and guidance from two of Europe's leading computational science research centres, the **Institute for Advanced Simulation (IAS)**[2] of Forschungszentrum Juelich in Germany and the **Barcelona Supercomputing Centre (BSC)**[3] in Spain, from now on referred to as the Twinning partners.

The underlining vision of the **Computational Science Twinning for Advancing Research (CoSTAR)** proposal is to mentor, network and train the three junior faculty and the associated researchers of CaSToRC in Computational Science through coordinated interaction with the research teams of leading scientists at the Twinning partners, and under the oversight of the Project Coordinator - the Director of CaSToRC. The proposed training and mentoring program aims to help CaSToRC create the vibrant, cross-disciplinary environment that is typical of high-performing institutions and is required to excel in research in this interdisciplinary field. Through teaming with European lead groups, the proposal aims at building long-term, sustainable research collaborations that will promote Computational Science of international calibre, helping to bridge the gap between Cyprus and high performing countries in Europe. The project will transfer the skills required to train the research staff to successfully compete for research funding and to ultimately take a regional leadership role in computational science.

The Twinning partners have a mission that is in harmony with that of CaSToRC, each partner operating national supercomputing facilities of their respective countries, as well as, promoting research activities in computational science. Furthermore, the Twinning partners bring world-leading competencies and are at the forefront of computational science, both within the current thematic focus of CaSToRC, namely **Future and Emerging Technologies, Atmospheric and Climate Modelling, Computational Physics and Chemistry,** and beyond. Their multifaceted expertise will be exploited to provide a well-rounded training and mentoring programme for faculty and their team members at CaSToRC, as well as to the technical personnel so as to better manage the High Performance Computing facilities that serve as the laboratories of computational scientists - the ultimate goal being to advance the research capabilities of CaSToRC and excel in computational science.

1.1 Objectives

The need for Europe to train computational scientists has been recognized and documented in several reports[4] as a crucial element for both solving large-scale scientific problems and for fostering innovation in industry. However, most Ph.D. programmes are still domain specific and the few Computational Science (CoS) programmes that exist in Europe are at the Master's level[5,6]. Thus, many talented young researchers receive training within the traditional

[1] CaSToRC Enterprise Plan, The Cyprus Institute, June 2009, http://www.cyi.ac.cy/castorc.html
[2] http://www.fz-juelich.de/portal/EN/AboutUs/organizational_structure/Institutes/InstituteAdvancedSimulation/_node.html
[3] http://www.bsc.es/about-bsc
[4] ETP4HPC (European Technology Platform for HPC), "Strategic Research Agenda", 2013; EESI (European Exascale Software Initiative), D4.4 Working Group report on software eco-system, PRACE scientific case report 2012[3].
[5] see e.g. http://www.siam.org/students/resources/cse_programs.php
[6] Examples of the CoS Ph.D. programmes in Europe are at CyI, http://www.cyi.ac.cy/education/programs/computational-sciences.html and at ICS, Switzerland http://icsweb.inf.unisi.ch/cms/index.php

domain-specific disciplines, but typically lack explicit mentoring on the use of HPC and simulation in modern scientific research. This is particularly acute in Cyprus which, until the establishment of CaSToRC, lacked HPC infrastructure and the associated expertise. The result is that even talented faculty either do not have the knowhow in, or even worse they are not aware of, the competitiveness that HPC can offer them in their research, leading to publications unnecessarily low in number or impact.

A tangible measure of the maturity of computational scientists, besides the quality of their publication record, is their ability to compete successfully for computational resources that require good scalability of application codes, such as those provided by, for example, the Tier-0 machines within the Partnership of Advanced Computing in Europe (PRACE)[7]. If an indicator for leadership in computational science is the success in accessing large computational resources then Cyprus, and indeed the whole Eastern Mediterranean region, is heavily underrepresented, with only a handful of groups being successful in competing for such resources. According to the statistics published by PRACE[8], the countries that perform best are those with long computational traditions and advanced infrastructure such as Germany, France, Spain and Italy, while the countries that are underperforming in research in general, such as those targeted by this call, typically have no or very low success rate in PRACE access calls. The necessary technical expertise for such access is very scarce, with most scientists in the region relying on their personal computers and having limited awareness of the possibilities of High Performance Computing (HPC), let alone expertise in parallel programming methods. CaSToRC was established in recognition of the potential of Computational Science and the reality of this deficiency of relevant expertise. It has taken crucial steps to improve the capabilities of scientists to excel in computational science: creating and operating the first supercomputing facility of Cyprus, recruiting technical personnel, establishing a user support group and establishing an innovative Ph.D. programme in Computational Science. It comes, perhaps, as no surprise that the only group in Cyprus that leads a Tier-0 allocation project is the one of the Director of CaSToRC, the Project Coordinator of this proposal, in the area of Computational Nuclear and Particle Physics.

CaSToRC has recently hired three talented junior faculty to expand its computational science research and education agenda into three new thematic areas that have been selected because of their relevance to the overall research priorities of CaSToRC and CyI as well as to Cyprus and the region. Indeed they align well with the Smart Specialisation Strategy of Cyprus announced recently. The motivation and driving force of CoSTAR is to help grow these scientists to become leaders in their research area through the implementation of a comprehensive training and mentoring programme with the Twinning partners. The mentoring component, which is lacking in most of the other training programmes, and provided here by the Twinning partners, is considered a crucial element for enabling high calibre research. Furthermore, creating a unified program that spans the three thematic areas of CaSToRC will greatly enhance the cross-disciplinary aspects of Computational Science and help CaSToRC take a crucial step forward in realizing its founding goal of excelling in this field.

CoSTAR will immerse the teams at CaSToRC in the interdisciplinary environment of the Twinning partners that will deliver training, mentoring and educational activities aiming at increasing the research capacity of these teams. It will catalyse high calibre research collaborations among the Twinning partners and CaSToRC, identify and promote long-term research projects, and develop the appropriate European networks to ensure long-term research sustainability. In order to further increase the research capacity of the teams, the scientific training and mentoring programme will be complemented by delivering computational skills and knowhow to the technical personnel operating the computational facility at CaSToRC to enable them to provide better services and the best utilization of these resources for research. In addition, CoSTAR will promote training of the staff at the Office of Sponsored Research of CyI and CaSToRC researchers aiming at enhancing their ability to better exploit the knowledge generated through research and to establish links to industry, leveraging the expertise at the Twinning partners, such as through the Technology Transfer Office at JUELICH[9] and the Project and Technology Transfer office at BSC[10]. The Twinning partners will closely work together with the Project Coordinator to implement the all-round training and mentoring programme laid out in CoSTAR.

The central goal of CoSTAR is, by the end of the project, to have established at CaSToRC a vibrant cross-disciplinary environment similar to that of the Twinning partners, one that fosters excellence in computational science within its research teams.

Before elaborating on the potential for excellence and the details of the training and mentoring programme to unleash it, we summarize the main objectives of the CoSTAR proposal:

[7] http://www.prace-ri.eu
[8] see e.g. http://www.prace-ri.eu/statistics (2012)
[9] http://www.fz-juelich.de/portal/EN/Expertise/UsingKnowledge/_node.html
[10] http://www.bsc.es/about-bsc/organization/support-structure/management

1. **Research capacity building:** Design and implement a comprehensive training and mentoring programme for the three junior faculty at CaSToRC to enhance their research capacity. The project will create European networks, increase the competitiveness of the three groups and promote the interdisciplinary nature of CaSToRC activities, leading to better quality and increased number of publications, more invited talks for the junior faculty, more successful proposals for research funding and ultimately to a regional leadership role in computational science.
2. **Educational capacity building**: Provide training and collaboration opportunities to the junior faculty to enable them to enrich the curriculum of the Ph.D. programme in Computational Science (CoS) with new training components, student exchanges, and common research opportunities with their peers at the Twinning partners. The outcome will be an increased level of collaboration and networking of students and young researchers at CaSToRC with the Twinning partners and, through their wide network, with other European research groups, leading to the establishment of long-lasting collaborations.
3. **Building advanced cross-disciplinary competencies:** Prepare both the researchers and infrastructure at CaSToRC for the challenges of the exascale era, by targeted training on porting codes to prototypes for new and emerging architectures, data post-processing and visualization. The outcome will be high level of HPC competencies transferred to the CaSToRC faculty, enabling them to participate and prepare for the forthcoming exascale era and allowing them to develop a competitive edge in their research activities.
4. **Building of training capacity:** Create a modern cross-disciplinary training program in computational skills such as parallel programming, performance analysis, data management and visualization that is sustainable and extensible by the researchers and technical personnel, and can be run by CaSToRC beyond the lifetime of this Twinning project.
5. **Supporting cutting-edge research of European relevance:** Mentor scientists to develop scalable algorithms and codes for petascale machines and for selected applications, for potentially exascale computing. A training program in a technologically-driven field of research of high relevance to the competitiveness of Europe, will provide the scientists with long-term opportunities for strong collaboration, access to state-of-the-art European facilities and enhanced funding opportunities. Allocations on petascale machines, such as those provided through PRACE or XSEDE, are highly competitive and granted both on scientific merit and on the performance of scientific applications codes being employed.. The outcome will be a marked increase in the amount of computational resources allocated to research projects at CaSToRC, in particular targeting resources provided at the European but also at the international level as for example by XSEDE[11] in the US, thereby contributing to enhanced research capacity for Cyprus and also for Europe.
6. **Aligning with the Smart Specialization Strategy (S3) of Cyprus:** The thematic areas of choice in CoSTAR align well with the S3 of Cyprus, primarily in the areas of Information and Communication Technologies (ICT) and Future and Emerging Technologies (FET), the Environment, Climate Change and Tourism, New Materials and Drug design. The outcome will be enhanced research, adaptation and mitigation activities in the priority areas chosen by Cyprus for their potential of improving the innovation capacity and economic prosperity of the country. Opportunities for national funding can thus be exploited to promote additional research activities of relevance to Cyprus. The training of both researchers and operations personnel will help better prepare for the upgrade of the facility at CaSToRC that will in turn better serve the scientific communities of Cyprus as a whole by increasing the country's research capacity.
7. **Building innovation capacity:** Provide faculty and support personnel at the Office of Sponsored Research (OSR) at CyI knowhow on best practices for management of intellectual property, exploitation of generated research results and forming links to industry. Collaborative work with the Twinning partners in projects involving European industry will network CaSToRC scientists with industrial partners and help establish long-term associations.

Enhancing the research and educational capacity of the junior faculty and their research teams, as well as providing the computational skills to the technical personnel to improve the operation of the supercomputing facility of CaSToRC and to deliver high level support, will in general strengthen and expand CaSToRC's participation in the European research area where HPC is recognized as central in pursuing 'Europe's place in a global race'[12]. Thus the objectives of the project are of high relevance not only to Cyprus but also to Europe. Furthermore, the research and technical capacity brought by the project will help establish CaSToRC as a hub for computational science in the Eastern Mediterranean increasing the qualified personnel in the region from which Europe can draw from. This

[11] https://www.xsede.org
[12] PRACE - The scientific case for HPC in Europe, http://www.prace-ri.eu/IMG/pdf/prace_-_the_scientific_case_-_executive_s.pdf

couples well with the regional role that CaSToRC has been pursuing through the FP7 infrastructure project LinkSCEEM[13].

1.1.1 Enhancing research capacity

Computational Science is a new cross-disciplinary field and finding the right leadership is difficult, in particular in countries like Cyprus that lack long tradition in simulation and HPC infrastructure. At CaSToRC the decision was made to **hire talented junior faculty and provide the environment and means to mature them into leaders**. It is these junior faculty members, their research teams and the students that they will train who form the nexus of CaSToRC going forward. Providing an optimal framework to allow for the realization of the potential of these teams is the purpose of this proposal.

The core element of CoSTAR's objectives is to enable and ensure sustainable competitiveness of the CaSToRC research teams, through the formation of persistent channels for idea and technology flow to and from the Twinning partners. This will be achieved by the provision of a comprehensive and persistent mentoring and training programme to these teams, which will involve a growing number of Ph.D. candidates and post-doctoral researchers over the project lifetime. The motivating force for these training programmes will be the realisation of specific aspects of the research programme of CaSToRC that have been identified and agreed with the Twinning partners.

Exploring Computational Science as a unified field of research is challenging due to its cross-disciplinary nature but, at the same time, creates many opportunities. As mentioned above, in spite of the recognized relevance of the power of simulation for scientific discovery as well as its industrial application, education and training of researchers is limited by being mostly discipline-oriented. This creates opportunities for a young institution like CyI to build excellence in a highly innovative area of European importance. It also provides opportunities for building a leadership role in the Eastern Mediterranean region, which lags behind Europe in HPC infrastructure and knowhow. Furthermore, the Cyprus Institute by the interdisciplinary construction of its research centres, provides an optimal environment to foster excellence in this inherently interdisciplinary area of research. These opportunities will be fully explored within the project leveraging the experience of the Twinning partners under the steering of the Project Coordinator who has been spearheading the development of CaSToRC since its establishment.

The timing of the proposal directly complements the development plan of CaSToRC. Until very recently CaSToRC concentrated its activities in the field of the Project Coordinator of CoSTAR, namely lattice Quantum Chromodynamics (QCD), where the centre has an established reputation. Research activities in prototyping, algorithms and novel computer architectures emerged from this lattice QCD group. During the last two years CaSToRC expanded its faculty by hiring three young assistant professors in the thematic areas of:

- Climate and atmospheric modelling (Th. Christoudias),
- Computational chemical kinetics (Y. Suleymanov),
- Lattice QCD for exascale (G. Koutsou),

who are, at the same time, expected to promote cross-disciplinary research in Future Emerging Technologies (FET). As postdoctoral fellows, these young scientists produced high calibre research and demonstrated potential for becoming the next leaders in their respective fields. CoSTAR's objective is to provide the mentoring, networking and intellectual environment for them to assume leadership in **both** their respective fields **and** in interdisciplinary research topics of computational science. The programme will also integrate them into pan-European research networks enhancing their competitiveness.

Building cross- disciplinary research capacity

The challenging and innovative aspect of this project is the inter-disciplinarity that it requires. Both Twinning partners have cultivated cross-disciplinary training and research activities and thus their mentoring role will be central in building in CaSToRC research capacity for interdisciplinary activities. This is a crucial component for growing leaders in computational science, particularly at this point in time, where programming paradigms need to be drastically revised to attain exascale performance. Thus the area of **Future and Emerging Technologies** will be a priority of the training and mentoring program of CoSTAR. In particular, the thematic area of lattice QCD will have a strong overlap with HPC Technologies and FET necessary for reaching exascale performances.

[13] https://www.linksceem.eu/ls2/

A crucial element of CoSTAR is that the research area to be promoted by this project aligns well with European research priorities, which is a prerequisite for creating strong vibrant collaborations. Developing common research interests between the collaborating scientists at the Twinning partners and at CaSToRC is a central element for sustainability: Long-term collaboration can only be sustained if the scientists at CaSToRc can carry out research of international scope and equal quality as that of the other European groups. The objective of the CoSTAR mentoring planned is, thus, to promote interdisciplinary thinking at the forefront of HPC to best couple to European research priorities connected to exascale computing where the Twinning partners have developed strong activities. The urgent need for such research on the European scale is connected to the realization that the disruptive evolution of HPC architectures requires to be accompanied by an equivalent evolution in algorithms that have to be adapted to future exascale architectures. Algorithms will thus need to evolve to ever more complex hierarchical memory concepts, to the increasing gap between memory bandwidth and floating-point performance, and to massive parallelism. Critical issues in allowing some of these algorithms to scale are generic, but the initial modelling of a physical problem can have a tremendous effect on its ability to be treated efficiently on massive parallel future exascale systems. The training will address two major challenges that are also applicable to the global computational science community, namely

- the ever-increasing gap between hardware advances and their effective utilisation in scientific research,
- disciplinary boundaries and the lack of education in computational thinking common to all areas of sciences.

Examples of the above problems are omnipresent in the current utilisation of computers in academia and industry. Typical application codes usually exploit at most 5% of the peak performance of the hardware they run on and there is widespread repetitive development of the same computational tools across disciplines. Application codes are written in ways that are case/problem/hardware specific and as such they tend to be impossible to maintain beyond a span of a few years.

Developing software for modern computer technologies is a challenge for many scientific applications and the existing experience at CaSToRC will be leveraged and combined with the expertise of the Twinning partners for advancing code development and for preparing the scientists for future and emerging technologies. In addressing the challenging task of software development keeping in pace with hardware, prototyping activities are to be pursued. Such activities aim at enhancing the opportunities for pioneering research that utilizes emerging multi-core technologies such as graphics cards (GP-GPUs) or other accelerators. In order for scientists at CaSToRC to participate, they need appropriate training and continuous access to prototype computers, so that they can reach a level that allows effective collaboration with colleagues in Europe. Although CaSToRC has initiated activities in this direction, with the lattice QCD group being the first group to import a GPU cluster in Cyprus, more training is needed to attain the required expertise expected at the highest level of the Twinning partners, as well as to spread it to other scientific areas.

This project will include training the technical personnel operating the facility so that it can better manage computational and storage resources, provide user support and most importantly plan for the upgrade of the CyI flagship machine in the next two years. In order to maintain a competitive edge in scientific software design and algorithms, CaSToRC researchers deploy prototype machines for performance evaluation and application code development. Such systems require cutting-edge expertise in novel computer architectures and systems administration, which is rare in Cyprus and the region. Thus this training will be crucial in keeping CaSToRC up to date with the rapid development in computer technologies.

Another big challenge inherent in almost all applications that will require and benefit from exascale computing is data post-processing and visualisation. Analyzing the deluge of data obtained from petascale and future exascale computing is a formidable task. Managing and visualizing the results is an important component in order to exploit simulation outcomes. CaSToRC has initiated efforts to adopt emerging computing infrastructures in storage for Big Data and high-volume data processing, provenance and curation. Initial efforts have been focusing in data for environmental and climate studies that rely on long-term temporal records specifying past, current and projected conditions over geographic regions. Another example is the adoption at CyI of Medici[14] as a data management system for data in cultural heritage and for an online Supercomputing Training Portal, which will be expanded within this project. A ***Visualization Laboratory*** **(VisLab)**[15] is necessary to allow researchers from all disciplines of science to better understand complex phenomena and translate large-scale data into high resolution images and visualizations to promote scientific understanding, knowledge dissemination and public outreach.

[14] http://medici.ncsa.illinois.edu/
[15] http://vislab.cyi.ac.cy

We list below some of the common challenges shared by the domain-specific applications that the CoSTAR training and mentoring programme will be addressing:

i. Load balancing at the pre-processing stage that can affect the performance of grid-based algorithms and may require new adaptive resolution methods or parallel grid generation.

ii. Modelling and algorithmic development in particular in view of the multi-core architectures that will prevail in the near future. These pose particularly challenging issues in coupling codes for multi-physics applications and multi-scale problems, such as those in Climate modelling, which need to be addressed if the field is to take advantage of exascale computing facilities.

iii. The post-processing stage that needs the development of visualization tools for the analysis and presentation of large data sets, as well as integrating computational models and data through uncertainty quantification and propagation techniques.

The researchers at CaSToRC have already built relevant core expertise for the mentoring programme to bear fruit. The objectives of the cross-disciplinary training will focus on:

i. *Expertise on HPC technologies***:** Researchers in lattice QCD have been participating in prototyping activities as part of the PRACE implementation projects. The CoSTAR exchange and training programme will enhance and extend research in HPC technologies focusing on understanding the performance of new computing devices, developing performance models, and finding optimisation strategies. As a mature application, lattice QCD is to be used for the FET and exascale performance activities within the lifetime of this project. The Climate and Atmospheric modelling group has been participating in the DEEP project and thus the mentoring programme will be designed to develop approaches for attaining better performance on current petascale machines as well as taking part in prototyping activities. The Computational Chemistry group is the newest at CaSToRC and the one to benefit most from expanded HPC training and initialization of further prototyping activities.

ii. *Modelling and algorithms***:** The three faculty members have experience in the development of methods and algorithms that are suitable for the various domain-specific applications. Thus the training programme will focus on new concepts for current hardware technology, in particular multi-threading technology and taking advantage of the massively multithreading architecture of GPUs in order to take the applications to the next level of performance. For lattice QCD this is exascale, and for climate and chemistry it is petascale. Development of multigrid algorithms for linear solvers scalable to exascale; hybrid particle-mesh methodologies incorporating adaptivity; integration of molecular dynamics and dissipative particle dynamics methods for describing flows at atomic and mesoscopic scales; adaptation of evolutionary algorithms for structure prediction for HPC, GPU-enabled quantum chemistry methods, are examples of what the advanced training will include.

iii. *Visualization of data***:** An equally important aspect is the post-processing of large data sets. Researchers in climate are already familiar with visualization of their data. The training programme will thus bring additional expertise and help them in the development of appropriate visualization tools, pipelines and workflows for simulation outputs and derived products for scientific visualisation, dissemination and outreach.

Building research capacity in the thematic research areas

Similarly to the mentoring on cross-disciplinary aspects of computational science, the training and mentoring in the domain-specific subareas aims at building research of international relevance and importance. Petascale computing has already had an enormous impact on research in particle and nuclear physics particularly in **Lattice Quantum Chromodynamics (QCD)**, while **Climate and atmospheric modelling**, and **Computational Chemistry applications** have seen a rapid evolution as growing processing capacity enables highly demanding, compute-intensive simulations. Exascale computing is expected to bring a major breakthrough in these areas, enabling complex simulations that are unthinkable today[16]. The mentoring programme of the CoSTAR project will train the three junior faculty and their teams to utilize the next generation of HPC technologies to advance their scientific field and make new discoveries. The areas of focus are:

i. *Climate and Atmospheric modelling (Th. Christoudias)*: There is already significant activity at CyI in climate research. However, most of the researchers are limited to using existing community codes due to lack of HPC training. The new faculty at CaSToRC is hired to spearhead model simulations to study the atmospheric transport and impacts of pollution, in the context of a changing climate in multiple spatial and temporal scales from Cyprus to the Eastern Mediterranean and Middle East region, and globally. The objective of the mentoring, besides the

[16] see e.g. http://extremecomputing.labworks.org/highenergyphysics/report.stm

inter-disciplinary competencies, is to enable improvements of the atmospheric model simulations, by including a mineral dust component and online emissions over the Eastern Mediterranean and Middle East region. The expertise of BSC in such atmospheric simulations, will be transferred to the group in Cyprus enabling them to couple the regional model to computationally optimised global climate-chemistry models, while the expertise of the Climate Simulation Lab at JUELICH with Lagrangian transport algorithms will enable the study of intercontinental tracer transport, and the effects of teleconnections on pollution and boundary conditions for downscaling and long-term climate change impacts studies.

ii. *Computational chemical kinetics (Y. Suleymanov)***:** This is a new group with high level expertise in theoretical organic chemistry but lacking the necessary HPC training that is needed for exploiting next generation computers. Prognosis of the chemical reactivity using molecular structure requires novel algorithms for quantum chemistry calculations that involve large datasets. This is a field of research that relies on community codes, many of which do not scale well. Critical kernels require rewriting and optimisation with potentially large impacts from the utilization of accelerators like GPUs. It also relies critically on efficient data management. Thus, in this field, potential gains from the cross-thematic interaction can be substantial in particular when facilitated by the advanced knowhow of the expert team at the JUELICH simulation laboratory "Molecular Systems" (see the training programme). The objective of the training is to enable the group to carry out improvement in algorithms to tackle problems such as automated analysis of 'unknown' chemical reaction pathways using freezing/growing string and evolutionary methods, automated generation of complex kinetics models relevant to combustion engineering, computational guidance of complex chemical synthesis, and computational studies of large molecular systems relevant to drug design.

iii. *Lattice QCD for exascale (G. Koutsou):* This is the only thematic subarea that, in addition to the junior faculty member, includes the Project Coordinator with an established research profile, serving as an example of the potential of the international level of research that can be achieved at CaSToRC. However, achieving a transition from petascale to exascale performance will require expertise beyond what is available. The junior faculty hired has worked with novel computer architectures and thus has the necessary qualifications to absorb the training provided and spearhead developments of lattice QCD in the exascale era, becoming the next leader of the field at CaSToRC. He is the appropriate person to be mentored in FET and take the lead for co-design activities within collaborative work with the exascale laboratories of JUELICH. Acquiring such cutting-edge expertise, the group can maintain its competitiveness in large-scale simulations of lattice QCD and in computations of observables relevant for searches of new physics beyond the standard model (BSM). These simulations are needed to answer fundamental questions like the identity of dark matter and dark energy, and the origin of the matter-antimatter asymmetry in the universe being sought by dedicated experiments.

The three domain-specific subareas of the project will depend on, and greatly benefit from, the use of HPC and exascale architectures and thus highly profit from mutual interaction. They also benefit from interaction with HPC experts and applied mathematicians. These cross- and inter-thematic elements will be interweaved into the training programme to address common algorithmic challenges such as allowing applications to tolerate less frequent communications, which is crucial for efficiently exploiting large parallel systems of co-processing accelerators. Researchers will simultaneously develop methodologies for modelling and predicting algorithmic performance that then can influence the future design of computational systems in collaboration with HPC industry. This co-design methodology, where scientific problem requirements influence computer architectures, and architectural constraints impact the formulation and design of algorithms and software, in turn affecting progress in the scientific areas, is a holistic approach that this training emphasizes. Examples of algorithmic research proposed are: the development of Monte Carlo (MC) methods for exascale platforms; development of efficient solvers for sparse matrices for exascale (that are important for lattice QCD and many other applications); exploring recently proposed ideas by the team at JUELICH such as domain decomposition multilevel algorithms[17] and extensions of deflation[18]. Addressing the Big Data challenges in climate simulations and chemistry applications will enable better understanding of the simulations and promote progress in e.g. computational simulations of biofuel combustion and the design of new drugs.

The CoSTAR project is thus designed to promote research capacity in a truly interdisciplinary manner that leverages the investment made by CyI in HPC infrastructure as well as building on CaSToRC current competencies. The project will be embedded in the simulation laboratory (SimLab) already initiated at CaSToRC, which to date fo-

[17] *An adaptive aggregation based domain decomposition multilevel method for the lattice Wilson Dirac operator: multilevel results,* A. Frommer *et al.*, arXiv:1307.6101

[18] *Deflation and Flexible SAP-Preconditioning of GMRES in Lattice QCD Simulation,* A. Frommer, K. Kahl, S. Krieg, B. Leder, M. Rotmann, arXiv: 1307.6110*; Hierarchically deflated conjugate gradient,* P. Boyle, arXiv:1402.2585.

cussed mainly in lattice QCD research being jointly developed with the SimLab "Nuclear and Particle Physics"[19] at the Institute of Advanced Simulation of JUELICH. While big computational centres like JUELICH have multiple thematic simulation laboratories, CaSToRC aims at establishing a truly interdisciplinary one serving its various computational disciplines, an important development enabled by CoSTAR.

The structure of the training and mentoring programme is discussed in Section 1.3 and illustrated in Figure 1.1. More details on the concept and approach will be given in Section 1.3.2.

1.1.2 Building educational and training capacity

The training and mentoring programme developed within CoSTAR also aims at preparing the faculty to train their own Ph.D. students and postdoctoral fellows within a similar framework. This will ensure the sustainability of research teams in the longer term and provide a legacy from the Twinning project for all future Ph.D. students and researchers at CaSToRC.

In addition, the project will train the technical personnel so that they can both optimise the administration of next-generation computational resources as well as provide adequate user support. This will enhance the research capacity of both the current staff but also of future users of the CaSToRC facility.

CaSToRC's role as a regional computing facility must also include broader education and training services in order to maximise the potential impact of its infrastructure. Technical expertise is scarce in the region, with most scientists relying on workstation computers and having limited awareness of the possibilities of HPC. An objective of this Twinning project is therefore to not only deliver the training programme to the researchers currently at CaSToRC, but to develop it in a way that will allow sustaining and extending it for future researchers. Given the rapid evolution of technologies used in HPC related topics, the programme must be designed to be flexible, allowing continuous updating of the material to include upcoming computing architectures and novel programming methods. This objective is in line with the goal of CaSToRC in supporting a regional Advanced Training Centre for HPC technologies, leveraging modern education techniques such as mixed-mode lectures (where high-level remote instruction is complemented by local tutors to provide direct assistance to learners) to give regional scientists access to the advanced training capabilities of the Twinning partners. To this end, one component of this project will focus on training CaSToRC staff in delivering the training programme in this context.

Furthermore all training carried out within the Twinning project will be leveraged to populate an existing online Supercomputing Training Portal[20] that integrates modern web technologies into a broader training programme. Establishing this training component at CaSToRC will strengthen the current doctorate programme with complementary material, increasing the faculty's capacity in attracting Ph.D. students and early-stage researchers and delivering sustainable and extensible HPC training beyond the lifetime of this Twinning project.

1.1.3 Implementing an innovative training and mentoring programme

The overall objective of the programme is to implement a three-year well-rounded training covering introductory to advanced topics, interweaved with intensive mentoring of scientific staff through secondments to the relevant teams of the Twinning partners. The mentoring component lacking in most of the other training programmes is considered crucial for enabling high-calibre research. Also, by teaming leaders in three HPC domains which can catalyse rapid development and innovation, we will train the young scientists to work in an interdisciplinary environment that is difficult to cultivate otherwise and to prepare the stage for successfully performing computational science in the exascale era. The innovation arises from both addressing all levels of expertise needed as well as implementing interdisciplinary structures in the training, transcending the traditional boundaries of individual disciplines.

The outline of the training programme, showing the competencies brought in by the Twinning partners and the departments involved, is shown in Figure 1.1. As can be seen, a spectrum of competencies is coupled to form a comprehensive HPC training program. An important component of the programme is that the training and exchanges are not limited to the scientific staff but include also the technical personnel. Training technical personnel how to best manage computational resources, prepare them for adapting new technology and how to handle long-term storage of Big Data is central to providing services of the same quality as other European national facilities. Providing well-managed resources and high level support will impact the centre as a whole increasing not only the research capacity of the researchers at CaSToRC but also the research capacity of all user communities in Cyprus. It is no coincidence that high-level computational science is produced by scientists in countries with well-

[19] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slnpp/_node.html
[20] http://supercomputing.cyi.ac.cy/

developed national computational facilities, and although CaSToRC will not be able to provide the large scale resources offered by the Twinning centres it is imperative that it offers Tier-1 resources to provide the knowhow and support for its' scientists to access the larger European resources. Choosing smaller appropriate hardware for prototyping is a crucial component to having the expertise locally to scale to the larger machines elsewhere. Developing collaborative programmes within the exascale laboratories of JUELICH and BSC and having access to such machines is a crucial hands-on component of the training programme. The advanced expertise brought to the centre will also help CaSToRC consolidate its regional role in the EM through the competencies gained.

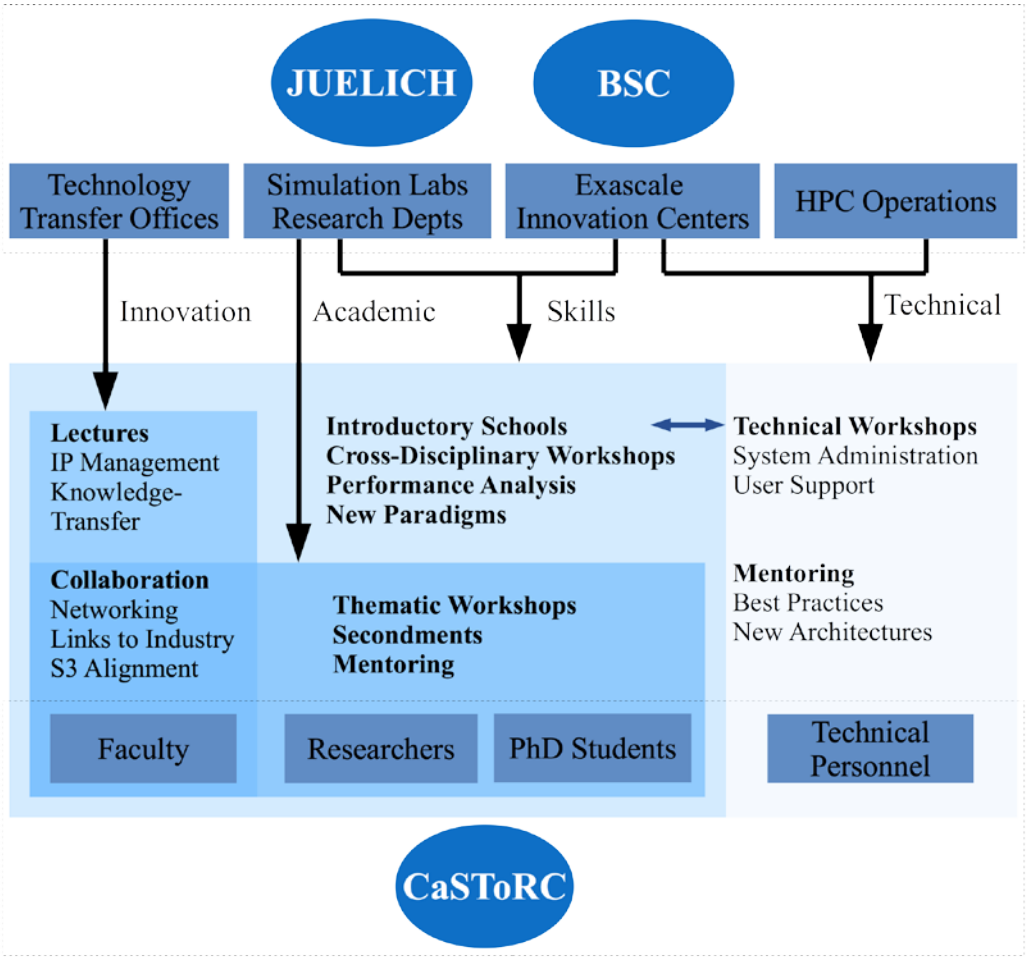

Figure 1.1: Components of the training programme of CoSTAR, with the groups at the Twinning partners involved and the teams at CaSToRC receiving the knowledge. A closing workshop near the end of the project will take place in Cyprus to disseminate the outcomes of the project.

A final important component is innovation training of CaSToRC researchers and CyI management staff. The two scientific coordinators of the project, one based at CaSToRC and one interfacing between JUELICH and BSC, will interact with the personnel at the Technology transfer office of JUELICH leveraging the course provided to researchers at JUELICH and transferring its knowhow to scientists and the personnel at the Office of Sponsored Research of CyI. This will help CaSToRC to promote interaction with experts from local and European industry and explore the innovation potential of the research results.

The training programme will be under constant evaluation throughout the project and additional training will be added when weaknesses or opportunities are identified.

1.1.4 Building innovation capacity

Research and innovation are strongly associated with economic growth and increased competitiveness[21]. While CaSToRC has already established an internationally recognised research branch in High Energy Physics (lattice QCD), the output in terms of innovation outflow has been low. One reason is the difficulty of identifying and subsequently exploiting innovation in fundamental science.

[21] http://ec.europa.eu/research/innovation-union/pdf/state-of-the-union/2013/research-and-innovation-as-sources-of-renewed-growth-com-2014-339-final.pdf

There is a lot of innovation potential in fundamental science that can result in economic impact. Examples can be drawn from Climate and Atmospheric modelling where accurate prediction of future weather and air quality conditions can help develop mitigation and adaptation policies and strategies, but also the development of more efficient algorithms can have significant innovation potential. Often, such potential is unrecognised and under-exploited. Interdisciplinary research environments where fundamental research is paired with applied science helps to overcome this limitation.

The training of this project will enhance research in fields with high innovation potential and with alignment with S3, such as FET, climate change projections in connection to tourism and agriculture, and chemistry simulation applicable to combustion chemistry of biofuels and computational drug design where links to local industry can be developed. Collaborative projects with the Twinning partners will network faculty with industry in Europe.

The scientific coordinators of CoSTAR will also interface with the personnel at the Technology Transfer Offices of JUELICH and BSC to transfer knowhow in IP management and in coupling basic scientific research to technological development. The first crucial objective that we will aim at is to help researchers to identify potential innovation of their research. The Office of Sponsored Research personnel at CaSToRC will be specifically trained to support CaSToRC scientists on how to identify and register intellectual property as well as subsequently exploit innovation. This will be supplemented with networking activities to develop ties to potential industrial partners in Cyprus and Europe.

1.2 Relation to the work programme

This proposal relates to the Call for Twinning of the work programme topic "Spreading Excellence and Widening Participation" to address networking gaps and deficiencies between research institutions in Member States with a low Composite indicator of Research Excellence and internationally-leading counterparts at EU level. It is part of the WIDESPREAD programme aiming at enhancing competitiveness by investing in research and innovation potential and increasing participation.

The Cyprus Institute (CyI), founded in 2005, is a newly established Science and Technology research and educational Institute that is built upon a novel issue-oriented, rather than discipline-oriented structure, conceived to help transform Cyprus into a knowledge-based economy. The three Ph.D. degree granting research centres of CyI are characterized by an interdisciplinary environment with objectives that align very much with the context of the current call. The research centre related to this project is the Computation-based Science and Technology Research Centre (CaSToRC), established in recognition of the pivotal role of computational science with respect to scientific discovery and innovation in the modern era. Its founding goal is in fact to address the HPC infrastructure gaps and deficiencies in computational science research between Cyprus and other European member states and to serve as a link between the Middle East region and Europe[22] perfectly matching the context of the call. More specifically, its missions are:

- To create a research programme of international calibre in computational science and scientific computing
- To provide forefront computing resources to enable Cyprus and the larger Eastern Mediterranean research community to pursue state-of-the-art computing-related research, with a portal function to the US and EU
- To act as catalyst for the development of an educational programme in computation-based science and technology in Cyprus and the Eastern Mediterranean region

Striving for the realization of these missions has required incremental progress since the foundation of the centre. CaSToRC has developed the first national HPC centre in Cyprus, with its primary HPC resource being the Cy-Tera[23] machine, which is a novel hybrid CPU/GPU architecture co-financed by the European Regional Development Fund and the Republic of Cyprus. It is **one of nine strategic research infrastructure projects in Cyprus** and the resource is open to Cypriot and regional scientists and industry through an internationally peer reviewed allocation process whose sole selection criterion is scientific excellence. In addition, CaSToRC obtained FP7 funding for the LinkSCEEM[24] projects that enabled the provision of computational resources and training to the Eastern Mediterranean region. In parallel, CaSToRC is the **Cypriot representative in PRACE** and allocates additional Cy-Tera resources to European researchers through the PRACE Tier-1 programme. These successes were spearheaded by the Coordinator of CoSTAR and provide the foundation upon which CaSToRC can build its primary mission: the creation of a research programme of international calibre in computational science. The

[22] CaSToRC Enterprise Plan, The Cyprus Institute, June 2009, http://www.cyi.ac.cy/castorc.html
[23] http://www.cyi.ac.cy/castorc/castorc-research-themes/the-cytera-hpc-facility.html
[24] http://www.linksceem.eu/ls2/

purpose of the current project is to mentor and network the junior faculty hired during the last two years as they gradually take leadership and expand the research capacity and impact of the centre.

By putting forward the CoSTAR proposal, CaSToRC recognises that to sustain the momentum and niche it has gained, it must ensure it continues to engage in region-relevant research of the **highest international standards,** as well as to deliver advanced expertise in HPC. It has therefore teamed up with two of the most advanced research and computational centres in Europe, both in terms of HPC infrastructure and expertise as well as world-leading research in the areas that CaSToRC seeks to excel. JUELICH and BSC are both founding partners in PRACE, highly respected European leaders in research in computational science, leading exascale initiatives (DEEP and DEEP-ER[25] coordinated by JUELICH and Mont Blanc[26] coordinated by BSC), and running very successful national supercomputing facilities, having a wealth of experience and expertise from both the operational and scientific perspectives of this project. JUELICH has world-leaders in lattice QCD and FET, as well as in Climate and Atmospheric modelling research and Computational Chemistry. BSC is a leader in scientific computing as well as climate, regional and air quality modelling. They are unquestionably capable Twinning partners who can help CaSToRC realise its mission to increase its research and innovation capacity and CoSTAR provides enviable scope to sustainably increase the level of collaboration and idea flow between CaSToRC and European research powerhouses.

The scientific and training teams at the Twinning partners to carry out the programme of activities have been identified and the conceptual development of a number of scientific research lines of common interest has occurred in concert with the Twinning Partners. These concepts leverage the existing research portfolio being developed at CaSToRC, pairing it with the additional research strengths and technical knowhow provided by the partners. Cross-cutting activities in modelling, algorithms, and HPC technologies will span across scientific disciplines while specific thematic training and secondment activities will focus on areas that are being targeted by CaSToRC: climate and atmospheric modelling, chemical kinetics, and lattice QCD for the exascale era.

Coupling scientists at CaSToRC to research and technical teams at leading European supercomputing centres, and aligning their interests and competencies, will strengthen and expand the research portfolio of CaSToRC, facilitate knowledge transfer, increase the potential for collaboration, as well as promote its innovation potential. With this in mind, a comprehensive training, mentoring and outreach programme, which benefits from current and future HPC technologies, has been developed to underpin and enable the scientific goals that drive CaSToRC as a research and educational centre. This programme is constructed of both horizontal cross-sectional components and vertical thematic elements and designed to ensure the sustained competitiveness of the researchers being trained at CaSToRC. Finally, it promotes the innovation potential of computational science that can positively impact the drive of Cyprus to become a knowledge-based society exploiting technology to improve economic growth.

Furthermore, the programme is aligned with the priorities as outlined in the Smart Specialisation Strategies of Cyprus and commits to a broader support of innovation. This proposal targets priority sectors chosen by Cyprus as part of S3 that are earmarked for their capacity in improving the competitiveness of Cyprus and benefiting its economic growth. Cyprus has selected the following priority sectors in its Smart Specialisation Strategy:

Horizontal:

i) Environment: Climate Change adaptation and mitigation, Pollution control and protection, Eco Systems, Eco – Innovation, Horizontal applications

ii) ICT: ICT Applications, Communication Technologies, Computer Science, Future and Emerging Technologies

Thematic:

i) Tourism: Sustainable Tourism, Alternative forms of tourism, Digital tourism applications, Management and promotion of tourism product

ii) Energy: Renewable forms of energy, Exploration of natural gas, Innovative applications (solar-thermal technology, solar photovoltaic, concentrated solar systems), Energy management

iii) Agriculture – Food Industry: Agricultural and livestock production, Food Security and Climate Change.

iv) Construction industry: Sustainable Urban Development, Sustainable Construction, Innovative and Intelligent Materials and Reuse of Building Materials, Cultural Heritage

v) Transportation- Marine: Road freight, Shipping, Air-transport, Intelligent Transport Systems

vi) Health: e-health, Prognosis - prevention and treatment of diseases, Health pharmaceutical industry, Health related tourism

[25] http://www.deep-project.eu/deep-project/EN/Home/home_node.html; http://www.deep-er.eu
[26] http://www.montblanc-project.eu

The proposed programme aligns with both of the horizontal priorities, namely ICT and the Environment, while the thematic research areas of CaSToRC targeted within this project align with tourism and agriculture through climate change, since projections of climate change will allow mitigation policies for tourism and in agriculture, Chemistry simulation is applicable to combustion chemistry of biofuels and computational drug design, and can bring competencies for material design. All topics involve an increasingly important simulation component, which makes future and emerging technologies a key enabler for innovation in these fields. As mentioned above, CaSToRC has received significant funding from the regional development fund (structural funds) for establishing its computational infrastructure of regional scale and this project will enhance activities that couple to the S3 priorities leveraging the investments made.

1.3 Concept and approach, quality of the coordination and support measures

1.3.1 Overall concept

The central concept of CoSTAR is to deliver a comprehensive, innovative training and mentoring programme in Computational Science that targets the needs of the junior faculty hired at CaSToRC within the last 2 years in three research areas where HPC plays a central role. Focusing on cross-disciplinary aspects as well as the specific thematic areas of CaSToRC's research portfolio, the programme will strengthen the research areas of these junior faculty members so as to realise the main objective of this call, namely to bridge the scientific performance gap between Cyprus and the rest of Europe. Computational Science is chosen as the overarching area of research because of its relevance to the centre, the catalytic effect of simulation in advancing a broad range of scientific and industrial applications, its relevance to the S3 of Cyprus and its connection to the European-level pursuit of scientific excellence.

The targeted thematic research areas of the Twinning project coincide with the areas of competency of the three junior faculty members, namely: Climate and atmospheric modelling, computational chemical kinetics, and lattice QCD for exascale. The thematic research will be complemented by cross-disciplinary research with emphasis in Future and Emerging Technologies**.** BSC and JUELICH have established expertise in these areas with the teams involved in this project being at the forefront of computational science research. They have strong collaborative links with other European and international institutions that will ensure networking of the faculty at CaSToRC. This project also builds upon existing relationships with these institutions, with an initial collaboration with both Twinning partners already established through PRACE**.** With the Institute of Advanced Simulation, stronger links are established mostly in the area of High Energy Physics/lattice QCD through the activities of the Project Coordinator, but also through the participation of Climate group in the DEEP project. These pre-existing links facilitated the teaming of the three institutions and provided the motivating force for identifying and designing the appropriate training and mentoring activities that are aimed to enhance the scientific and innovation capacity of CaSToRC.

The Twinning partners are also both leading national computational centres that can provide expertise to the technical personnel of CaSToRC, providing training in optimal management of computational resources that can lead to their better utilization for research. They have established exascale labs with pioneering co-design activities in collaboration with HPC vendors. Thus secondments of CaSToRC researchers and technical staff will benefit from the advanced infrastructure provided at the Twinning centers.

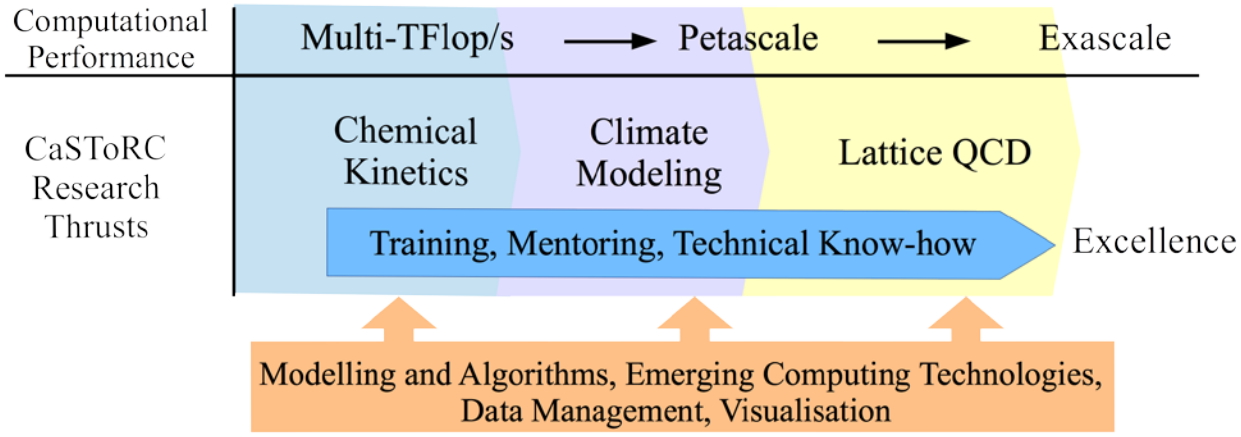

Figure 1.2: Concept of the project showing the research areas to be enabled by the proposed training and mentoring programme, the current state as far as code performance of these research areas and the knowhow that JUELICH and BSC will provide.

The level of adoption and utilization of supercomputers is neither uniform across countries nor across scientific disciplines. The research thrusts in CaSToRC, as shown in Figure 1.2, display non-uniformity in HPC capacity and capability, with scientists in high-energy physics/lattice QCD being the most advanced, followed by climate and atmospheric modelling and computational chemical kinetics. The interdisciplinary nature of the computational science field presents challenges as well as a number of opportunities when designing a training and mentoring programme. Synergies from various thematic areas need to be exploited to create an integrative approach, enabling scientists to develop software and algorithms for effective hardware use in order to achieve excellence in their research. The programme that will be implemented within this project, therefore, necessitates developing training material at all levels of expertise, targeting **academic training and mentoring** but also including, **computational skills building**, **technical** and **innovation** training.

1. Academic training focuses on the needs of faculty and their research teams (currently comprising 16 members). Cross-disciplinary and thematic workshops will be complemented by targeted short-term visits from the Twinning partners and longer-term secondments of CaSToRC researchers to BSC and JUELICH where they will be **mentored by established leaders in their fields**. This aspect is important both in ensuring the effectiveness of the training received in workshops, but also to establish long-term collaborations beyond the end of the project. The cross-disciplinary training will cover topics such as: i) HPC technologies; ii) Mathematical modelling and algorithms, iii) data management and visualization; all of which are relevant to each research theme. In addition mentoring on FET and co-design activities will form part of the programme. The thematic workshops will target the specific competencies of CaSToRC: i) In climate and atmospheric modelling mentoring will be provided to produce a regional air quality model focused on Cyprus, including mineral dust component and online emissions over the Eastern Mediterranean and Middle East region, coupled to a computationally optimised global climate-chemistry model with Lagrangian transport to study intercontinental tracer transport, the effects of teleconnections on pollution and boundary conditions for downscaling and long-term climate change impacts studies; ii) Computational chemical kinetics with training and mentoring on novel algorithms for quantum chemistry calculations that involve large datasets; iii) Lattice QCD for exascale where mentoring on evolving petascale codes to exascale will be provided.

Exascale computing is expected to bring a major breakthrough in these areas enabling simulations that are unthinkable today[27]. Thus this component is crucial for ensuring the long-term competitiveness of the teams.

2. Computational skills building focuses on both foundational and advanced computational skills, complementing the academic training. Foundational training targets researchers who have been trained in traditional scientific disciplines with little or no training in parallel or massive computation.

The advanced training component targets researchers experienced in scientific computing, in extending their skillset to advanced topics in parallel computing and preparing them for the exascale era. Examples include i) programming and performance optimisation of accelerators, ii) parallel I/O, parallel data formats, and visualising large data sets iii) new programming paradigms. An additional component includes training of CaSToRC researchers in delivering the training material developed (i.e. a **training the trainers** programme), thus building the **training capacity** of the centre. To ensure sustainability, an online Supercomputing Training Portal developed through previous project activity in FP7 will be expanded with material from the core and advanced training schools as well as cataloguing dedicated content for each represented discipline. This will maximize the impact of the training, maintaining it for future researchers and enhancing the existing Computational Science doctoral programme at CyI. This computational skills training will include a number of workshops in Cyprus that will aim, besides the capacity building for CaSToRC, in educating scientists outside of CaSToRC.

3. Technical training targets mostly the supercomputing support staff including user support, systems administrators and operations personnel. This element will enhance the quality of CaSToRC services, via training workshops and secondments for implementing best practices and advanced resource and user management at the centre's facilities. This in turn will help researchers better utilize the available resources for their research. In addition, this knowledge will be important for the upcoming upgrade of the CaSToRC main supercomputer, expected to happen midway through this project that will significantly impact research resources. As in the case of the researchers, another pillar of this component is training technical staff to deliver the programme beyond the duration of the project as part of the **training the trainers** programme and the online Supercomputing Training Portal. Thus this particular training programme will: i) Recognise and develop the service role of CaSToRC for other researchers by providing training for the technical personnel at CaSToRC; ii) Develop the HPC user support through dedicated workshops and secondments for the support personnel of CaSToRC as well as establishing a direct line of support with the user support offices at JUELICH and BSC; iii) Train systems administration staff of

[27] see e.g. http://extremecomputing.labworks.org/highenergyphysics/report.stm

CaSToRC within the context of the planned upgrade of the main production machine of CaSToRC; iv) Train technical staff and researchers in the adoption and integration of relevant technologies; v) Provide training for the best practices for managing the computing resources provided by CaSToRC.

4. Innovation Training will be aimed at faculty as well as research and innovation support personnel of the Office of Sponsor Research of CyI. Cyprus lags behind in innovation with an economy that is not founded on research and education and which still mostly relies on low-level technologies. There are a number of reasons for this but most relevant to the project is the reduced understanding regarding the application of computational science in the commercial world. We address this aspect here by providing knowledge transfer on intellectual property (IP) management and enhancements of contacts with stakeholders. This will focus on recognising, protecting and exploiting IP. The Technology Transfer offices of JUELICH and BSC run dedicated lectures for their scientists and have a track record of making knowledge and know-how available to researchers and interested parties in industry. The scientific coordinators of CoSTAR will interface the Technology Transfer offices of JUELICH and BSC to OSR at CyI in order to prepare and deliver a programme of lectures for the researchers at CaSToRC and to train the personnel of OSR. Application of HPC in relevant industries (e.g., in the pharmaceutical industry), as well as, policy recommendations based on the resulting research (e.g., in climate services to better define the regional risks of climate change) and subsequently adaptation measures in the private and public sectors, that may be associated with emerging opportunities for business development will be targeted.

These four elements form the core concept of the training programme proposed in this Twinning project. Opening communication channels among the different scientific domains by promoting computational thinking and by utilizing unprecedented computing capabilities will generate new science and set the state-of-the-art in Computational Research, Innovation and Education. These are not only priorities for the Twinning partners in this proposal but are also recognised European priorities[28].

1.3.2 Approach, Coordination and Support activities

The project is designed to maximize the flow of knowledge and create strong collaborative links between the partners through a coordinated series of training and support actions. The four main components of the training programme detailed above will be implemented through a series of schools, cross-disciplinary and thematic workshops, secondments and mentoring of staff. The project will also fund participation in about 30 conferences to increase the visibility of the research at CaSToRC. These conferences will be selected together with the leaders at the Twinning partners to be the most relevant in the field. A closing workshop will be held in Cyprus to present the results of the project to a wide audience from academia, industry, government agencies and stakeholders to address important issues in HPC and applications of computational science of societal interest.

In Figure 1.2 we underline the overall approach of our methodology, indicating the competencies that will be brought to CaSToRC from the Twinning partners. We show the approach of CoSTAR towards these training and mentoring activities as well as the teams involved (with an indicative scheduling of the events foreseen shown in the Gantt chart in Section 3.1). Academic training will involve secondments to the individual JUELICH Simulation Labs under the Institute of Advanced Simulation (IAS), and the BSC Atmospheric Modelling Group under the Earth Sciences Department, and via thematic workshops. The JUELICH Exascale Labs will be linking all activities and thematic areas under the Future and Emerging Technologies horizontal component. Training in core and advanced computational science topics and technical skills, best practices and know-how will be provided by the BSC Education and Training Team and the JUELICH Application Support Division through cross-disciplinary workshops and schools. The inter-linking of all activities will benefit the CaSToRC faculty, researchers and technical personnel.

Although the schedule and types of training may be adapted either to respond to additional needs or to leverage yet-to-be-scheduled training opportunities arising within the three-year span of the project, we expect that to a large extent the proposed scheduling can be followed. A summary of the types and frequency of the training and mentoring events follows:

[28] see e.g. http://ec.europa.eu/priorities/jobs-growth-investment/plan/what/index_en.htm

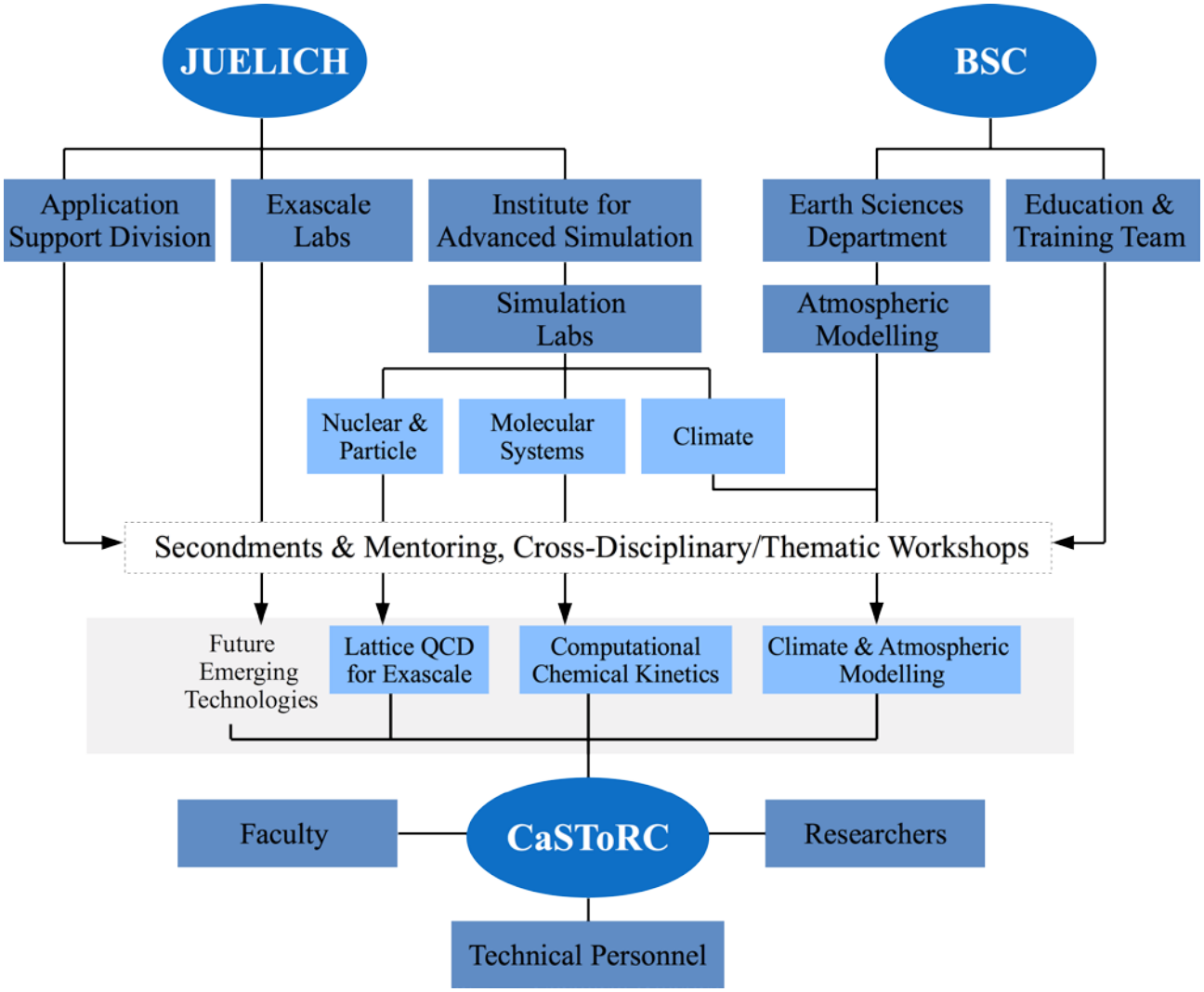

Figure 1.3: Diagram showing an overview of the events detailed in the proposal. Cross-disciplinary training includes an annual school on core computational skills and a series of advanced training workshops attended by all involved researchers of CaSToRC. Thematic workshops and secondments will target specific research groups. Training is also provided to the technical personnel either by targeted training and secondments or by their participation to the annual cross-disciplinary school.

Cross-disciplinary training events.

The interdisciplinary training events include both foundational and advanced HPC skill building aimed at training the researchers and technical personnel of CaSToRC. The main core skill-building event will be a seasonal school, developed in collaboration with the Twinning partners. Advanced HPC training will be in the form of training workshops such as the PRACE Advanced Training Centres[29] (PATC) trainings that are regularly organised by BSC and JUELICH.

Schools on core skills: The core skills school will be held annually with a four-day duration. The first will be held during the initial stages of the project as the initial, common training event and a seed activity for further development. It will train the trainees in the core HPC skills required to succeed in the training programme that will be delivered under the guidance of the Twinning partners. Topics of the core-skills school will introduce attendees to concepts such as:

- **Parallel architectures and programming:** Distributed (MPI) and shared memory (OpenMP)
- **HPC system workflows:** Automation using scripts, job scheduling and monitoring, batch job processing
- **Concepts of code scalability and performance:** Amdahl's law, measuring performance, measuring code scalability

[29] http://www.prace-ri.eu/prace-advanced-training-centres/

The school will be held at CaSToRC with experts from JUELICH and BSC providing lectures and hands-on sessions. It will be open to faculty, postdoctoral fellows and Ph.D. students of CyI but also from other Cypriot institutions. In the second and third iteration of the school, CaSToRC staff will offer many of the sessions, as part of their training in delivering the material so as to sustain the training programme beyond the end of the project. The created content will be gathered and integrated into the online Supercomputing Training Portal.

Training Workshops: Training workshops will be followed by CaSToRC researchers and some of the technical personnel aiming at advancing their skills in a specific advanced HPC topic. These workshops will leverage overlaps with planned training events at JUELICH and BSC, such as PATC training courses held regularly by both centres. Selected training events will be held at CaSToRC when such overlaps will not be possible, in which case they will be open to all Cypriot institutions. The advanced topics that will be covered include:

- **Programming of co-processor accelerators:** GPU programming and optimization including CUDA, OpenCL and OpenACC; Xeon Phi programming and optimization, including vectorisation. These topics will be covered over two to three training workshops.
- **New programming paradigms:** Languages implementing PGAS paradigms including CoArray Fortran and UPC; OmpSs; Architecture-specific models such as TBB, Cilk**.** These topics will be covered in one training workshop.
- **Performance analysis tools and performance modelling:** Tools for measuring code performance and scalability (Scalasca, Periscope); modelling performance of simple computational kernels. These topics can be delivered within one to two training workshops.
- **Parallel I/O and data management:** Parallel I/O file-systems; Scientific data formats; Advanced MPI – I/O topics; Parallel I/O libraries. These topics will be delivered within one to two training workshops.

Researchers and technical personnel will follow these training events on a case-by-case basis, depending on their needs, although we expect that the majority of the researchers will follow all training workshops planned.

Future and Emerging Technologies: Secondments to JUELICH Exascale labs will follow the training workshops. Mentoring on FET and co-design activities will be intensified after the second workshop, in particular, in the area of lattice QCD but also in Climate and Atmospheric modelling. Two secondments related to co-design activities in lattice QCD are planned to the exascale laboratories of JUELICH. In addition, during the last half of the project, the co-design potential of climate and quantum chemistry codes will be explored during the secondments of the relevant researchers to the respective SimLabs. Short-term visits of relevant JUELICH scientists to CaSToRC are also foreseen.

Thematic training events

This set of events covers thematic training of CaSToRC researchers, including secondments to BSC and JUELICH for training and mentoring, as well as attending thematic workshops, which in certain cases will include specialized tutorial sessions. We detail the events by discipline below:

Computational chemical kinetics: The chemical kinetics track will include five secondments to the SimLab "Molecular Systems" at JUELICH. These secondments will be complemented by short-term visits of leading members of the JUELICH group for project coordination to CaSToRC.

Climate and Atmospheric modelling: The Climate and atmospheric modelling track has two components: i) Global climate modelling and ii) Regional atmospheric modelling. An initial workshop will be held at CaSToRC and BSC for each of these tracks respectively attended by all researchers of the domain. Five secondments will follow, two to the IAS Climate SimLab at JUELICH for training and mentoring in global climate modelling and three to the BSC for regional climate modelling.

Lattice QCD for exascale: A workshop will be organised by the Nuclear and Particle Physics Simulation Lab of IAS at JUELICH, which will include lectures and hands-on sessions from the local experts on lattice solver methods. Three secondments to the IAS simulation laboratory will complement the two secondments to the POWER Acceleration and Development Centre, the former for mentoring on solver methods and the latter for performance modelling and prototyping activities on new architectures. A second workshop on lattice QCD algorithms and codes for exascale will be organised at CaSToRC drawing from expertise built during the secondments. The secondments will be complemented by two short-term visits of JUELICH scientists to CaSToRC.

Technical training

Targeted technical training will be provided to CaSToRC operations, user support staff, and systems

administrators. The goal is to equip CaSToRC technical staff with the means to employ advanced user support for Cy-Tera, knowledge of new HPC technologies, and to implement best practices in HPC operations.

HPC operations best practices: The user support staff of CaSToRC will be seconded to the Twinning partners to be mentored on best practices in HPC systems administration, which includes accounts management, resource monitoring, systems maintenance and cyber security. Workshops will also be held for training administrative staff in managing systems of tens of thousands of nodes.

Emerging technologies: HPC systems administrators will, during their secondments to the Twinning partners, be mentored on managing emerging HPC technologies. New computing technologies, innovations in infrastructure such as cooling, power supply and power management will be transferred to CaSToRC staff.

Advanced user support: CaSToRC user support staff will be mentored in assisting researchers in completing requests for computational resources. Such proposals include a technical component, requiring application scaling and performance information. As part of their advanced user support role, the technical staff of CaSToRC will be trained in supporting scientists in obtaining this information from their application codes, as well as offering technical advice on ways to identify optimization opportunities.

Innovation training

The scientific coordinators of CoSTAR will interface with the relevant technology transfer offices at JUELICH and BSC to prepare appropriate training material to be offered to the personnel of the OSR at CyI, as well as, to CaSToRC researchers. The training will target the development of transferable skills training for contact with industry, intellectual property management, efficient project management, proposal writing and quality control, and knowledge transfer and dissemination. The goal is to create at OSR capabilities to help enhance the center's innovation potential and impact.

1.3.3 Linked research and innovation activities

Related competitively funded projects

The potential of this proposal should be taken in the context of some of the previous and on-going national and European funded projects that CaSToRC is or has been engaged in. Programmes that are linked to the activities of this project are the following:

- **The Cy-Tera project (on-going):** The infrastructure project Cy-Tera was one of nine strategic projects funded by the Cyprus Research Promotion Foundation (RPF) and EU structural funds. It created a research facility including a high-performance computing (HPC) infrastructure supporting cutting-edge scientific applications, with associated user support and computational science research and training programmes. The Cy-Tera facility is the first HPC facility at multi-Tflop/s level in Cyprus, serving the needs of the Cyprus Institute (CyI) and its partners for frontier research applications in many fields of great scientific and/or societal importance. The facility is also used by scientists in the EM region establishing it as a research facility of regional scale. It is a hybrid machine of CPUs and GPUs and will provide a platform for code development and optimization for this project. The Project Coordinator of CoSTAR is the Scientific Leader of this project.
- **The PRACE implementation projects (on-going):** CaSToRC represents Cyprus in PRACE and has been participating in the implementation projects. Scientists in the area of lattice QCD have actively participated in the prototyping activities. CaSToRC co-funded small prototype machines used for the development and optimization of linear solvers used in lattice QCD research. Through the CoSTAR activities, and in particular the further development of the Supercomputing Training Portal, CaSToRC aims at establishing a regional PATC to pursue training in HPC technologies and computational science.
- **LinkSCEEM project series (ended 28 Feb. 2015):** These FP7 projects, coordinated by the Project Coordinator of CoSTAR, created an eco-system of computational infrastructure in the EM regional in similar spirit to PRACE albeit at a much smaller scale. CaSToRC contributed 30% of its computational resources to projects coming from scientists in the EM region develop with the main objective to enable scientific research through computation in the region. It also provided user-support and basic training. Climate research was one of the research foci of the project. The climate codes developed in LinkSCEEM as well as the Supercomputing Training Portal it began will be leveraged in the current project.
- **The HPC-LEAP project (on-going)**: The European Joint Doctorate programme funded recently within H2020 recognises the innovation potential of the Ph.D. programme setup at CaSToRC for cross-disciplinary doctoral training in computational sciences. It involves mainly physicists using simulation in their field of study. Lattice

QCD is a dominant component of the project, the maturity of the field signified by the collaboration proposed in this project with the exascale laboratories of JUELICH. There are mutual benefits from synergies between the HPC-LEAP and CoSTAR projects since the graduate fellows will benefit from the interaction and extra training possibilities of the current proposal, while additional scientists can utilize funding from this project to attend training events of HPC-LEAP.

- **The DEEP project (on-going)**: The CaSToRC climate group is participating in this FP7 Exascale project that aims at developing a novel, exascale-enabling supercomputing platform. Climate kernels being benchmarked and optimized in the context of DEEP will be the starting point for codes for the current project.
- **The Clusterware project (on-going)**: This is a project funded by the Research Promotion Foundation of Cyprus under a call to promote connections between academic institutions with industry. The project brings together computational scientists and an industrial company, IBM, to work together to address issues related to the efficient management and usage of distributed clusters of co-processor accelerators, such as general-purpose graphics processing units (GPGPUs). It is coordinated by G. Koutsou.

Synergy with existing research activities and exploitation of research infrastructure

CoSTAR leverages other activities both within CaSToRC but also with the other two research centers of CyI, which are the Energy, Environment and Water Research Center (EEWRC), and the Science and Technology in Archaeology Research Center (STARC).

- CaSToRC has developed the first research HPC facility in Cyprus with the installation of the Cy-Tera machine[30] that allows membership of Cyprus through CaSToRC to PRACE. The training provided by CoSTAR to the technical personnel operating the facility, will crucially influence the quality of services offered to CyI and Cypriot scientists. Equally importantly, it will prepare them for best planning of the upgrade of the machine in the next two years. In addition, CaSToRC deploys several small prototype machines mainly of graphic cards. Within the objectives of the SimLab is to deploy prototype machines, which requires cutting-edge expertise in novel computer architectures. Such expertise is rare in Cyprus and the EM region. Thus the training program of CoSTAR will be crucial in keeping CaSToRC up to date with the rapid development in computer technologies. Such advanced knowhow will enable CaSToRC to introduce new methodologies and computer hardware to the academic environment in Cyprus and to enhance its engagement into the training opportunities that are being created by e.g. the CaSToRC participation in PRACE such as having a regional PATC. Commercial organisations such as SMEs are allowed to use the computational facilities at CaSToRC, given that results are published openly. The uptake of this has been slow as companies could not find regional academic partners to team up with to help them to this endeavor of using HPC to solve their challenges. Building in-house expertise in how to transfer knowhow will allow to approach and support non-academic users.

  Within CaSToRC a ***Simulation Laboratory*** *(*SimLab) has been setup in collaboration with the Jülich Supercomputing Center (JSC) to provide advanced user support and develop HPC software and tools that are crucial for competitive research and innovation, focusing mainly up to now in high energy physics (lattice QCD) applications. In particular, researchers in lattice QCD work closely with those at the SimLab 'Nuclear and Particle Physics' at JSC and DESY-Zeuthen to develop common strategies for software development for the user community. CoSTAR will strengthen the existing activities and expand to other areas coupling to the SimLabs 'Molecular Sytems' and 'Climate' at JUELICH. Given the size of CaSToRC its SimLab is planned to have cross-disciplinary competencies hosting under the same unit the three areas of focus in CoS. CoSTAR will enrich the SimLab cross-disciplinary activities, expand the range of algorithms, applications and specialized expertise that can be offered. This will be a crucial upgrade of the SimLab, in particular, as it takes the necessary steps to prepare for the next generation of supercomputing technologies.

  Recognizing that many research domains already require researchers to interpret and visualize massive amounts of data in an easily comprehensible manner a ***Visualization Laboratory*** **(VisLab)**[31] is setup at CaSToRC led by Th. Christoudias of the CaSToRC Climate and Atmospheric modelling group. Exascale computing will bring new challenges with the vast amount of data that need to be handled. The CoSTAR program will provide expertise and knowledge transfer through visits and workshops and advanced user support enabling CaSToRC to address some of these challenges targeting applications with direct relevance to CyI and Cyprus.

[30] http://cytera.cyi.ac.cy
[31] http://vislab.cyi.ac.cy

CaSToRC has also initiated efforts to adopt emerging computing infrastructures in storage for Big Data and high-volume data processing and curation. ***Data repositories*** have been focused on environmental and climate data that rely on long-term data sets to specify the current and past conditions over geographic regions, as well as on cultural heritage data. An example is the adoption at CyI of Medici[32] as a data management system for data in cultural heritage, which is adopted by the Supercomputing Training Portal of this CoSTAR proposal. The Medici Content Repository System is a web and desktop-enabled content management system that allows users to upload, collate, annotate, and run analytics on a variety of files types. Its design enables to be further developed to hold a variety of data types. It has advanced query functionality that is scalable and enables processing very large amounts of data. Training the technical staff of the CaSToRC will expand their capabilities in providing support to the CyI and other Cypriot scientists in need of these services.

- EEWRC is pursuing research in **Environment** that will benefit from the advanced computational skills of the computational scientists at CaSToRC who will be able to spread it in other areas thus strengthening the research and innovation capacity of the whole institute. In particular, researchers at EEWRC investigate the atmospheric dynamics that influence changes in precipitation and hot weather, and their interdependencies. An air quality monitoring station has been established in Cyprus that samples regional background air, being representative of the Eastern Mediterranean. Scaling of atmospheric chemistry and climate models, using massive parallel HPC, is difficult due to the complex interconnected physical processes. Developing the computational skills of the scientists at CaSToRC in this area will greatly affect their ability to contribute in the EEWRC activities by improving their modelling and better couple them to observational data.

  In addition, the cross-disciplinary competencies that CoSTAR training will bring will impact EEWRC activities of its Energy group that pursues research, adaption, development and testing of concentrated solar power CSP devices primarily for electricity production but also (in co-generation) with desalination of sea water. Modeling and simulation of energy storage devices can result in better design options and computing can enable the investigation of multiple scenarios for desalination and the feasibility of technologies such as carbon nanotube-based membranes for which experiments may be expensive or even impossible to conduct.

- STARC is pursuing activities in Digital cultural heritage and Visualization. The development of realistic animations, the processing of available data and the related visualisation techniques are highly intensive computational processes that require the development of novel algorithms that can effectively harness modern computing architectures. As such they will benefit from the core expertise of the envisioned training programme that involves complex data storage and management and visualization techniques, in particular in relation to the expanded capabilities of the VisLab.

1.3.4 Sex and gender analysis

The PC is an accomplished female scientist with a long-term experience in mentoring women in science. Nevertheless male scientists dominate the field and measures will be taken to encourage women researchers to participate. A number of female trainers has been identified and will be invited to the training programme to provide role models for the researchers. Even though the sex balance at the Twinning partners is also not satisfactory, two well-established women scientists from BSC will be leading the training program (Nia Alexandrov and Maria-Ribera Sancho). The training workshops already include another three women from BSC who will deliver OMPS and COMPS training. The direct involvement of these women will serve to ease the gender gap as well as provide role models. Additional women scientists will be invited as speakers at training events and sessions will be organised within the events of the program to discuss gender related issues and career prospects. The project website will highlight success stories of women scientists. Hiring policies and practices for couples at the participating institutions will be examined and good practices promoted to the administration for consideration.

2 Impact

Background

Academic research and development (R&D) began about two decades ago in Cyprus with the creation of the first University in the country in 1992. Although there has been progress in the percentage of GDP spent on R&D, Cyprus still ranks last among EU countries[33]. As a result many graduates of the three local public universities, which typically attract the best quality of students, find themselves either in jobs that are unconnected to their

[32] http://medici.ncsa.illinois.edu/

[33] Discussion of this topic can be found in the EU Commission's report on Research and Innovation Performance in EU member states (2013): http://goo.gl/IetQ0G .

training, unemployed or forced to leave the country. One reason for the establishment of the Cyprus Institute about ten years ago was, in fact, to increase research prospects in Cyprus. Another ambitious goal was to interconnect the Middle East with Europe by establishing itself as a scientific excellence hub in the Eastern Mediterranean (EM). Of particular relevance to the CoSTAR project is the Computation-based Science and Technology Research Centre (CaSToRC) established to promote computational science in Cyprus and EM in order to keep pace with the advances in the rest of Europe. Since 2012 it operates the largest supercomputer for academic access in the EM region, a hybrid machine of peak performance 33 Tflop/s. Indeed, the regional role of CaSToRC was established through the FP7 infrastructure project Linking Scientific Computing in the Eastern Mediterranean and Europe (LinkSCEEM) providing knowhow and computational resources to the scientists in Cyprus and the EM region. This demonstrates both the potential of CaSToRC to lead as well as and the impact that coordination and support actions can bring in realizing the mission of the centre.

This proposal aims at supporting and advancing the ambitious goal of establishing CaSToRC as a research hub for computational science in Cyprus and the EM region. To ensure maximum local impact, the thematic research areas have been chosen to align with the Smart Specialization Strategy (S3) of Cyprus, thereby helping to establish Cyprus as a knowledge-based economy.

2.1 Expected impacts

For this Twinning call, the work programme defines the expected impacts to be:

- measurable and significant improvement in the overall scientific and innovation capacity of the initiating institution
- positive impacts on the overall research and innovation potential of the Member State or the region

In order to provide measurable quantification of, and track, the expected impacts created by the CoSTAR project, a list of **Key Performance Indicators (KPI)** have been produced. The KPIs incorporate basic scientific research output indices that are applicable to the proposed project and, to the extent possible, indices relevant to the elements of the Composite Indicator of Research Excellence[34] included in the WIDESPREAD Work Programme[35].

In the subsections below, we discuss the various aspects that the impact of this proposal is expected to have and relate them to particular KPIs, providing a final complete list of the KPIs at the end of this section with both their initial values and those expected at the project end.

2.1.1 Raising Scientific and Technical Capacity

Increased research excellence in the specific field

Computational Science research is the core field of research at CaSToRC. The centre has put a lot of emphasis on making highly specialised computer hardware available to researchers (albeit at a relatively small scale by the highest European standards) to enable cutting-edge research in novel HPC technologies and new algorithms. Equal emphasis is given to embedding faculty in an interdisciplinary environment that promotes idea and innovation flow between the various thematic research specialisations in computational science. Adapting to the academic environment in which it finds itself, CaSToRC has selected to cultivate its faculty from junior roles. This project is designed to increase the research capability of these promising young scientists by mentoring and training them within leading groups at the Twinning sites, exposing them to the methods and collaboration networks of the internationally-leading researchers at these sites.

The impact on the research output is expected to be significant both in the specific thematic areas of focus as well as the cross-disciplinary aspects that bridge them. The inherent potential of the junior faculty has already been demonstrated by their past research track-record (see Section 4.1). Embedding them in teams with established leadership in the respective fields will serve to open new horizons and capabilities, greatly enhancing their potential productivity. Of equal importance is their exposure to the strong cross-disciplinary interactions that this project emphasizes. Developing cross-disciplinary thinking is difficult and the envisioned training programme aims to cultivate interactions among the three teams via cross-disciplinary events and secondments. It is envisioned that creating such a cross-disciplinary environment that transcends the traditional boundaries of individual disciplines will have a catalytic effect in generating new science and innovation at the intersections of the scientific domain, computer science and applied mathematics.

[34] http://ec.europa.eu/research/innovation-union/pdf/state-of-the-union/2012/innovation_union_progress_at_country_level_2013.pdf
[35] Available at http://ec.europa.eu/research/participants/portal/doc/call/h2020/common/1635101-part_15_widening_participation_v2.1_en.pdf

The Project Coordinator, active in the field of lattice QCD research is the only senior faculty at CaSToRC, with a group that has already established itself internationally and has strong links with leading collaborations in Europe. Thus this particular field serves both as an example of the present leadership, and showcases the potential success of further expansions in new thematic areas for CaSToRC. Even in the case of lattice QCD, the addition of the junior faculty is crucial and very timely, given the challenges to progress the field to the exascale era. Expertise in novel computer architectures is key to preparing for exascale. The aim is to expand the breadth of the research of this junior faculty in HPC technologies and associated algorithms and network the group with leading HPC industry, made possible by collaboration with the exascale laboratories in JUELICH.
Relevant KPI: Journal publications (peer reviewed), scientific publications in TOP-10 impact factor journals of the field, average h-index of junior faculties, conference publications.

Increased attractiveness of the institution, country and region for internationally excellent and mobile researchers

The Cyprus Institute has already demonstrated its ability to attract foreign staff to Cyprus (comprising more than 20 nationalities as of 12/2014). The English language working environment, attractive research scope of the institute, and Cypriot membership of the EU have proven very attractive to researchers, especially in the early stages of their research careers. The particular thematic areas targeted in this proposal are being led by junior faculty whose publication records and previous research posts serve to highlight their understanding of the necessity of mobility in modern research and the calibre of internationally acknowledged work. They now seek to establish an international reputation for their own research groups emerging at CaSToRC. This project will offer a fertile environment for these young research groups, enabling them to couple to their peers in leading European collaborations. The opportunity and momentum generated by the project will help to create critical mass within the research teams, attracting further talented young scientists and students to join the institute, thereby increasing its research potential.

Networking young researchers with leaders in Europe will have a tremendous impact on their career paths. It is natural to expect that some non-faculty researchers will move back to their home countries or elsewhere to assume higher research positions after a number of years. What this programme of activities seeks to do is to fashion a sustainable mentoring programme built upon the establishment of channels for idea and expertise flow between the Twinning partners and CaSToRC research teams. Under the stewardship of CaSToRC faculty who are the focal point of the initial activities, this mentorship programme will continue between the current and next generations of research groups. In this sense, the international mobility of members of the research group is considered an advantage since established bonds often remain and contribute to the expansion of the international network of the research group. Coupled with the appeal that recognised research excellence gives CaSToRC, such an international network creates a sustainable source of future team members to further the institute's research goals and expand its collaborative opportunities.
Relevant KPI: Researchers engaged (full time equivalent), successful research proposals.

Improved capability to compete successfully for internationally competitive research funding

By leveraging the international contacts of the strong research network of the Director of CaSToRC (and Project Coordinator of CoSTAR), the centre succeeded in gaining competitive funding in high profile infrastructure and coordination projects within FP7 (LinkSCEEM, PRACE, DEEP). This success highlights both the capability of CaSToRC to compete for funds internationally when leadership is in place, and the importance of strong networks in having success.

The expertise that CaSToRC has gained from these projects from an organisational and project management perspective enable it to support its junior faculty in their efforts to obtain research funding. It is the distinct relative advantage that the strong network of collaborators and contacts built by this project gives that can provide the additional weight to their proposals to achieve success in a highly competitive environment. The project explicitly targets such success through support measures for the writing of proposals and the deliverable "Initiatives and opportunities for further funding of research activities" of Work Package (WP) 1.
Relevant KPI: Submitted proposals with Twinning partners, successful research proposals, increased funding secured from submitted proposals.

Linking regional challenges to international excellence

A unique aspect of this project is that it will provide training and support to research activities linked to **climate change and adaptation**, which are scientific challenges of high priority and importance to Cyprus and the wider EM region. This will help to scientifically address regional issues such as air quality, spread of vector borne disease due to climate change, water management and planning for the tourism industry, all of which are crucial societal

and economic issues for Cyprus. The research methodology applied in climate and atmospheric studies has to be of international calibre in order to satisfactorily address these critical issues for the region. The interaction with leading scientists in regional modelling, such as the team at BSC, will enable research of international calibre for addressing the regional challenges (through the seeding of collaborative research in WP6). This will enhance CaSToRC participation in international partnerships and fora (FAIRMODE, AQMEII, HTAP).
Relevant KPI: Collaborative proposals involving institutions in the Eastern Mediterranean. Scientific publications on Climate and Atmospheric modelling results for the EM region.

Improved capability to compete successfully for internationally competitive large-scale HPC Resources

Excellence in computational science requires solid knowledge in current HPC methodologies. Such HPC knowhow is crucial for the development of new algorithms and scalable codes. The channels created by this project for local researchers to access future and emerging technologies will positively impact their **ability to compete effectively for much larger computational resources provided in Europe and in the USA** that are necessary for maintaining competitive research in computational science. This knowhow will in turn be transferred to CaSToRC graduate students and postdoctoral fellows as well as to other young researchers in Cyprus, helping them acquire skills that are in high demand in technologically driven fields relevant for Cyprus and Europe, thereby having positive impact in the job prospects of young scientists and providing them with better opportunities in jobs both locally and at the European level.
Relevant KPI: Successful proposals for HPC resources.

Increased competitiveness of the scientific community helps CaSToRC pursue its regional role

The advanced knowhow and increased research capacity will solidify CaSToRC as leader in computational science in the region enabling the continuation of its front-runner role in the Easter Mediterranean in promoting computational science. This will in turn promote regional collaborations with institutions enhancing further the research capacity. The foundation for such collaboration already exists through contacts with various groups in the region, established with the provision of computational resources on the Cy-Tera facility through the LinkSCEEM-2 project to scientists in the EM region, in the fields of Earth Sciences and Climate Modelling, Chemistry and Materials, Drug Design and Life Sciences[36].
Relevant KPI: Successful research proposals involving institutions in the region.

Increased knowhow of the HPC operations and user support groups helps establish CaSToRC as a leading supercomputing center in Cyprus and the region

The technical training of the systems administrators and user support personnel will bring best practices in the running of supercomputing facilities as well as better prepare for the upgrade of the facility. Given the limited HPC expertise in Cyprus and the region in running such research facilities this project will highly impact the services provided to scientists at CaSToRC, Cyprus and the region
Relevant KPI: Increased number of successful proposals for HPC resources, increased number of publications.

2.1.2 Educational Impact

Ph.D. programme in Computational Science (CoS) at CaSToRC

Excellence in research goes hand in hand with excellence in education, and increases in research quality and capacity will attract and generate better students in the Ph.D. programme in Computational Science of CaSToRC, where students are trained in computational methods. Within this project, students will also have possibilities to interact with international experts from the Twinning sites as well as experts from industry (in particular through the exascale laboratories maintained by JUELICH[37] and the established links of both JUELICH and BSC to HPC vendors). Such highly versed HPC professionals subsequently enter the work force and increase the professional capacity of local stakeholders and the innovative thinking of local enterprises. This supports the long-term goal of the Cyprus government to become a regional hub for research and education, in particular in a technologically-driven field where the region is lagging behind.
Relevant KPI: Increased number of doctoral students.

[36] http://cytera.cyi.ac.cy/index.php/allocations/past-allocations.html
[37] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/Technology/_node.html

Regional Training Role

The further expansion of the Supercomputing Training Portal established at CaSToRC during the LinkSCEEM project will help spread HPC skills and knowhow in the country and even in neighbouring institutions, which collaborate with the Cyprus Institute. Coupling this capability with modern teaching methodologies will strengthen the possibility of the creation of a regional PRACE Advanced Training Centre under the leadership of CaSToRC, providing funding for sustainability and enabling CaSToRC to further pursue its regional role.
Relevant KPI: Submitted proposals involving regional institutions and Twinning partners.

Better exploitation of the European Joint Doctorate Programme in HPC

CaSToRC has demonstrated its potential to attract EU funding for computational science by coordinating a European Joint Doctorate programme in computational sciences (HPC-LEAP)[38]. Many teams involved in HPC-LEAP have the lead scientists coming from the area of lattice QCD research. This demonstrates once more the potential of cultivating leadership at CyI as this project aims to do in areas like computational chemistry, climate and atmospheric modelling, HPC technologies and algorithms. Thus this project will strengthen the educational component provided by HPC-LEAP by bringing complementary expertise to CaSToRC not covered by the programme.
Relevant KPI: Submitted proposals with Twinning partners, new doctoral students.

2.1.3 Impact on the Smart Specialisation Strategy for Cyprus

The applications of the research portfolio of the project align with the Smart Specialization Strategy priorities of Cyprus, in both horizontal areas namely ICT and future emerging technologies (FET) and the Environment (in particular environment and climate change). Computational chemistry relates to pharmaceutical design within the health thematic sector. These applications share common challenges in developing scalable algorithms, and in managing and visualising complex data sets. More specifically the topics within the S3 priorities addressed by this proposal are:

ICT and FET

Capitalizing on the expertise of the lattice QCD researchers at CaSToRC and the already existing collaboration ties of this group with JUELICH in co-design projects, this project will promote closer collaboration aiming in particular to network these CaSToRC scientists with HPC vendors that are involved in the exascale laboratories of JUELICH.[39] This will bring cutting-edge expertise in HPC technologies and new programming models to CaSToRC enabling it to participate in forefront research in exascale computing alongside other leading European centres. In addition, collaboration with JUELICH and BSC will enable extending the range of applications benefiting from co-design efforts to encompass Climate and Atmospheric modelling and chemical kinetics applications. Attaining good performance for these applications on novel architectures will require rethinking some of the computational kernels, a challenging task. This objective couples well to the European efforts in co-design and prototyping activities thus bringing excellent collaboration prospects and increasing the funding opportunities of the centre within FET calls.

Furthermore, when considering the ICT horizontal Smart Specialisation of Cyprus, the LinkSCEEM project has shown that there exists a **regional lack of technical expertise in HPC-related technologies**. HPC is the "Formula 1" of the computing world, with technical expertise in this field holding huge potential economic value. CaSToRC has trained a number of local systems administrators to the level required to efficiently manage its HPC facility. This project seeks to further localise the knowhow and expertise of the Twinning partners in world-leading HPC hardware and software. Further training of such technical personnel in best practices in HPC administration will be crucially impacted by their interaction with experts at JUELICH and BSC (see WP3). Their ability to provide researchers with better facilities will not only enhance the research output of CaSToRC and all users of the CyI facility, but such skills in technologically driven fields will help to cultivate an ICT environment in Cyprus that can be competitive with those offered by other European countries. Furthermore, this provides a solid foundation for the technical requirements that will be necessary for advancements in the other Smart Specialisations of Cyprus, in particular e-Health.
Relevant KPI: Successful proposals for HPC resources, funding secured from submitted proposals.

[38] http://www.cyi.ac.cy/education/programs/hpc-leap.html
[39] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/Technology/_node.html

Climate and Atmospheric modelling

Given the projected increase in temperature in the EM region[40], the decrease in water availability and the resulting health hazards from a changing climate and air pollution, our ability to accurately forecast climate change and air quality in the EM region is of paramount importance. Cyprus is located downwind of arid regions and airborne sand and dust presents serious risks to the environment, property and human health. The implementation of air quality models for research and forecasting will help to improve capacity building to combat air pollution. Therefore, this project, besides improving the research capacity and output in the area of Climate and Atmospheric modelling, which is one of the areas identified in the S3, will also greatly impact the mitigation policies and adaptation measures to be implemented, extending to crucial sectors of the economy like tourism. In addition, the knowhow in data management and new algorithms for visualization can be applied to projects impacting the field of cultural heritage, another S3 priority identified for Cyprus. Such an activity has already started within LinkSCEEM involving one of the three faculty members of CaSToRC involved in this project, who leads the visualization lab.

Relevant KPI: Scientific publications in TOP-10 impact factor journals of the field.

Computational chemical kinetics

The design of new materials and drugs are S3 priorities. This area of research is emerging at CaSToRC, with codes that are intended to progress from the multi-TeraFlop/s to the petascale era. Coupling this effort to leading experts at JUELICH will be crucial for the development of this team. The expected scientific outcomes of the activity focus on the simulation of biofuels combustion, design of new chemical reactions and materials, drug design (of particular relevance to the pharmaceutical industry and an area of economic importance locally).

Relevant KPI: Journal publications (peer reviewed).

2.1.4 Expected Innovation Impact

The interdisciplinary nature of Computational Science can potentially impact a wide range of technology driven applications and catalyse academic and HPC related industry cooperation (see letter of support from NVIDIA and IBM Cyprus). The sectors related to S3 that are the most likely to have the largest impact are ICT, Climate Change and Environment with consequences for Tourism and Health, and Drugs Design. We give indicative examples of specific impacts that might arise in these sectors.

Enhanced Profile of Computational Science

Computation-based science and technology has evolved from a technology crucial to the academic research community to being central in the industrial and commercial world. While the Cypriot economy lags behind in the utilization of HPC (as does most of the EM region with possibly the exception of Israel), there are companies that have activity which is often computation driven. Prominent examples are IBM-Cyprus and Hyperion[41], a Cyprus based engineering consulting company that is globally active in process engineering. Building academic expertise in computational science will support the growth of such highly innovative businesses in Cyprus. Computation-based science and technology is a key competency that countries like Cyprus, which are underperforming in innovation, need to integrate into their research and education system. While there are traditional academic departments in science and engineering in the country, the interdisciplinary nature and utilization of massive computation is missing. The project will enhance this critical knowhow promoting the development of computation-based science and technology in Cyprus.

ICT: The project will potentially greatly impact the information technology component of scientific applications in topics such as development of advanced algorithms for multi-core architectures, co-design activities and energy efficiency, visualization tools for large data sets, digital documentation and semantics. As already mentioned, another important aspect is the training of the technical staff that operates the supercomputing facility of CaSToRC. This expertise will spread to other institutions in Cyprus and the EM region, providing the human resources for maintaining such systems.

Climate and Atmospheric modelling: The project will enable cutting-edge high-skill forecasting of weather and air quality which is important in the EM with pronounced topography and many cities in coastal areas. It will establish a dust forecasting system to serve the needs and requirements of the private and public sectors in Cyprus and the Eastern Mediterranean and Middle East region and link to global pollution pathways to aid in policy formula-

[40] Lelieveld, J., P. Hadjinicolaou, E. Kostopoulou, J. Chenoweth, M. El Maayar, C. Giannakopoulos, C. Hannides, M.A. Lange, M. Tanarhte, E. Tyrlis and E. Xoplaki (2012) Climate change and impacts in the eastern Mediterranean and the Middle East. Clim. Change, doi: 10.1007/s10584-012-0418-4.

[41] http://www.hyperionsystems.net/

tion and risks and impacts assessments. The meteorological service department of Cyprus is supporting the project since it regards the expertise that it will bring beneficial for its activities (see Letter of support).

Drug design: The project will enable efficient molecular simulation on advanced HPC systems applied to complex organic chemistry processes relevant to the design of new materials such as drugs are some areas there can be impacted. Companies, like Medochemie,[42] potentially can benefit from the expertise developed in this proposal (see Letter of support from Medochemie, a local pharmaceutical company).
Relevant KPI: Researchers engaged (full time equivalent).

2.1.5 Key performance indicators

In order to track the impact created by the Twinning project, a list of Key Performance Indicators (KPI) have been produced. Mentioned already in the previous subsections, the KPIs incorporate basic scientific research output indices that are applicable to the proposed project and, to the extent possible, indices relevant to the elements of the Composite Indicator of Research Excellence[43] included in the WIDESPREAD Work Programme.[44] Here we reproduce the complete list of KPIs listed in the above subsections together with their current values and those expected after the project is completed.

This category of KPIs comprises, inter alia, scientific publications, research proposals for grants, prizes, invited talks, etc. This will assess whether the programme will exploit the resources provided in conjunction with the intellectual expertise and collaboration networks foreseen to produce high quality scientific output and secure substantial funding from various funding schemes, including EU Grants, such as ERC or Marie Skłodowska-Curie ITNs and other grants of equivalent magnitude. While allowing performance assessment by the European Commission, the KPIs will also enable CaSToRC to evaluate itself and identify areas for further improvement. The KPIs listed in Table 2.1.a, which will be monitored throughout the project.

Table 2.1.a: Key performance indicator for academic excellence foreseen by the proposed Twinning project. The values concern the last two-year periods before and at the end of the Twinning programme. Proposals and publications include those of the PC.

Key Performance Indicators	Current value over 2013-14	Target value after twinning over 2017-18
Successful research proposals	2	4
Successful proposals for HPC resources[a]	2	4
Submitted proposals with Twinning partners	3	8
Funding secured from submitted proposals	1.2 million euros	>2.0 million euros
Submitted proposals involving institutions from the EM region	4	7
Journal publications (peer reviewed)	29	~ 45
Scientific publications in TOP-10 impact factor journals of the field[b]	18	36
Invited talks of junior staff at international conferences	6	>10
Average h-index[c] **of junior faculty**	6.33	>12
Conference publications	29	~ 45
Total number of doctoral students associated with the junior faculty	1	6-8
Researchers engaged in the targeted fields including Ph.D. students (full time equivalent)	17.5	~ 28

[a] Counting PRACE Tier-0 or equivalent allocations (i.e. in excess of 30 million core-hours);
[b] from the *2013 Journal Citation Reports® Science Edition* (Thomson Reuters, 2014));
[c] over last 5 years, from scopus.com.

[42] http://www.medochemie.com
[43] http://ec.europa.eu/research/innovation-union/pdf/state-of-the-union/2012/innovation_union_progress_at_country_level_2013.pdf
[44] http://ec.europa.eu/research/participants/portal/doc/call/h2020/common/1635101-part_15_widening_participation_v2.1_en.pdf

2.2 Measures to maximise impact

An effective dissemination and communication strategy will be put in place, focusing on traditional dissemination, outreach and communication methods for scientific output, but also exploring innovative methods for education and training communication, knowledge management and exploitation of data.

2.2.1 Dissemination and exploitation of results

The project has created a specific work package, WP2, to engage in all aspects of the dissemination and exploitation strategy. The dissemination strategy employed there will build on traditional measures such as a well-maintained online presence and publications of related results in high-impact scientific journals and international conferences. In addition to this it will engage in a number of more specific initiatives to disseminate the project and maximise the exploitation of the results generated by it.

From a dissemination perspective the strategy includes:

- A **Project website** to disseminate the activities and research outcomes of the project.
- A **Conference attendance programme,** which will support the attendance of CaSToRC researchers at relevant international conferences. The programme intends to support the attendance at ~30 conferences over the project lifetime.
- A **Local awareness programme,** which to generate awareness of the extended scientific capability. This will include public colloquia and permission for the local scientific community to attend workshops organised in Cyprus. Dissemination material tailored to the general public will be produced in the CyI visualisation laboratory and appearances in local TV programs (see videos at www.youtube.com/user/cyprusinstitute), press releases and a well-maintained Internet presence will complement the outreach. Interaction with local schools does already exist and will be intensified. Local schools frequently visit the institute and are offered guided tours by researchers. The visualisation lab is often the highlight of these tours.
- Educational dissemination through the online **Supercomputing Training Portal**. The project will leverage and expand the Supercomputing Training Portal that CaSToRC maintains to incorporate additional material and capabilities. This will be advertised during the Local awareness programme.
- Organisation of a **final project meeting** to be held in Cyprus that will showcase the outcomes of the project to local scientists, and stakeholders as well as relevant policy makers.

From an exploitation perspective, the strategy includes:

- **Integration of modern education techniques and web technologies** in the training and education programme of CaSToRC, leveraging the capabilities of the Supercomputing Training Portal and integrating it into the local educational community
- Through the collaboration with, and training by, the Twinning partners CaSToRC researchers will become more competitive in securing PRACE Tier-0 resources[45] leading to high impact research publications and conference contributions. Furthermore, expertise in future computing technologies will **future-proof their scientific applications** allowing them to maintain an edge when competing for resources on the latest supercomputing infrastructures
- An additional key component will be the **direct link to stakeholders**. Given that JUELICH and BSC are PRACE hosting partners, the scientists will be integrated into existing networks (e.g. PRACE) and new networks will be explored (ETP4HPC, HTAP, FAIRMODE, AQMEII, EuCheMS, EFCE). This explicitly includes local relevant companies like IBM Cyprus and Medochemie.
- Activities such as the **regional networking and training programme** that CaSToRC has already implemented through the LinkSCEEM[46] project to promote HPC in the Eastern Mediterranean region will also be a part of the broader strategy to position CaSToRC as a regional leader in HPC training.

2.2.2 Communication Strategy

CaSToRC already communicates its activities through well-established channels. The Cyprus Institute has a communication unit that supports this work. Media outlets are targeted through a contracted media agency and social media are engaged. The CaSToRC visualisation lab also maintains a website[47] and social media channels (YouTube, Vimeo, Facebook, Google+) for easy access to the latest visualisations by the general public. The

[45] http://www.prace-ri.eu/prace-resources
[46] Linking Scientific Computing in Europe and the Eastern Mediterranean coordinated by CaSToRC (www.linksceem.eu/ls2/).
[47] http://vislab.cyi.ac.cy

training programme will reinforce existing research with direct impact on public health and safety, such as the regional atmospheric modelling component. Public media regularly quote research conducted at CyI that impact public health, and this Twinning project will help strengthen this presence.

More importantly, The Cyprus Institute keeps open channels to government agencies and the government itself. A prime example is the Meteorological Department, which uses the CyI computational infrastructure for weather prediction. These links are essential, especially in a small country like Cyprus without a strong research and innovation tradition. The Institute's vision and mission is continuously broadcasted along these channels jointly with success stories to ensure the vital political backing. The results generated by the project will be promoted through these media, explaining to the general public the societal impact that they may have. CaSToRC scientists and visitors from the twinning sites will be assisted in giving Public talks and interviews to communicate research results.

2.2.3 Knowledge management and innovation

The overall innovation strategy of the Cyprus Institute is currently being developed jointly with Isis Innovation[48] the knowledge management agency of the University of Oxford as part of an initiative of the government of Cyprus. CoSTAR will enable the next step and implement the innovation strategy with a special focus on HPC related technologies. The Office of Sponsored Research (OSR) at CyI will work closely with the Innovation offices at JUELICH and BSC to set the appropriate mechanisms for the best utilization of the generated knowledge and results in all CaSToRC computational science domains (see WP2). Links with HPC vendors and software companies in Europe and the region will be pursued and collaboration in ICT and FET will be promoted.

Identifying and securing intellectual property is not yet part of the wider scientific culture in Cyprus. Unlocking the innovation potential will require a dedicated support structure that sensitizes researchers towards creating and identifying innovation opportunities and also supports the research centre on the path towards innovation. This will be promoted by special training of the researchers leveraging the experience of innovation officers at JUELICH and BSC. The OSR personnel at the Cyprus Institute will need to adapt best practices from the Twinning partners to the Cypriot environment in order to pursue opportunities in Cyprus in addition to those on the European scale. The two scientific coordinators of the project (one of which is local, one shared between the Twinning partners) will act as bridge contact between the officers at the OSR and innovation officers at the Twinning sites in order to implement a localised innovation strategy.

Below we give a list of potential innovation activities:

Education in IP and knowledge management: The two scientific coordinators will organise training specifically targeting research scientists and the other scientific coordinators at CyI. The training will directly target faculty and also include a screening of existing potential IP. The Twinning partners will perform this IP assessment jointly with the OSR to enable full knowledge transfer. This targeted training will be complemented with more general workshop sessions hence educating researchers at all levels. This will include also material available from the European Patent Academy[49] and similar organisations. The innovation training will help scientists to identify innovation and cultivate dedicated activity.

Understanding the private sector: There is a "cultural gap" between the academic and private sectors. A better understanding of the objectives of either side will help to successfully transfer knowledge and innovation. Strong connections to relevant industry representation groups will help build this understanding. On a European scale, JUELICH and BSC have enormous experience and will network the scientists with the relevant European commercial partners such as the NVIDIA EU branch, EUROTECH, IBM etc. Locally CyI has developed links to local alliances, such as IBM Cyprus, the Cyprus Chamber of Commerce and Industry[50] (CCCI) and the Cyprus Employers and Industrialist Federation (OEB).

2.2.4 Data exploitation

Research activity in computational science towards exascale is generating a deluge of data. This is expected to increase significantly with the advancement of computational power and available resources. CaSToRC has already established limited expertise in the design of cutting edge content management systems that can deal with Big Data

[48] http://www.isis-innovation.com/
[49] http://www.epo.org/about-us/office/academy.html
[50] http://en.oeb.org.cy/, http://www.ccci.org.cy/

and Big Data analytics. One example is the MEDICI content management system that was recently adapted to the data specific to cultural heritage and being used to manage the content of the Supercomputing Training Portal.[51]

Given the expertise of BSC and JUELICH in Big Data, CaSToRC will gain tremendous knowhow in the design of the appropriate storage and data management solutions to fit the needs of both CaSToRC scientists but also the wider user base of its facilities, thus impacting the broader scientific community in Cyprus (see WP5). This will also include the joining of federated community databases that might be of interest to specific research activities. CaSToRC believes strongly in and advocates open access. All scientists involved in the project will make codes and research data available, unless specific agreements with companies call for confidentiality during the development phase.

The same philosophy holds for publications. This is already standard in communities such as High Energy Physics and is being followed by the scientists at CaSToRC. The Supercomputing Training Portal will be publicly available to form a primary education dissemination channel (see WP4). In addition the "Computational Science Skills" training programme will be maintained and continue to be delivered by CaSToRC beyond the lifetime of the project, as both a project legacy and as the springboard for integrating additional educational methodologies in CaSToRC. This programme is something that could form a core aspect of any future regional PRACE Advanced Training Centre (PATC), and CaSToRC would be a prime candidate to assume leadership of such a centre.

3 Implementation

The coordination of the project will be undertaken by the Project Coordinator (PC) with the assistance of two scientific coordinators who together will comprise the Project Management Office (PMO) at CaSToRC. The PC is experienced in managing large EU projects including coordination and support project such as LinkSCEEM. She is also experienced with managing computational science research and education, having overseen the creation and development of CaSToRC. She will oversee the implementation of the training programme, coordinate with the research teams to access progress and in particular to meeting the performance indicators, identify weakness and gaps, and propose corrective actions. She will also seek complementary supportive actions and opportunities outside the CoSTAR project.

A simple but effective management structure is adopted to best implement the activities of the project keeping the cost of the management low (12% of total budget). The project will engage two scientific and management coordinators. The support activities of the scientific coordinators will be optimised by having one coordinator based at CaSToRC and the second one interfacing between the two Twinning partners. This will allow constant contact between the scientific coordinators with the research teams and technical personnel at CaSToRC and at the Twinning partners. These two coordinators will track the day-to-day implementation of the project, assist the scientists and technical personnel in their planning, gather the training material and maintain the online Supercomputing Training Portal. In particular the scientific coordinators will help identify trainers, help organise the schools and workshops and provide information to trainers on training needs. Measures to ensure the quality of the training programme delivered will consist of: i) a constant tracking of the training quality of the schools and workshops and their outcome as far as knowledge transfer and integration; ii) adaptation and expansion of aspects of the training programme to the needs of the CaSToRC teams; iii) assessment and suggestions for improvements of the content of the online Supercomputing Training Portal to more effectively support the training programme; iv) interface of the scientific coordinators with the Technology Transfer offices for gaining know-how and expertise and transferring it to CaSToRC researchers and OSR.

PMO will also be in constant contact with the scientific groups to monitor progress and suggest adjustments of the mentoring programme, if needed, according to the evolution of the research areas during the lifetime of the project. Identification of collaborative lines of research between CaSToRC and the Twinning partners will be promoted by regular teleconferences of the PC with the leaders of the research teams at JUELICH and BSC in coordination with the research teams at CaSToRC.

PMO will also assess the training of the technical personnel of CaSToRC provided by CoSTAR and monitor the impact on the support provided to scientists for accessing new computers e.g. within PRACE. Furthermore, PMO will monitor the identification and implementation by the technical personnel, based on the size of CaSToRC, particular aspects from the partner infrastructures that are both achievable with the available human resources and provide the highest possible impact for the researchers that use CaSToRC HPC resources. Finally PMO will liaise with the Twinning partners to facilitate (remote) access for CaSToRC to the bleeding-edge training events provided by them.

[51] http://www.linksceem.eu/ls2/developed-codes-software/medici.html

PMO will put emphasis on the identification of funding opportunities; identification of access calls for computational resources; identification of new software and hardware technologies and changing trends in HPC; and interfacing with PRACE for the development of a regional Advanced Training Centre for HPC technologies (PATC); support for proposal writing; organisation of lectures on knowledge transfer in IP management and innovation; identification of gender issues and organisation of special sessions to promote women scientists.

3.1 Work plan – Work packages, deliverables and milestones

Detailed descriptions of the work packages and deliverables are given in Table 3.1.a-c. The project implementation will be carried out within six work packages (WP) as illustrated in Figure 3.1: a coordination WP, a dissemination WP, and four WPs that will implement the training, mentoring and secondment programmes. A brief description follows with more details given in Section 3.2.1.

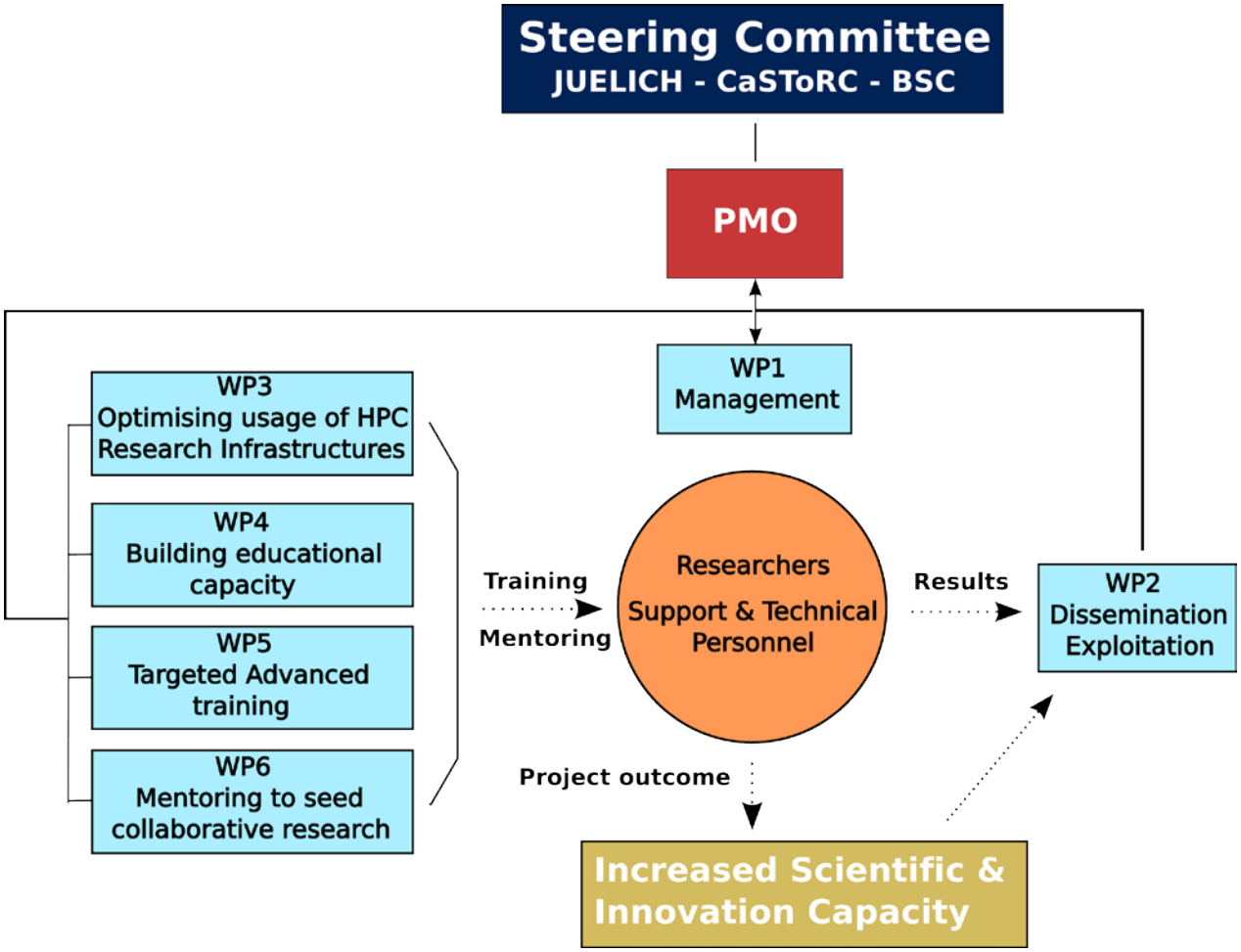

Figure 3.1: Organisational structure of the project.

Management and coordination (WP1): The management of the project will be assumed by the project management office (PMO) setup at CaSToRC chaired by the PC with the participation of two scientific coordinators, one based at CaSToRC and one based at the two Twinning sites. The PMO will have the responsibility of implementing the training and mentoring programme, promote the dissemination activities and monitor the research teams and their scientific progress. A steering committee (SC) will be setup consisting of representatives from each partner. The SC will be the governing and decision making body of the programme.

Dissemination and exploitation (WP2): The PMO will promote dissemination and outreach activities of the project, aimed at local, regional and international forums, as well as, raise the profile of the local researchers and, consequently, of CaSToRC internationally. It will also promote knowledge transfer from the Twinning partners in exploitation of research outcome. A range of approaches will be implemented, including presentation of the researchers' work at international conferences, innovative use of social media platforms, and presentations to key local government agencies and policy makers. A closing workshop will be organized towards the end of the project

to highlight the scientific results of the project and disseminate the outcomes to the stakeholders.

Optimising usage of HPC research infrastructure (WP3): This work package will implement a series of training workshops and secondments targeting the HPC support and operations staff of CaSToRC. It will expose the technical staff to the best practices and procedures followed by their colleagues at BSC and JUELICH. Furthermore, the HPC operations staff will be trained in upcoming HPC systems and infrastructure technologies, such as new computing and network devices, novel cooling technologies, and approaches for advanced power management.

Building educational capacity (WP4): The goal of this work package is two-fold. Firstly, it will develop and implement a "Computational Science Skills" training programme, with the objective of educating researchers and technical staff in core, cross-thematic computational science skills. Secondly, this work package will oversee educating a target set of research and technical CaSToRC staff to deliver this programme, both within the project timeline and beyond the duration of the project. This task will also include populating an online Supercomputing Training Portal with the content developed within the "Computational Science Skills" programme, as well as complementing it with training material from WP5 and WP6.

Targeted advanced training (WP5): This task will organise and oversee the training of CaSToRC researchers in advanced cross-disciplinary HPC topics, as well as thematic training workshops. The first goal is to advance the HPC skills of the researchers at CaSToRC in programming and optimising their applications through courses in programming of novel computer architectures such as GPUs and Intel Xeon Phis, parallel I/O and management of large datasets, and performance analysis and parallel debugging tools. The second goal is to train CaSToRC researchers in state-of-the-art algorithms and computational methods of their scientific field, through topical training workshops given by the collaborating research groups at BSC and JUELICH.

Mentoring to seed collaborative research (WP6): The mentoring of the CaSToRC faculty and their teams will involve longer visits to the research teams at BSC and JUELICH. For the duration of the secondments, CaSToRC researchers will be embedded in the corresponding BSC and JUELICH research groups, and will be mentored in the topics of novel computing architectures, chemical kinetics, regional and global climate modelling, and lattice QCD algorithms for exascale. The mentoring will be on-going with the groups at CaSToRC and at the Twinning partners being in constant contact remotely. Regular discussions will take place to assess progress. This activity is considered central for the success of the programme since mentoring aims to seed research collaboration activities that will extend beyond the end of the Twinning project.

The scheduling of events foreseen in WP3 to WP6, including schools, thematic and cross-disciplinary training workshops, and secondments is given in detail in the Gantt chart of Table 3.1.d.

Table 3.1.a: Work package description

Work package number	1	**Start Date or Starting Event**			Month 1		
Work package title	Management and coordination						
Participant number	1	2	3				
Short name of participant	CaSToRC	JUELICH	BSC				
Person/months per participant:	10	4	4				

Objectives

- To ensure an effective and timely implementation of the programme by coordinating the activities of all participants, including the reporting and financial management of the network.
- To evaluate the impact of each of the project activities and, when necessary, define and implement corrective action.
- To work towards long-term sustainability of activities enabled by the project.

Description of work

The Steering Committee (SC) will be the governing and decision making body of the programme. It will comprise from representatives from the three partners chaired by the Project Coordinator. All decisions will be taken by simple majority of present participants on an equal basis.

A Project Management Office (PMO) will be setup consisting of the Project Coordinator and two scientific coordinators, one based at CaSToRC and one shared between the Twinning sites. PMO will be responsible for coordinating the day-to-day activities of the programme including administrative and financial matters, as well as communication among the Twinning partners. The scientific coordinators will work closely together to evaluate

and optimise the training events as well as monitor the scientific secondment programme and dissemination activities.

A continuous assessment of the activities will be a main focus of WP1 aiming at devising corrective actions to optimally exploit the training opportunities and research potential.

An equally important component is the development and sustainability of research collaborations beyond the project. In this regard, research topics for long term collaboration will be identified by the scientists in charge early on in the project and resources for their implementation will be sought well ahead of the end of the project through, e.g., collaborative proposals to funding agencies, internal possibilities of funding etc. This WP will assist in organisational aspects of such opportunities, as well as provide assistance for proposal writing.

The main tasks of the work package will be:

Task 1.1: Steering and coordination of the project activities (CaSToRC, JUELICH, BSC**)**
The PMO will be responsible for coordinating the overall project activities and fulfil the administrative requirements. This includes administrative and financial matters, as well as communication among the twinning partners. PMO will evaluate and optimise the training events from an organisational perspective, working towards an efficient framework for event planning and implementation. Scientific coordinators will assist in monitoring event quality and impact as well as monitoring the progress of the scientific secondment programme.

Task 1.2: Submission of publication list of CaSToRC researchers involved in the CoSTAR proposal (CaSToRC)
List of publications in the computational science research areas of CaSToRC during the three years preceding the start date of the project.

Task 1.3: Communication among partners (CaSToRC, JUELICH, BSC**)**
Setting up teleconferences, face-to-face meetings and other communication activities as needed.

Task 1.4: Management of project resources (CaSToRC)
Managing and monitoring all project resources, including event and personnel resources as well as overall financial management.

Task 1.5: Event support (CaSToRC, JUELICH, BSC**)**
Support all other work packages in the organisation of training events, secondments as well as dissemination and outreach activities. This includes event logistics, coordination of travel, and overall budget management for each project activity.

Task 1.6: Reporting to and communication with the EC (CaSToRC)
Submission of deliverables of all WPs, after internal review, in addition to all periodic reports, financial reports, the final report and any other necessary information to the EC.

Task 1.7: Project monitoring (CaSToRC, JUELICH, BSC**)**
Monitor project activities, evaluate their effectiveness and devise any necessary corrective measures. PMO will be responsible for assessing effectiveness of activities and defining corrective actions in consultation with the Steering Committee with implementation through PMO.

Task 1.8: Support actions for securing resources for long term research collaboration (CaSToRC, JUELICH, BSC**)**
Source possible funding opportunities for collaborations derived from the project and assist them in proposal preparation.

Deliverables
D1.1: One-page statement on the completion of the task 1.2 (M2).
D1.2: Midterm project report (M18)
D1.3: Report on initiatives and opportunities for future funding of research activities (M30)
D1.4: Final project report including mentoring outcomes as per KPIs (M36)

Work package number	2	**Start Date or Starting Event**		Month 4		
Work package title	Dissemination and exploitation					
Participant number	1	2	3				
Short name of participant	CaSToRC	JUELICH	BSC				
Person/months per participant:	5	3	2				

Objectives

One of the overall goals of both the Call and the project is to increase the impact and potential of research in Cyprus and raise the research profile of CaSToRC. This work package is responsible for a dissemination and exploitation programme to highlight the activities of the programme both internationally and in particular within the local research community.

From a dissemination perspective, the work package will engage in:

1. Supporting participation of CaSToRC researchers in targeted international conferences and workshops.
2. Communication and public engagement through presentations at other institutions including local and other European research institutes, government agencies and public events.
3. Local outreach activities (such as a webpage for the project, a yearly open day for local stakeholders and policy makers, visits from high schools).

Organisation of a closing workshop in the last six months of the project in Cyprus, including an open day to highlight the achievements of the project and to disseminate the outcomes to stakeholders and relevant government agencies. We will seek participation from the academia and industry to address important issues in HPC and computational applications of societal impact.

From an exploitation perspective, the work package will engage in:

1. Exploitation of the research results enabled by the project through their publication in high-impact journals.
2. Leveraging the training content and expertise generated by the project to position CaSToRC as a regional leader in advanced HPC training.
3. Utilise the online Supercomputing Training Portal as a fully featured training platform for incoming research staff at CaSToRC.
4. Leverage the content integrated in the portal to encourage the incorporation of the portal in local and regional University courses.
5. Training on intellectual property rights and knowledge transfer from academia to the industrial.

Description of work

Task 2.1: Project website (CaSToRC)

A project webpage to disseminate the activities and research outcomes of the project.

Task 2.2: Conference attendance programme (CaSToRC, JUELICH, BSC**)**

Faculty, in coordination with the leaders of the research teams at the Twinning partners, will identify the most appropriate conferences for CaSToRC researchers. The project will provide funding for attending up to 30 conferences and it is expected that faculty will be regularly attending major conferences. Other members of the research teams will also be encourage to participate in international events. It is expected that Ph.D. students and postdoctoral fellows of the teams will be participate at least once during the duration of the project

Task 2.3: Dissemination and awareness (CaSToRC, JUELICH, BSC**)**

Local dissemination of the project to generate awareness of the extended scientific capability. This will include public colloquia and opening workshops organised in Cyprus to the local scientific community.

Implementation of an outreach programme to target the general public, stakeholders and policy makers in Cyprus to promote research awareness.

Organisation of a closing workshop in Cyprus during the last six months the will include an open day. The event will highlight the achievements of the project targeting participation from academia, local stakeholders, government agencies and industry.

Task 2.4: Enabled research exploitation (CaSToRC)

Dissemination of research results enabled by project activities will be pursued through high-impact open access journals. In addition, the overall research enabled over the project lifetime will form part of the programme for the open-day of the final closing workshop targeting a wide audience from academia, government agencies and industry.

Task 2.5: Exploiting advanced training potential (CaSToRC, JUELICH**)**

Within the project, there will be significant development of advanced training capabilities at CaSToRC. This will come in terms of trained personnel at CaSToRC, the training content developed by the project and the capabilities of the supercomputing training portal used by the project.

Internally, this potential will be used by CaSToRC to train incoming researchers. In addition, it will be used as an outreach platform targeting local universities, encouraging them to utilise these capabilities in relevant lectures and providing support as necessary.

Task 2.6 Innovation workshop (CaSToRC, JUELICH, BSC**)**
Coordination with the relevant Technology Transfer offices of JUELICH and BSC to introduce scientists at CaSToRC to the intellectual property rights, the innovation process and how to network them with the industrial sector focussing on companies where HPC-related hardware and application technology is most relevant.

Deliverables
D2.1: Project webpage (M2)
D2.2: Interim report on dissemination and exploitation (M18)
D2.3: Report on dissemination and outreach activities (M36)

Work package number	3	**Start Date or Starting Event**			Month 6	
Work package title	Optimising usage of HPC research infrastructure					
Participant number	1	2	3			
Short name of participant	CaSToRC	JUELICH	BSC			
Person/months per participant:	4	4	4			

Objectives
Advanced technologies underpin the "laboratory" of computational scientists. This work package is to ensure that the HPC facilities at CaSToRC are optimised for the scientific community they serve, from both a hardware and software perspective. This includes aspects such as network optimisation, large data capabilities, facility management, software availability, resource monitoring, etc.

This work package will foster communication and collaboration between the technical and support teams of the consortium through the organisation of yearly best practices workshops for these teams. This will expose each team to the particular tools and advances of other teams. In addition, it will provide the platform for a secondment programme of CaSToRC staff to other centres to allow them to integrate new tools and workflows.

The specific objectives of the work package are:

1. Sharing of best practices regarding system operation, optimisation, monitoring and control.
2. Training of CaSToRC technical staff in emerging HPC technologies and tools relevant to the research portfolio of the centre.
3. Implementation of a programme to assist researchers in the preparation of the technical components of HPC resource request proposals at national and European levels.

The final point above stems from the fact that typical application processes for HPC resources involve a technical as well as a scientific review. As the support teams at JUELICH and BSC typically act as technical reviewers in such cases, they are in a strong position to assist in the creation of a programme that will ensure applicants meet all technical requirements of resource request proposals.

Description of work

Task 3.1: Best practices workshop (CaSToRC**, JUELICH,** BSC**)**
An annual workshop for administrators and user support will be carried out to highlight particular aspects of the workflow, tools and technologies of each of the teams. The workshops will rotate across the three sites with the initial workshop to be carried out in Cyprus. The workshops will cover both general and thematic topics. A candidate for a thematic topic would be "Big Data and HPC", while general topics will include best practices in user account management, resource management and reporting, and system administration and maintenance. The programme will be coordinated such that all content will have a potential impact on the facilities and services of CaSToRC.

Task 3.2: Technical secondment programme (CaSToRC, JUELICH, BSC**)**
The workshops of Task 3.1 will provide an opportunity for CaSToRC technical staff to be exposed to the cutting-edge tools and concepts being implemented at JUELICH and BSC. From these workshops, CaSToRC staff will identify tools or technologies that they expect will improve the performance of the services or facilities of CaSToRC. The secondment programme under this task will provide CaSToRC staff with the opportunity to train on-site, at the Twinning partners, to learn more about their tools of choice and begin the process of implementing these at CaSToRC. A total of 6 secondments, one week in duration, are foreseen over the project lifetime.

Task 3.3: Technical review support (CaSToRC, JUELICH, BSC**)**
Together with the Twinning partners, CaSToRC will define a set of guidelines for completing the technical parts of requests for HPC resources (in particular focussing on the PRACE proposal process, in which both JUELICH and BSC are hosting sites). CaSToRC will then work with researchers applying for such resources to ensure that, from a technical perspective, their proposal meets the standards expected in such calls.

Deliverables

D3.1: Midterm report on optimising research infrastructures (M18)
D3.2: Final report on optimising research infrastructures (M36)

Work package number	4	**Start Date or Starting Event**			Month 1		
Work package title	Building educational capacity						
Participant number	1	2	3				
Short name of participant	CaSToRC	JUELICH	BSC				
Person/months per participant:	8	4	9				

Objectives

CaSToRC seeks to deliver the highest quality training to local as well as regional researchers who use its resources, just as its Twinning partners do. It must, however, operate within the limitations of its relative size. With this in mind, this work package seeks to leverage, adapt and integrate emerging education material and techniques (such as mixed-mode lecturing and flipped classrooms) to provide a complete spectrum of HPC learning to its user community. Coupling this with modern web technologies in innovative ways will allow CaSToRC to position itself as regional leader in the advanced training of HPC capabilities.

The specific objectives are:

1. Train members of CaSToRC research and support teams in delivering HPC related training material, for both intensive workshops and regular classes.
2. Develop a "Computational Science Skills" training programme that CaSToRC will provide to both internal and external computational scientists using CaSToRC facilities.
3. Deliver the "Computational Science Skills" training programme annually, firstly to train Ph.D. students and postdoctoral fellows of the consortium on core computational skills, and secondly to build the training expertise of CaSToRC staff.
4. Integrate modern web technologies in the training programme of CaSToRC, in particular to leverage the educational opportunities provided by mixed-mode and flipped-classroom lecturing methodologies.
5. Populate the online Supercomputing Training Portal used by CaSToRC with the training material generated within the project.

Description of work

Given the objectives of the work package, the tasks described here work towards the goal of creating a core set of standardised training material that covers the basic skillsets typically required of a computational scientist to effectively use HPC resources. It is also part of this task to deliver this material to CaSToRC researchers, such that they build the core computational skills required to move on to the more advanced, targeted HPC training.

HPC is of course a very dynamic subject and the novelty of the technologies it uses means one can never cover the entire spectrum of potential subject matter with standardised content. For this reason the work package also seeks to integrate appropriate technologies into the training methodologies of CaSToRC such that the target community of CaSToRC can also benefit a mixed-mode or flipped classroom lecture model together with the Twinning partners. Particular use cases for this approach would be with respect to future and emerging technologies as well as discipline-specific content such as community-developed applications.

Task 4.1: **Design of a "Computational Science Skills" training programme** (CaSToRC, JUELICH, **BSC**)
This task will be in collaboration between all partners, led by BSC, to identify the scope of the proposed training programme. This will be done using the Delphi technique to evaluate the appropriate scope within the restrictions of the foreseen 4-day workshop. It is expected to include topics such as:

- Automating tasks using the POSIX shell
- Structured programming
- Version control
- Data management
- HPC architectures
- Resource management and queuing systems

Such a list of topics would extend the existing 2-day programme of the Software Carpentry Foundation[52] for scientific computing with additional topics that are seen as essential in the specific environment of HPC. Where necessary, appropriate software solutions will be selected to serve as examples of the concepts that the programme wishes to convey.

Task 4.2: **Training the trainers** (**CaSToRC**)
Through the LinkSCEEM[53] project, both CaSToRC and JUELICH have had very positive interactions with the Software Carpentry Foundation. There is significant overlap between the goals of this WP and the efforts of Software Carpentry, which is a well-established volunteer organisation that seeks to make scientists more productive, and their work more reliable, by teaching them basic computing skills.

Software Carpentry offers a training course that teaches scientists how to teach other scientists how to programme. This course covers the basics of educational psychology and instructional design, and looks at how to use these ideas in both intensive workshops and regular classes. This task will oversee the training of a set of target instructors at CaSToRC via the Software Carpentry, and more precisely via the "Software Carpentry" instructor training course. The target instructors will be drawn from both the technical and research staff of CaSToRC. The goal will be to enable this staff to deliver the "Computational Science Skills" training course beyond the duration of this project.

Task 4.3: **Standardising the computing environment for training material** (CaSToRC, **JUELICH**)
Many computing centres provide the computing environment, and even the applications used by the majority of users, through environment modules. Tools such as EasyBuild[54] allow centres to collaborate on the HPC software build and installation procedure for these tools, providing a standardised and potentially vast module environment.

The standardised environment that EasyBuild provides can be leveraged to create a common platform for the creation of practical content for training material. This task will integrate the software requirements of Task 4.1 into EasyBuild such that no modification of training material is required when moving between HPC training systems. The expertise to achieve this already exists within the collaborations as EasyBuild is being used by both JUELICH and CaSToRC on their production systems.

[52] http://software-carpentry.org/
[53] http://www.linksceem.eu/ls2/
[54] http://easybuild.readthedocs.org/

Task 4.4: Creation of content for the "Computational Science Skills" training programme (**CaSToRC**, BSC, JUELICH)
The collaborative workflow of Software Carpentry will be leveraged in the creation of the additional lessons required for the "Computational Science Skills" training programme. Practical content will be created in the framework provided by Task 4.3.

Training content will be created in a collaborative manner between Twinning partners and will leverage the existing expertise available at each site. The content will be iteratively improved over the project lifetime as the programme is implemented. The task will be driven by CaSToRC, with all partners contributing, in particular BSC with their advanced education programme.

Task 4.5: Delivery of the "Computational Science Skills" training programme (**CaSToRC**, BSC, JUELICH)
Once the initial training programme design and software environment is in place, the consortium will work towards the first implementation of the programme in Cyprus. Instructors from all three partners will contribute to this event. The programme will then be delivered each year increasing the participation of CaSToRC instructors, for all new users of CaSToRC HPC facilities.

Task 4.6: **Content integration in Supercomputing Training Portal** (CaSToRC, **JUELICH**)
The previous tasks create a framework through which basic training can be sustainably provided within the region. This task addresses the issue of material that goes beyond the introductory. Given the potentially large number of specialised, advanced HPC workshops that computational scientists can benefit from, delivering this type of material on a regular basis is an expensive prospect since high quality trainers with the necessary knowledge will need to be flown in to a particular location and the trainees also have to reach that location. Many regional institutions do not have travel budgets for such activities so attendance to any such event is likely to be highly localised.

Online training is by necessity an important component of any training programme in the region, especially in mitigating costs and certain impracticalities involved in organising regional schools. For basic, but in particular advanced, training researchers need to be provided with adequate means for self-learning. The Supercomputing Training Portal[55] developed within LinkSCEEM provides such capabilities and includes an in-browser connection to HPC resources for the purposes of carrying out practical training components.

In this task, material generated during the training events over all work packages of this project will be integrated into the Portal. In addition, further capabilities will be added to the Portal as required in order to adequately service the needs of the CaSToRC research community.

Deliverables
D4.1: Report on "Computational Science Skills" training programme (M9)
D4.2: Software configuration application to provide the standardised computing environment required by Task 4.1 (M8)
D4.3: Report on training content creation and integration (M24)
D4.4: Final report on the development of advanced training capabilities (M36)

Work package number	5	**Start Date or Starting Event**		Month 6			
Work package title	Targeted advanced training						
Participant number	1	2	3				
Short name of participant	CaSToRC	JUELICH	BSC				
Person/months per participant:	3	8	7				

Objectives

To be on the cutting edge of computational science, researchers must be both aware of, and be able to effectively utilise, the advanced computing technologies that underpin the field. The technologies that are likely to bring us to exascale will require expertise in areas such as:

1. Vectorisation
2. Performance analysis and improvement of application codes
3. I/O performance and methods at large scale

[55] http://supercomputing.CaSToRC.ac.cy/

4. Accelerator programming

Furthermore, currently used algorithms and models will need to be rethought and adapted for the increased parallelisation and new storage and memory hierarchies, which will necessarily arise to achieve exascale. The objective of this work package is to provide CaSToRC researchers with targeted training in the advanced HPC topics listed above. In addition, this WP foresees thematic workshops covering the codes, algorithms, and methods used in the computational science topics portfolio of CaSToRC researchers, thus connecting them with the specialised groups at JUELICH and BSC.

Description of work

This work package will leverage the activities of the experienced partners within other collaborations such as PRACE[56] and VI-HPS[57] to expose CaSToRC researchers to some of the advanced technologies required to run on exascale systems.

Task 5.1: Performance analysis (CaSToRC, **BSC**, JUELICH)
Both JUELICH and BSC are members of the Virtual Institute - High Productivity Supercomputing (VI-HPS) whose mission is to improve the quality and accelerate the development process of complex simulation codes in science that are being designed to run on highly-parallel computer systems. For this purpose, they are developing integrated state-of-the-art programming tools for high-performance computing that assist programmers in diagnosing programming errors and optimising the performance of their applications. A VI-HPS training workshop (with the assistance of Dr. Judith Gimenez, manager of the "Tools" group at BSC) will be held in Cyprus offering hands-on experience and expert assistance using the tools with the applications of interest to CaSToRC.

In addition to this, CaSToRC researchers will be funded to attend relevant PATC courses in Performance Analysis to be held at BSC.

Task 5.2: Parallel I/O and portable data formats (CaSToRC, BSC, **JUELICH**)
CaSToRC researchers will be trained in advanced data management topics, including parallel I/O and parallel file systems and data formats. The application support division of JUELICH, under Norbet Attig, will offer this workshop, with Wolfgang Frings leading the instructors. The course will start with an introduction to the basics of I/O, including basic, I/O-relevant terms, followed by an overview over parallel file systems with a focus on GPFS and the HPC hardware available at JUELICH, and giving detailed insight into the I/O subsystem of the BlueGene/Q architecture. I/O strategies will be presented including the use of specialised libraries such as HDF5, netCDF and SIONlib, as well as of lower-level parallel I/O (MPI I/O). Optimization potential and best practices will be discussed.

Task 5.3 Programming of accelerators and vectorisation (CaSToRC, BSC, **JUELICH**)
Computational devices designed for high-throughput, multi-threaded workloads are becoming increasingly prominent in supercomputing systems. Accelerator type technologies, which currently include GPUs and Intel Xeon Phi (MIC) architectures, are expected to be the dominant computing component on the road to exascale. It is, therefore, crucial for researchers that aim to be competitive in scientific computing to learn how to efficiently programme such devices.

This task will train the researchers at CaSToRC in programming these devices. The workshop will combine and extend training material already delivered by JUELICH, including the vectorisation and OpenCL course given by Willi Homberg, and the CUDA programming course by Jan Meinke. The workshops will include not only training in the relevant programming languages and frameworks but also understanding the underlying technologies, to ensure codes make optimal use of the devices. For the case of the Xeon Phi and similar architectures, techniques in vectorisation of codes and optimisations in cache and memory use will be taught. Trainings will cover the features of new architectures that make vectorisation increasingly relevant, the tools to assist in this approach and best practices in the implementation. Courses covering basic aspects of GPU architectures and their programming are the other component of this task. Trainings will focus on both lower and higher level programming paradigms. For the former, the usage of the parallel programming language CUDA-C will be taught, allowing maximum control of NVIDIA GPU hardware when this is required by the application. For more high-level programming, pragma-based languages such as OmpSs and OpenACC will be taught for cases where rapid development is required such as proof-of-concept algorithms and prototyping of applications. Examples of increasing complexity will be used to demonstrate optimisation and tuning of scientific applications.

[56] http://www.prace-ri.eu/
[57] http://www.vi-hps.org/

Task 5.4 Programming models and novel programming paradigms (CaSToRC, **BSC**, JUELICH)
As supercomputing systems grow more diverse, with complex memory hierarchies and multiple levels of computational components, new programming paradigms are emerging to ease their programmability. Within this task the researchers at CaSToRC will be trained in using new programming paradigms, including pragma based programming models allowing fast development of otherwise complex application codes. Partner expertise will be leveraged, such as that of BSC in the OmpSs paradigms using the Nanos runtime and Mercurium compiler (Dr. Rosa Maria Badia, manager of the "Grid computing and clusters" group at BSC). Other topics will include UPC, CoArray Fortran, OpenCL and OpenACC.

Task 5.5 Thematic workshops (**CaSToRC**, BSC, JUELICH)
This task will oversee the organisation of topical training workshops in the computational science domains of CaSToRC. The workshops will focus on training CaSToRC researchers in the algorithms and application codes used in the respective fields. The workshops, which will involve both lectures and hands-on training, will be provided by the experts of the simulation laboratories of JUELICH, namely the molecular systems simulation laboratory (SimLab), the climate science Simlab and the Simlab in nuclear and particle physics, as well as the Earth Sciences department of BSC.

Deliverables
D5.1: Interim report on targeted advanced training (M18)
D5.2: Final report on targeted advanced training (M36)

Work package number	6	**Start Date or Starting Event**		Month 6			
Work package title	Mentoring to seed collaborative research						
Participant number	1	2	3				
Short name of participant	CaSToRC	JUELICH	BSC				
Person/months per participant:	15	10	5				

Objectives

Consolidation of the training received in workshops and schools will be done by secondments and mentoring of CaSToRC researchers working towards the development of common research activities with the teams at JUELICH and BSC. This aims at building long-term collaborative links that will extend beyond the lifetime of the project. Common research interests have been identified, which are expected to be expanded in the course of the programme. The objectives of the secondment and mentoring programme will have the following foci:

1. Development of new algorithms for climate and atmospheric modelling and computational chemical kinetics for current and future computers.
2. Development of exascale algorithms and codes for lattice QCD and co-design activities using lattice QCD as a prototype application.
3. Handling of big data and their visualization.
4. Improvement of the evaluation of atmospheric transport over Cyprus and the Eastern Mediterranean via the development of emission models and the implementation of the Nonhydrostatic Multiscale Model on the B-grid for Air Quality (NMMB/BSC-AQ) model; an online (fully online coupling meteo-chemistry) multi-scale (from global to regional scales) atmospheric model that integrates a mineral desert dust module[58].
5. Improvement of current quantum chemistry codes to enable solving organic chemistry problems ranging from kinetic modelling of combustion chemistry of biofuels to computational drug design
6. Development of multiple right-hand-side and multi-grid algorithms for lattice QCD capable of exascale performance. This aims at ensuring the competitiveness of the team for performing calculations of observables probing beyond the standard model physics.

Description of work

Task 6.1: Mentoring in Co-design and prototyping of new computing architectures (JUELICH, CaSToRC**)**

[58] http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast

A number of secondments will take place for mentoring CaSToRC scientist in the co-design approach for developing new computing architectures, initially using lattice QCD as a prototype application, and eventually including kernels from climate modelling. Codes related to chemical kinetics are even more challenging and the goal is to first port to GPUs and then assess the potential for co-design. For making progress in lattice QCD towards exascale performance, understanding of new HPC technologies and developing optimal algorithms will be crucial. Therefore lattice QCD will form the core of the co-design activities between the group of G. Koutsou at CaSToRC and the group led by D. Pleiter, head of the POWER Acceleration and Design Centre (PADC) at JUELICH, with links to both IBM and NVIDIA. This training and mentoring will include a total of **two secondments** of G. Koutsou and members of his team to **JUELICH** for periods of **1-2 months. In the last half of the project** Th. Christoudias and, depending on progress Y. Suleymanov, during their last secondment at JUELICH will interact with the exascale labs for co-design training. A short-term visit of Dirk Pleiter, or a member of his team, to CaSToRC is also foreseen. The seconded researchers will be mentored by experts at PADC on programming novel architectures and various aspects of the co-design approach such as:

- understanding the details of their application codes, their bottlenecks, computational hot-spots, and data access patterns;
- understanding the performance of contemporary and of upcoming novel computing systems, such as novel co-processor accelerator technologies;
- understanding how design factors of prototype machines can be influenced to match the requirements of their applications and vice-versa, i.e. how to develop their scientific codes based on direct knowledge of the architecture by interacting with hardware developers.

During the secondments, mentoring of the CaSToRC researchers will take place through collaborative work with JUELICH researchers for developing performance models for their applications, following the performance analysis advanced training workshops detailed in WP5. Application benchmarks and optimised mini-applications on prototype computer hardware will subsequently be used to evaluate the performance models developed. Examples of the evaluation that will be carried out include investigating different opportunities for GPU-acceleration based on the underlying models the codes implement and the impact of a given algorithm on the scalability of codes.

Lattice QCD kernels will be used as a pilot application, investigating initially the performance of Wilson-like hopping terms, and subsequently extending the performance evaluation to include such features as optimising for multiple grid layouts. For climate, the numerical temporal integrator kernel of the Kinetic PreProcessor[59] (KPP) atmospheric chemistry solver algorithms used in the European Centre HAMburg[60]/Modular Earth Submodel System[61]: ECHAM/MESSy (EMAC) climate model will be considered for GPU acceleration. For chemical kinetics, the goal will be optimising GPU-enabled quantum chemistry calculations, namely analysing and balancing GPU performance of quantum chemistry codes that underpin their approach. In this case, the impact on scalability of different aspects of quantum chemistry theory will be investigated such as to identify opportunities for GPU acceleration.

Task 6.2: Mentoring in computational chemical kinetics (CaSToRC**, JUELICH)**
We plan **five secondments of Y. Suleymanov** and his group members to the JUELICH **IAS simulation laboratory "Molecular Systems"** in the group led by Godehard Sutmann, and three short-term visits of members of the JUELICH group to CaSToRC. Within this task the researchers from CaSToRC will take advantage of the twinning partner's expertise in the field of materials informatics and quantum chemistry calculations on HPC systems. During the **first visit for 1 week**, the scope of the secondment programme and the prospective collaborative projects will be discussed and the needs of training during the secondments of the students clearly defined. During the **first two secondments** of **3-4 weeks** to the JUELICH team, CaSToRC researchers will be trained on relevant application codes for quantum chemistry problems of common interest. This will give the visiting researchers an introduction to the interfaces of the applications (both in terms of input and output) and provide a platform for discussing the codes themselves and their capabilities. The **third and fourth secondments** of about **one month** will focus on training for error detection and analysis, and the management of the quantum chemistry results, respectively. This will allow researchers from CaSToRC to adapt their approaches to I/O, replacing simple serial approaches implemented in current codes, which are inappropriate for massively parallel systems. This will expose efficiently their codes to various quantum chemistry packages and enable efficient data

[59] http://people.cs.vt.edu/~asandu/Software/Kpp/
[60] http://www.mpimet.mpg.de/en/science/models/echam.html
[61] http://www.messy-interface.org/

management approaches, which are of great importance for computational chemistry when hundreds (or thousands) of structures are analysed simultaneously. The **fifth secondment** of **one month** will focus on algorithms and optimisation. This secondment will enable researchers from CaSToRC to design and assess an efficient algorithm and to restructure their application for efficient execution in parallel, on multicore architectures with accelerator capabilities. The last secondment of one month will involve mentoring on GPU-enabled quantum chemistry calculations as describe in task 6.1 and interaction with the exascale labs.

Task 6.3: Mentoring in Climate and Atmospheric modelling (CaSToRC, JUELICH**, BSC)**
This task will include secondments to the **BSC Earth Sciences department** led by Francisco Doblas, and the **JUELICH IAS Climate Science Simulation Lab**, led by Lars Hoffmann, focusing on their world-class core competences for regional air quality modelling and global climate modelling respectively, that link to the science programme of the CaSToRC Atmospheric and Climate modelling group led by Theo Christoudias. **Three secondments** of Th. Christoudias and his team members for **1-2 months** each to the **Earth Sciences department of BSC, complemented by two intermediate shorter visits of members of the Earth Sciences department to CaSToRC,** will allow CaSToRC researchers to be exposed to the research environment and train on regional air quality model development with particular focus on the NMMB/BSC-AQ atmospheric model and the High-Elective Resolution Modelling Emission System[62] (HERMES), respectively. The target is the development of an efficient regional air quality model for Cyprus that can be extended over the Eastern Mediterranean and Middle East region, incorporating a detailed aerosol component including mineral dust with online emissions and a high-resolution regional emission inventory.

The regional modelling will be complemented by developments in global chemistry-climate modelling. **Two additional secondments** to the **JUELICH IAS Climate Science Simulation Lab** and a short term visit of researchers from the simulation lab, will focus on the coupling of the new Langrangian particle dispersion model MPTRAC (Massive-Parallel TRAjectory Calculations), under development in the simulation laboratory to the dynamical core of the EMAC global climate model developed and used by CaSToRC, and work towards full integration with atmospheric chemistry to allow for new applications. The dispersion model will also have the capacity to be driven with meteorological reanalysis data at JUELICH for validation and applications such as inverse modelling, made available to CaSToRC researchers. During the last secondment mentoring on GPU-acceleration of the KPP atmospheric chemistry solver will take place as well as on its applicability for co-design activities.

Task 6.4: Mentoring in Linear solvers for lattice QCD capable of exascale (CaSToRC**, JUELICH)**
This task will include **three secondments** of G. Koutsou and a member of the group for about **1 month each** to the JUELICH **IAS simulation laboratory "Nuclear and Particle Physics"**, overseen by Thomas Lippert and led by Stefan Krieg, with close collaboration with the Applied Mathematics group of Andreas Frömmer. Two short-term visits from members of the JUELICH group to CaSToRC are also foreseen. Within this task the researchers will be trained on developing advanced solver algorithms for lattice QCD capable of scaling to exascale. The competencies of JUELICH in multiple right-hand-side methods such as multi-gird solvers will be leveraged, combined with their expertise in novel computer architectures and in application codes capable of sustaining multi-petaflop performance. During the initial secondments CaSToRC researchers will be trained in the state-of-the-art in solver algorithms and specifically in those developed at JUELICH, following a workshop with hands-on exercises in linear solver methods for lattice QCD. The seconded researchers will subsequently gain expertise in developing these solver algorithms targeting lattice QCD topics of interest to CaSToRC, including hadron structure observables impacting searches for beyond the standard model physics. The final secondment will involve mentoring in the implementation of these algorithms in lattice QCD codes. The resulting codes will be made publicly available. These will include the open-source codes tmLQCD and QUDA of interest to CaSToRC researchers. The code development component will leverage the expertise of JUELICH in code design and accelerator technologies. This training will ensure the competitiveness of the group in compute-intensive calculations of observables probing new physics beyond the standard model.

In all tasks above, these visits will establish direct links between the research units at the Twinning partners and will be followed by continual mentoring through constant interactions and remote collaboration.

[62] http://www.bsc.es/earth-sciences/hermes-emission-model

Deliverables

D6.1: Intermediate report on researcher secondments (M18)
D6.2: Report on mentoring for code development (M36)
D6.3: Final report on researcher secondments (M36)

Table 3.1.b: List of work packages

Work package No	Work Package Title	Lead Participant No	Lead Participant Short Name	Person-Months	Start Month	End month
1	Management and coordination	1	CaSToRC	18	1	36
2	Dissemination and exploitation	1	CaSToRC	10	4	36
3	Optimising usage of HPC research infrastructure	2	JUELICH	12	6	36
4	Building educational capacity	3	BSC	21	1	36
5	Targeted advanced training	3	BSC	18	6	36
6	Mentoring to seed collaborative research	2	JUELICH	25	6	36
				104		

Table 3.1.c: List of Deliverables[63]

Deliverable (number)	Deliverable name	Work package No	Short name of lead participant	Type	Dissemi-nation level	Delivery month
1.1	One-page statement on the completion of the task 1.2	1	CaSToRC	R	PU	2
1.2	Midterm project report	1	CaSToRC	R	PU	18
1.3	Report on initiatives and opportunities for future funding of research activities	1	CaSToRC	R	PU	30
1.4	Final project report including mentoring outcomes as per KPIs	1	CaSToRC	R	PU	36
2.1	Project webpage	2	CaSToRC	DEC	PU	2
2.2	Interim report on dissemination and exploitation	2	CaSToRC	R	PU	18
2.3	Report on dissemination and outreach activities	2	CaSToRC	R	PU	36
3.1	Interim report on optimising research infrastructures	3	JUELICH	R	PU	18
3.2	Final report on optimising research infrastructures	3	JUELICH	R	PU	36
4.1	" Computational Science Skills" training programme	4	BSC	R	PU	9
4.2	Software configuration application to provide the standardised computing environment required by Task 4.1	4	CaSToRC	OTHER	PU	8
4.3	Report on training content creation and integration	4	JUELICH	R	PU	24
4.4	Final report on the development of advanced training capabilities	4	BSC	R	PU	36
5.1	Interim report on targeted advanced training	5	BSC	R	PU	18
5.2	Final report on targeted advanced training	5	BSC	R	PU	36
6.1	Intermediate report on researcher secondments	6	JUELICH	R	PU	18
6.2	Report on mentoring for code development	6	JUELICH	R	PU	36
6.3	Final report on researcher secondments	6	JUELICH	R	PU	36

[63] If your action is taking part in the Pilot on Open Research Data, you must include a data management plan as a distinct deliverable within the first 6 months of the project. This deliverable will evolve during the lifetime of the project in order to present the status of the project's reflections on data management. A template for such a plan is available on the Participant Portal (Guide on Data Management).

Table 3.1 d: Gantt chart showing the schedule of the events (workshops, secondments, and conference etc.) as well as the various WP reports.

Months		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
WP1- Management and coordination																			R												R						R	
Meetings		K					T						F						T					F						T							
WP2 - Dissemination and exploitation																			R																	R	E
Conference attendance programme																														R							
Innovation workshop																			W																		
Closing workshop																																	W				
WP3 - Optimising usage of HPC research infrastructure																			R																	R	
Best practices workshop								W												W											W						
Technical secondment programme									S					S						S				S				S		S							
WP4 – Building educational capacity										R															R											R	
“Computational Science Skills” training programme workshops							W												W											W						
Supercomputing training portal integration																																					
Training the trainers workshop									W																												
WP5- Targeted Advanced Training																			R																	R	
Cross-disciplinary training workshops							W			W					W			W						W				W									
Thematic workshops	Regional atmospheric modelling												W																								
	Lattice QCD algorithms for exascale													W																								
	Global climate modelling																			W																		
	Lattice QCD algorithms & codes for exascale																					W															
WP6 – Mentoring to seed collaborative research																			R																	R	
Future and Emerging Technologies	Co-design for exascale using lattice QCD applications										V					S											S										
Computational chemical kinetics	Quantum chemistry								S					S																							
	Error detection and data							V								S									S												
	Optimisation and performance analysis																												S								
Lattice QCD	Algorithms for exascale								V	S					S								V														
	Optimized codes for exascale								V																		S										
Climate & Atmospheric modelling	Global modelling											V			S								S														
	Regional modelling							S				V								S						V					S						

E = End of project; F = Face-to-face meetings; K = Kick-off meeting; R = Report; S = Secondment; T = Telco; V = Visits; W = Workshop

3.2 Management structure and procedures

Table 3.2.a: List of milestones

Mile-stone No	Milestone name	Related work package(s)	Est. date	Means of verification
1	Delivery of developed "Computational Science Skills" training material in a first training workshop	4	12	Workshop website with attendance and training material
2	CaSToRC technical staff trained in HPC administration best practices	3	18	Secondments and training of technical staff
3	Qualified Software Carpentry instructors at CaSToRC deliver "Computational Science Skills" training workshop	4	24	Workshop website with the list of trainers
4	Number of publications and invited talks satisfying anticipated KPIs	2,5,6	24	Conference invitations and proceedings
5	HPC administration best practices adopted by CaSToRC operations staff	3	24	CaSToRC user support website
6	Large-scale computer time allocation (>30 Mi core-hrs) awarded to CaSToRC research group (e.g. PRACE Tier-0)	3,5,6	24	Awarding computer site webpage
7	First submission of joint proposal for research funding (with CaSToRC and one or both of the Twinning partners)	3,4,5,6	24	Project proposal submitted
8	First proposal submission with local partners and from the region aligned with Cyprus' smart specialisation strategy	3,4,5,6	30	Project proposal submitted

3.2.1 Organisational structure

The organisational structure of the project is illustrated in Figure 3.1. We define a simple organisational structure to allow more effective support of the training, mentoring, secondments and research support envisioned in the project. The following bodies will be created to oversee the general implementation of the programme:

The steering committee (SC) will be the governing and decision making body of the programme. It will comprise of representatives from the three partners chaired by the Project Coordinator. All decisions will be taken by simple majority of present participants on an equal basis. The PC takes the final decision in case of a draw. The SC will have a kick-off meeting and at least another two face-to-face meetings (once per year) with frequent teleconferences in between. The main responsibility of the SC will be the monitoring of the activities of the project to ensure that the objectives and milestones are achieved according to schedule, as indicated in Table 3.2.a, as well as to recommend improvements, if needed. The SC will coordinate closely with PMO. The SC will be responsible for the distribution of the budget as agreed in the consortium agreement (CA). The coordinating site will hold the budget for all training events.

A **programme management office (PMO)** will be set-up at the CaSToRC chaired by the PC, and will be supported by the two scientific coordinators. The PMO will have a dual function as project management office and as the supporting body of the SC. The SC, in close coordination with PMO, will monitor the progress of the training and mentoring programme, the implementation of the secondments, address deviations and conflicts and take corrective measures when needed. The PMO will implement decisions taken by the SC. It will be responsible for the day-to-day implementation of the programme including administrative and financial reporting internally and externally. This includes communications with the EC. The PMO will be responsible for the management of intellectual property rights (IPR). PMO will be in constant contact with the scientists participating in the project regarding safeguarding the exploitation of results generated by the programme.

The **work package (WP) leaders** will be responsible for coordinating the WP activities, organise meetings and enable the effective communication among the WP participants. The leaders will monitor WP progress and ensure that all tasks, deliverables and milestones of the WP are completed in accord with the project plan. They will be working closely with the two scientific coordinators of the project who will help in drafting the internal reports from each WP and preparing project deliverables to be approved by the SC. The WP leaders will be in regular contact with PMO. The scientific coordinators will report the progress to the SC during the annual meetings. The management and the dissemination and outreach WPs will be coordinated by the two scientific coordinators as part of PMO, while the training WPs will be led by scientists at the leading institutions with the support of the two scientific coordinators. This structure will relieve the scientists of extensive administrative burden allowing them to pursue training and research activities. The scientists in charge will monitor the scientific progress and the effectiveness of the mentoring

3.2.2 Innovation management

PMO will coordinate with the office of sponsored research (OSR) operating at CaSToRC and the Technology Transfer offices at JUELICH and BSC for supporting the researchers in innovation management. The consortium Steering Committee will identify the activities with high innovation potential and handle the associated knowledge transfer, based on past and pre present patterns of successful research-innovation interface at the Twinning Partners. To achieve this, PMO in collaboration with the OSR at CaSToRC, will explore successful practices at JUELICH and BSC and implement policies to develop equivalent services for CaSToRC researchers. Ultimately this activity will contribute to the drafting and compilation of the CyI intellectual property policy, an effort undertaken by the OSR jointly with Isis Innovation Ltd, the international knowledge transfer organization founded by the University of Oxford, appointed by the National Research Foundation of Cyprus to consult research organisations in Cyprus.

A major component of innovation management includes intellectual property management and knowledge transfer from academia to the industrial sector (see Task 2.6 in Section 3.1). PMO will coordinate with JUELICH and BSC to transfer knowhow to the scientific coordinators of CoSTAR and to the personnel of OSR at CyI so they can convey lectures specifically targeting the scientists and all other scientific coordinators at CaSToRC. Material available from the European Patent Academy[64] and similar organisations will also be utilized. PMO will pursue these educational opportunities and guide academics towards the most effective workshop programme.

One of the major tasks of PMO will be to identify and promote opportunities for collaboration and links to industry through the European technology platforms, local and international industrialist federations[65] and relevant government agencies[66]. The scientific coordinators who will be technically trained will serve as liaisons between the academic and private sector using the established communication channels of the Twinning partners. PMO will also be in charge for managing short term visits to CaSToRC of experts identified from industry in order to acquaint them with the work of the researchers and probe for potential synergies both on the national and the European scale.

3.2.3 Risk management

The critical challenge of this project is to ensure the right level of training and networking creating the collaborative environment that will result in improving the research output of the local teams. An equally challenging component is to sustain the research capacity and innovative structures beyond the life-time of the programme. The key risks related to these challenges are detailed in Table 3.2.b.

Table 3.2.b: Critical risks for implementation

Description of risk	Work package(s) involved	Proposed risk-mitigation measures
Insufficient number of qualified Ph.D. students and postdoctoral fellows joining the research teams	WP1, WP4, WP5, WP6	Use network of the Twinning partners to advertise and identify qualified researchers (medium to low).
Conflicting or non-overlapping research agendas between CaSToRC researchers and the twinning partners	WP1, WP4, WP5, WP6	PMO will coordinate the Twinning activities with the trainers and mentors to resolve such issues. Secondments will be considered to other simulation laboratories at JUELICH and other BSC departments with similar overlap (low).
Insufficient number of publications and other dissemination activities, leading to lower than expected target	WP6	Intensify mentoring and analysis of the shortcomings of the secondment programme that lead to delays in the dissemination. Increase number of secondments

[64] http://www.epo.org/about-us/office/academy.html
[65] e.g. Cyprus Chamber of Commerce and Industry, Cyprus Employers and Industrialists Federation, ETP4HPC
[66] e.g. Directorate General for European Programs for Coordination and Development (formerly Cyprus Planning Bureau), Cyprus Research Promotion Foundation

KPIs		and remote interaction (low to medium).
Difficulties encountered in scaling scientific applications for petascale and exascale architectures, resulting in low Tier-allocation	WP5, WP6	Intensify secondments to partners to identify suitable approaches add secondments to exascale laboratories (medium to low).
Low success rate in proposals for securing Tier-0 computational resources	WP3, WP4, WP5, WP6	Intensify mentoring for code development and scalability (low risk)
Sustainability of research activities beyond the project's duration	WP1, WP3, WP4, WP6	Identify research topics of common interest to scientists at CaSToRC and the Twinning sites by end of year-1. Identify resources for implementation and proposal submission (low to medium).
Low number of successful proposals	WP6	Coordinate closely with leaders at Twinning sites to identify opportunities and seek their help in forming strong consortia (low to medium).

3.3 Consortium as a whole

3.3.1 Consortium composition and exploitation of partners' complementarities

The consortium links the Computational Science and Technology Research Centre (CaSToRC) of the Cyprus Institute with two internationally leading European counterparts: the JUELICH Research Centre (JUELICH) in Germany, and the Barcelona Supercomputing Centre (BSC) in Spain to strengthen research in Computational Sciences in the joint European effort towards meeting the Exascale challenge. This is facilitated by the strong overlap of the requirements set by the research activities, training, technical know-how and user support needs among all consortium members. At the same time there is complementarity in individual research themes and technical, technological and training competencies of the two advanced partners, to cover all components in the research agenda and necessary supporting activities for the advancement of CaSToRC towards excellence.

Both BSC and JUELICH are PRACE advanced training centres[67] (PATC), hosting regular training workshops on advanced HPC topics. They already utilize their extensive in-house expertise to provide training programmes aiming at both local users and visitors in the technologies and skills required by competitive research utilising HPC resources. The partners are therefore optimally suited to jointly carry out the cross-thematic training programme of this project.

JUELICH and BSC systems are regularly ranked among the top ten supercomputers in the world according to the Top500 list[68], and therefore have extensive expertise in user support and systems operation and administration. This ensures that the training of CaSToRC technical staff will be of the highest quality and relevance. The expected gain in knowledge transfer and in best practices and technical know-how will extend CaSToRC services as it establishes itself as the national supercomputing facility for Cyprus and a regional leader in South-East Europe and the Eastern Mediterranean in the provision of HPC resources.

CaSToRC will also gain through linking of the scientific officers essential networking contacts and transferable skills in the identification of funding opportunities, successful competition and management of research grants and proposals and links to industry and enterprise for innovation and knowledge transfer.

The Twinning partners conduct world-class research in computational sciences, in disciplines spanning the research portfolio of CaSToRC, which is to a very large part aligned with the Smart Specialization Strategy for Cyprus. A prime example is the cutting-edge research on FET performed at the exascale labs of JUELICH led by Th. Lippert and D. Pleiter that resulted in the group coordinating large infrastructure projects such as DEEP and DEEP-ER. In addition, Th. Lippert has a joint affiliation with the University of Wuppertal working closely with the lattice QCD group of Z. Fodor and the Applied Mathematics group of A. Frömmer. These groups have pioneered new

[67] http://www.prace-ri.eu/prace-advanced-training-centres/
[68] http://www.top500.org/

algorithms such as the multi-grid algorithm for lattice QCD solvers and Hybrid Monte Carlo overlap operator [69] and performed the first simulation of lattice QCD with physical parameters of the light quark mass[70]. Another example is the cutting-edge work in the JUELICH simulation lab "Molecular Systems" led by G. Sutmann on multiscale modelling methods for applications in computational chemistry and materials science[71], in particular, the development of advanced algorithms with high parallel scalability for the calculation of long-range interactions in many-particle systems. Furthermore, expertise in the development of advanced algorithms with increased heterogeneity and locality, as well as resiliency to equipment failure and highly scalable I/O[72] in atmospheric and climate models, will also be a critical component of the training to enable CaSToRC research to advance to the exascale era.

While both Twinning partners excel in computational science research and services there are complimentary aspects between them. Leveraging previous common activities with JUELICH such as the development of a joint SimLab in Nuclear and Particle Physics mentoring in lattice QCD for exascale and FET will be exclusively involve JUELICH. Climate and Atmospheric modelling will benefit from both Twinning partners equally. Two mentoring track will be pursued one provided by the SimLab of JUELICH and the other by the group at BSC. The CaStoRC team pursuing computational chemistry kinetics matches best to the SimLab activities of JUELICH. BSC, on the other hand, will bring its strong cross-disciplinarily competencies leading advanced training and computational skills building.

We describe in more details in what follows the competencies of each Twinning partners and the demonstrated of relevant research groups at BSC and JUELICH involved in the mentoring and secondments of CaSToRC researchers.

Future and emerging technologies - Exascale computing: The research and support activities in all consortium partners are tightly integrated with the adoption and application of future and emerging technologies in High Performance Computing (HPC). JUELICH has established links with major HPC technology vendors, including IBM and NVIDIA, through a number of joint centres, such as the Exascale Innovation Centre[73] (EIC), the NVIDIA application lab[74], and the ExaCluster laboratory[75] (ECL). One of the main research activity thrusts at the JUELICH is the evaluation of future HPC architectures for scientific applications, led by the group of Dirk Pleiter, where CaSToRC is expected to benefit and contribute with the aim to meet exascale performance requirements. BSC has established an Exascale Lab[76] in collaboration with Intel, carrying cooperative research on complementary areas considered key for future exascale computing, concentrating on programming models and performance analysis tools.

JUELICH, in partnership with technology leaders IBM and NVIDIA, plan for a new competency centre, the POWER Acceleration and Design Centre[77] (PADC), to advance the creation and optimization of research codes on GPU-accelerated OpenPOWER compatible systems. The mentoring and secondments of CaSToRC researchers will be embedded in PADC, training them on architectures of future supercomputers and on the necessary knowledge and tools to prepare their applications in order to exploit new technologies as early as possible, at an internationally competitive stage.

Computational chemical kinetics: JUELICH operates the simulation laboratory "Molecular Systems"[78] under Godehard Sutmann, developing advanced many-body algorithms for solving problems in physics, chemistry and engineering. The simulation laboratory competencies will be leveraged to advance the computational chemistry group of CaSToRC led by Yury Suleymanov, in automated algorithms for prognosis of chemical reactivity of organic molecules from first principles,[79] advanced quantum dynamics approaches for chemical rate calculations,[80] and reaction paths analysis for detecting new 'unknown' types of chemical reactions[81] using evolutionary and

---

[69] N. Cundy, S. Krieg (Wuppertal U.), G. Arnold (Julich, NIC), A. Frommer (Wuppertal U., Dept. Math.), Th. Lippert (Julich, NIC & Wuppertal U.), K. SchillingN. CusComput.Phys.Commun. 180 (2009) 26-54

[70] S. Durr *et al.* Science 322 (2008) 1224-1227

[71] http://juser.fz-juelich.de/record/138015

[72] See for example "Enabling Climate Simulations at Extreme Scale (G8 ECS)" project with participation by both Twinning Partners

[73] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/EIC/_node.html

[74] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/NVLAB/_node.html

[75] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/ECL/_node.html

[76] http://www.bsc.es/intel-bsc-exascale-lab

[77] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/PADC/_node.html

[78] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slms/_node.html

[79] http://www.mit.edu/~~ysuleyma/prognochem

[80] Yu. V. Suleimanov, J. W. Alen, and W. H. Green, Comp. Phys. Comm. 183, 833 (2013).

[81] K. Prozument, Y. V. Suleimanov, B. Buesser, J. M. Oldham, W. H. Green, A. G. Suits, and R. W. Field, J. Phys. Chem. Lett. 5, 3641 (2014); Y. V. Suleimanov and W. H. Green, in preparation (2015).

freezing/growing string algorithms. The simulation laboratory expertise in HPC complements the CaSToRC expertise in quantum dynamics. Building on the experience of the simulation laboratory, the achievement of massive parallelism in the codes developed and used by CaSToRC researchers will open doors into new application areas in combustion engineering, modelling and guiding organic synthesis, and drug design.

Climate and Atmospheric modelling: Groups at both BSC and JUELICH carry out internationally leading research in complementary aspects of climate and atmospheric modelling. The Earth Sciences department at BSC[82] led by Francisco Doblas develops and implements high-resolution meteorology-chemistry and emissions **regional modelling** systems to understand the physico-chemical processes taking place in the atmosphere, including air quality and dust forecast. Through secondments and mentoring, Theo Christoudias and his team will be enabled to develop regional chemical weather and air quality forecast and hind-cast modelling capability for the Eastern Mediterranean and Middle East, centred on Cyprus, including mineral dust. This project will enable leveraging the world-leading know-how of BSC in air quality forecasting, comprising the HERMES emission model and the NNMB/BSC-AQ air quality forecast model.

JUELICH operates the simulation laboratory "Climate Sciences"[83], led by Lars Hoffmann, that together with the CaSToRC Atmospheric and Climate Modelling Group are founding members of the consortium[84] developing the EMAC model, a numerical atmospheric chemistry and climate simulation system. The JUELICH simulation laboratory is leading the development of Lagrangian transport algorithms, with the Lagrangian particle dispersion model MPTRAC to be developed in tandem to be driven by the EMAC dynamical core, a computational tool instrumental in advancing the research of the CaSToRC Climate and Atmospheric modelling group in **global** pollution transport with teleconnections and inverse modelling.

Lattice QCD for exascale: The JUELICH Simulation Laboratory "Nuclear and Particle Physics"[85] primarily carries out research in lattice QCD through which it provides expertise on present and future supercomputing architectures. Its research programme encompasses both fundamental physics topics and algorithmic developments. The Nuclear and Particle Physics SimLab is developed jointly with the Simulation Laboratory of CaSToRC. Thomas Lippert, Director of IAS and JSC, oversees its development, led by Stefan Krieg, with links to the applied mathematics groups of Wuppertal University. The IAS simulation laboratory members have pioneered calculations in lattice QCD including one of the first scientific applications to demonstrate the general-purpose capabilities of GPUs and a range of multiple right-hand-side solver methods. They have also developed optimised codes achieving unprecedented performance on the BlueGene series of supercomputers[86]. Giannis Koutsou and his team will be mentored on solver methods, such as multi-grid, specialized for the hadronic calculation programme of CaSToRC and for efficient use with co-processor accelerators such as GPUs. They will also mentor CaSToRC researchers in implementing and optimising the algorithms on novel computing devices, to deliver production-ready open source codes.

3.3.2 Commitment of beneficiaries and partner organisations to the programme

All participants and their institutions are fully committed to the proposed programme, with the intention of building on the relationships established under this project beyond the 36 months allocated. Beyond the research staff identified above, which include the simulation laboratories of the JUELICH and the Earth Sciences Department of BSC, the user support and supercomputing operations staff of the JUELICH are committed to mentoring and training CaSToRC support staff under the technical training programme, and maintaining these links beyond the duration of the project The consortium has also secured letters of support from HPC vendors that have an interest in seeing Computational Sciences developed in Cyprus and the region. These technology vendors have committed assistance that will be provided to CaSToRC researchers through the secondments to the twinning partners.

3.4 Resources to be committed

The budget for this project is grouped into three main categories:

- The personnel costs for the management and coordination of the activities of the project.
- The costs for the training events and mentoring program
- Other costs associated mainly with dissemination and outreach

[82] http://www.bsc.es/earth-sciences
[83] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slcs/_node.html
[84] http://www.messy-interface.org/
[85] http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slnpp/_node.html
[86] http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/dynQCD/_node.html

Personnel costs

A summary of the person month (PM) effort is shown in Table 3.4.a. One new scientific coordinator will be assigned to CaSToRC, the site responsible of the organization of all training events and following the day-to-day implementation. The second scientific coordinator, already employed at JUELICH, will be interfacing between the two Twinning partners and also contribute to core skills training. The coordinators will populate the Supercomputing Training Portal with material generated within the project. Most of the rest of the PMs are allocated for the delivering of the training events as well as for the mentoring the CaSToRC staff while on secondments to the Twinning sites.
In more detail:

- PM costs including overheads for WP1 are €120,358 (or 12% of the total project budget) and for WP2 €68,769
- PM costs for WP3, WP4 and WP5 are €84,358, €140,858 and €132,217, respectively
- Funded PMs for WP6 are €178,396 while CaSToRC will contribute additionally 5 PMs (i.e. 30% of its allocation in WP6) bringing the budget to €208,396. These PMs are included in the work effort of the project.

The EC requested total personnel costs are €724,956 including 25% overheads, with CaSToRC receiving €240,000, JUELICH €283,456 and BSC €201,500.

Costs for training events and secondments

Costs for the training events and secondments are primarily travel and accommodation costs, either of CaSToRC researchers to the training site or for trainers from the Twinning sites to CaSToRC. The budget also includes small funding for running of the events such as coffee breaks and lunches. The budget for the training events will be managed by the coordinator and transferred to the partner holding the training event to cover the expenses. Visits of researchers from the Twinning partners to CaSToRC are also budgeted. These will be coordinated with training events to minimise travel expenses. The budget for the training events is **€**140,979 and for the secondment program **€**66,281, amount to a total budget of **€207,260** including 25% overheads.

Dissemination and outreach

The project will allocate funds in a specific program that will enable CaSToRC researchers to participate in conferences. Up to 30 such participations will be supported. It is expected that towards the final 12 months of the project, faculty will be securing invited talks and support for participation will be provided.
A closing workshop will be organised including an open-day where the research highlights enabled by this project will be presented to the local research community and stakeholders.
The total budget for these dissemination and outreach activities is about **€65,154**, including 25% overheads.

The total budget of the project is: €1,027,370

The total EC contribution required for the project: €997,370

Table 3.4.a: Summary of staff effort

	WP1	WP2	WP3	WP4	WP5	WP6	Total person months per participant
Participant 1: CaSToRC	10	5	4	8	3	15	45
Participant 2: JUELICH	4	3	4	4	8	10	33
Participant 3: BSC	4	2	4	9	7	5	31

Table 3.4.b: 'Other direct cost' items

CaSToRC	Cost (€)	Justification
Travel	272,414	Funding for: i) training events by the Twinning partners and CaSToRC (**€**140,979); ii) secondments for mentoring of CaSToRC researchers and technical personnel to the Twining sites and short visits of staff from the Twinning sites to CaSToRC (**€**66,281); iii) CaSToRC researchers to attend international conference (**€**55,000); iv) closing workshop (**€**10,154). All amounts include overheads.
Total	272,414	

Section 4: Members of the consortium
4.1. Participants (applicants)

1. The Cyprus Institute

The Cyprus Institute (CyI), founded in 2005, is a non-profit research and educational institution with scientific and technological focus. It consists of issue-oriented research centres that address challenging interdisciplinary questions both at the regional and international levels. The Government of Cyprus supports The Cyprus Institute, viewing its establishment as important to its overall policy of transforming Cyprus into a regional centre for research and education. It has established up to date three research centers that are characterized by an interdisciplinary environment. These are the Energy, Environment and Water Research Center (EEWRC), the Computation-based Science and Technology Research Center (CaSToRC), and the Science and Technology in Archeology Research Center (STARC). The founding goal of CaSToRC is to combine a supercomputing infrastructure with research and education in computational science. Since 2012 it provides computational resources for Cypriot researchers with the installation of the Cy-Tera machine, a hybrid cluster of peak performance 33 Tflop/s, since 2012. HPC training programs and a user support team have been established to best serve the needs of the Cypriot scientific community. Through LinkSCEEM-2, a 4-year FP7 infrastructure project that ended recently, CaSToRC created an e-infrastructure committing up to 30% of its computational resources to scientists in the Eastern Mediterranean. Cy-Tera is the largest academic supercomputing of open access available to scientists in the Eastern Mediterranean. CaSToRC aspires to maintain its role as a hub in the region bridging the Middle East to the EU. CaSToRC is the representative of Cyprus to PRACE contributing 10% of Cy-Tera to Tier-1 resources. It has recently established an accredited Ph.D. program in Computational Science and succeeded in coordinating a Marie Skłodowska-Curie European Joint PhD program in Computational Science entitled HPC-LEAP. Lattice gauge simulations, climate modelling, computational chemistry, prototyping activities and visualization are research areas of current focus.

Lead participants in the project:

Constantia Alexandrou (female) obtained a BSc in Physics from the University of Oxford and a Ph.D. in Theoretical Nuclear Physics from the Massachusetts Institute of Technology. She is Institute Professor at CyI and Professor of Theoretical Physics at the Department of Physics at the University of Cyprus. She has over 20 years of experience in mentoring young scientists in the area of Computational Nuclear Physics and in particular Lattice QCD. Prof. Alexandrou is Director of CaSToRC and was the coordinator of the LinkSCEEM projects that promoted HPC capacity in the Eastern Mediterranean. She is the coordinator of HPC-LEAP and the representative of Cyprus to the PRACE council.

Giannis Koutsou (male) obtained a BSc in Physics and a Ph. D. in Lattice QCD from the University of Cyprus. After a three year postdoctoral appointment at the University of Wuppertal and a visiting scientist position at the Julich Supercomputing Center he become Assistant Professor at CyI in 2013. His research focuses on HPC algorithms for lattice QCD and HPC technologies. He has been engaged in evaluating novel supercomputing architectures as part of PRACE prototyping activities, as well as, code development of lattice QCD applications on novel systems such as the QPACE machine, GPUs and the Intel Xeon Phi. He is coordinating the *GPU-Clusterware* project funded by the Cyprus Research Promotion Foundation that to evaluate new accelerator technologies.

Theodoros Christoudias (male) has a BSc in Physics and a Ph.D. in Experimental High Energy Physics from Imperial College London. He joined the Climate and Atmospheric modelling group of CaSToRC as a Research Scientist and since 2014 became Assistant Professor at CyI. He is carrying out research in atmospheric and climate modelling and simulations and he leads the visualization lab of CaSToRC. He is actively involved in porting state of the art climate models onto next generation system architectures in an effort to pave the way towards exascale systems. He serves as Consortium Responsible for CyI in the Consortium Steering Group of the multi-institutional consortium that oversees the development of the ECHAM/MESSy (EMAC) Earth System Model.

Yury Suleimanov (male) He has an MSc in Chemistry and a Ph.D. in Physical Chemistry from Moscow State University. He held a Princeton Combustion Energy Frontier Research Center Fellowship allowing him to be at the Massachusetts Institute of Technology, USA and a Royal Society Newton International Fellow at the University of Oxford. He assumed the position of Assistant Professor at CyI in 2014 to lead the establishment of the computational chemistry group at CyI. His research interests are in the area of Theoretical and Computational Chemistry and in particular chemical reactivity from quantum chemistry calculations, combustion chemistry, computational discovery of unexpected chemical reactions, theoretical study of non-adiabatic effects in chemical dynamics, and computational optimization of heterogeneous catalysis.

Relevant Publications:

1. C. Alexandrou, T. Korzec, G. Koutsou and T. Leontiou, "Nucleon Excited States in N_f=2 lattice QCD", Phys. Rev. D **89**, 034502 (2014).
2. C. Alexandrou, M. Constantinou, V. Drach, K. Hadjiyiannakou, K. Jansen, G. Koutsou, A. Strelchenko and A. Vaquero, *"Evaluation of disconnected quark loops for hadron structure using GPUs"*, Comput. Phys. Commun. **185,** 1370-1382 (2014).
3. T. Christoudias and J. Lelieveld, "*Modelling the global atmospheric transport and deposition of radionuclides from the Fukushima Dai-ichi nuclear accident*", Atmos. Chem. Phys. **13**, 1425-1438 (2013).
4. Yu. V. Suleimanov, J. W. Allen, and W. H. Green, *"RPMDrate: bimolecular chemical reaction rates for ring polymer molecular dynamics"*, Comput. Phys. Commun. **183**, 833 (2013).
5. K. Prozument, Y. V. Suleimanov, B. Buesser, J. M. Oldham, W. H. Green, A. G. Suits, and R. W. Field, *"A signature of roaming dynamics in the thermal decomposition of ethyl nitrite: chirped-pulse rotational spectroscopy and kinetic modelling"*, J. Phys. Chem. Lett. **5**, 3641 (2014).

Relevant Projects:

1. **PRACE:** CyI is a partner and amongst other activities participated in the prototyping work packages of PRACE 1IP and PRACE 2IP. It currently participates in the code development in PRACE 4IP.
2. **LinkSCEEM projects:** CyI is coordinated the FP7 LinkSCEEM project series, a coordination and support project followed by an infrastructure project creating an HPC user community base in the Eastern Mediterranean region.
3. **HPC-LEAP:** CyI coordinates a Marie Skłodowska-Curie Innovative Training Network for a European Joint Doctorate entitled "*High Performance Computing for Life Sciences, Engineering and Physics*" (HPC-LEAP).
4. **DEEP:** CyI participates with the climate modelling application in the *"Dynamical Exascale Entry Platform"* (DEEP) project.

5. **GPUCW:** CyI coordinates a project titled *"GPU Clusterware"* funded by the national Research Promotion Foundation of Cyprus aimed to promote cooperation of academia with local industry. Project partners include CSCS, IBM Cyprus and the University of Cyprus. The purpose of the project is to evaluate new accelerator technologies for scientific computing as well as build appropriate cluster management tools for heterogeneous systems.

Infrastructure:

- CyI runs Cy-Tera, the national computing facility of Cyprus, a 33 Tflop/s hybrid CPU/GPU cluster open to all academic researchers in Cyprus and the region. Beyond the computer system, CyI maintains all relevant computer centre infrastructure including support staff, help-desk and ticketing system, and storage and backup services.
- CyI maintains small prototype systems for evaluating new computer technologies, including a system of 12 Intel Xeon Phis and 4 NVIDIA GPUs.

2. Forschungszentrum Juelich GmbH

Forschungszentrum Jülich (FZJ), a member of the German Helmholtz Association, is with about 5,500 employees one of the large interdisciplinary research institutions in Europe. Continuous strategic development ensures that it can successfully perform its tasks for society and economy in a rapidly changing environment. Forschungszentrum Jülich has nine research institutes with 53 sub-institutes working in the areas of energy and climate research, bio- and geosciences, medicine and neuroscience, complex systems, simulation science, and nanotechnology. One of these nine institutes is the Institute for Advanced Simulation (IAS) which unites Simulation Sciences and supercomputing under one roof. Thus, disciplinary, methodological and technological competences can be combined to manage the future challenges in the Simulation Sciences. The close cooperation of the scientific users with the staff of the Jülich Supercomputing Centre (JSC) leads to a prolific usage of the highly attractive European supercomputing centre in Jülich - especially in method development and scientific visualisation. The institute consists of the Jülich Supercomputing Centre and six simulation laboratories (SimLabs).

The Jülich Supercomputing Centre (JSC) has 145 staff and 40 third-party funded members. It provides outstanding supercomputer resources, IT tools, methods and know-how for researchers at FZJ and for more than 200 German and European projects through the John von Neumann Institute for Computing (NIC), the Gauss Centre for Supercomputing (GCS) and the Partnership for Advanced Computing in Europe (PRACE). To ensure optimal mapping of methods, models and algorithms needed by users of state-of-the-art supercomputing JSC provides teams for mathematical methods and algorithms, performance analysis or visualisation by community oriented high-level research and support units called Simulation Laboratories (SL). Several of these Simulation Laboratories target applications in biology, medicine, and biotechnology. Furthermore, through the JSC and the Institute of Neuroscience, FZJ is leading the HPC Platform subproject of the Human Brain project, a EU flagship project that aims at understanding the human brain and its diseases and ultimately at emulating its computational capabilities. In addition to providing access to supercomputers, JSC focuses on technology developments, in cooperation with industrial and academic partners. This involves exploration of opportunities provided by new architectures, innovative networks or accelerator processors like GPUs, FPGAs or Intel MICs. Last but not least, JSC carries out educational activities in cooperation with the Aachen University of Applied Sciences and the German Research School for Simulation Sciences (GRS), a collaboration between FZJ and RWTH Aachen University, which offers an innovative master's degree program in simulation sciences and a simulation-oriented PhD program.

Furthermore, JSC is significantly involved in high-level training activities like the GCS PRACE Advanced Training Centre.

Lead participants in the project:

Thomas Lippert (male) is Head of the JSC and Director of the Institute for Advanced Simulation. He is also a member of the board of directors of the John von Neumann Institute for Computing (NIC), and holds the chair for Computational Theoretical Physics at the University of Wuppertal. His research interests include lattice gauge theories, quantum computing, numerical and parallel algorithms, and cluster computing.

Norbert Attig (male) is Deputy Head of the JSC. He also heads the Application Support division of JSC, which is responsible for the high-level user support of the centre, with the goal of supporting users to make efficient use of their applications on the HPC systems at JSC. This high-level support includes education and training. The Application Support division of JSC will oversee allocating the trainers to the workshops foreseen in this project. His interests centre on diverse aspects of high performance computing, particularly the seamless integration of state-of-the-art architecture with applications and high-level user support.

Lars Hoffmann (male) is the team leader of the Simulation Laboratory Climate Science at the Jülich Supercomputing Centre. The research activities of this laboratory include climate modelling and numerical weather prediction, data analysis of remote sensing measurements, modelling of atmospheric radiative transfer, inverse modelling and data assimilation, high-performance computing, scientific visualization. He is the main developer of the Lagrangian particle dispersion model MPTRAC to be used in this project. He co-authored nearly 40 peer-reviewed publications. is the leader of the JSC Simulation Laboratory “Climate Science”.

Dirk Pleiter (male) is a research group leader at the Jülich Supercomputing Centre and professor of theoretical physics at the University of Regensburg. At JUELICH he is leading the work on application oriented technology development. Currently he is principal investigator of the Exascale Innovation Center and the NVIDIA Application Lab at Jülich. He has played a leading role in several projects for developing massively-parallel special purpose computers, including QPACE. He is also the head of the POWER Acceleration and Design Center (PADC) at JSC, a new competence centre to support scientists and engineers using OpenPOWER technologies and architectures to address problems requiring supercomputing resources. At this lab experts from the IBM labs in Böblingen and Rüschlikon as well as from JSC and NVIDIA combine their efforts to pool know-how and experience on applications, mathematical methods and algorithms, performance analysis and engineering as well as computer architectures.

Godehard Sutmann (male) is the leader of the JSC Simulation Laboratory "Molecular Systems”. The research fields covered by this laboratory include techniques covering a wide range of time and length scales: ab initio calculations using electron correlation methods, density functional theory, force-field-based molecular dynamics and mesoscopic fluid simulations. The group is also interested in developing new global models combining multiscale techniques from both molecular physics and quantum chemistry.

Stefan Krieg (male) is the leader of the JSC Simulation laboratory “Nuclear and particle physics”. This laboratory builds and provides expertise on present and future supercomputing architectures with a particular emphasis on applications in the fields of theoretical Nuclear and Particle Physics. Its research program encompasses both fundamental physics topics and algorithmic developments.

A particular focus of active research is Lattice Quantum Chromodynamics, which allows for ab initio simulations of the strong force of the Standard Model of elementary particle physics.

Alan O'Cais (male) is a member of the Application Support division of JSC with a research background in algorithm development for lattice quantum chromodynamics. He is the main developer of the Supercomputing Training Portal and led two work packages within the successful LinkSCEEM-2 project, helping to develop a Virtual Research Community in Computational Science in the Eastern Mediterranean region. He has been an invited speaker at a number of PRACE Advanced Training events covering topics such as performance optimisation, benchmarking and profiling.

Wolfgang Frings (male) is a research scientist at Jülich Supercomputing Centre of Forschungszentrum Jülich. He now heads the application optimisation team, after 25 years at JSC. He organised the 2009, 2010 & 2011 Jülich Extreme Scaling Workshops and is a member of the High-Q Club committee. He works together with developers and users on porting and optimizing codes, especially focusing on parallel file I/O. He is author of several software tools used at many HPC centers. Among these are SIONlib, a library to support task-local parallel file I/O on large-scale systems; LLview, a batchsystem monitoring software; JuBE, a benchmarking environment; and LinkTest, a highly scalable MPI point-to-point network benchmark used for interconnect veri fication on various HPC systems. He has contributed to a number of national and European projects including PRACE, being involved in the development and management of the technical review process for access to Tier-0 resources.

Markus Geimer (male,) is the deputy team lead of the cross-sectional team "Performance Analysis" at JSC. He is involved in the design and development of the Score-P instrumentation and measurement infrastructure, and the lead developer of the trace-analysis component of the Scalasca performance analysis toolset. In this context, he taught a number of tutorials at major HPC conferences (SC, ISC) and was involved in various multi-day hands-on tuning workshops.

Relevant Publications:

1. A. Orr, J. S. Hosking, L. Hoffmann, J. Keeble, S. M. Dean, H. K. Roscoe, N. L. Abraham, S. Vosper, P. Braesicke, *"Inclusion of mountain-wave-induced cooling for the formation of PSCs over the Antarctic Peninsula in a chemistry-climate model"*, Atmos. Chem. Phys. **15**, 1071 (2015).
2. R. Spang, G. Günther, M. Riese, L. Hoffmann, R. Müller, S. Griessbach, *"Satellite observations of cirrus clouds in the Northern Hemisphere lowermost stratosphere"*, Atmos. Chem. Phys. **15**, 927 (2015).
3. S. Borsanyi, S. Durr, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg, L. Lellouch, T. Lippert, A. Portelli, K. Szabo, B. C. Toth, *"Ab initio calculation of the neutron-proton mass difference"*, Science **347**, 1452 (2015).
4. C. Begau, G. Sutmann, *"Adaptive dynamic load-balancing with irregular domain decomposition for particle simulations"*, Comp. Phys. Comm. **190**, 51 (2015).
5. A. Frommer, K. Kahl, Th. Lippert H. Rittich, *2-norm error bounds and estimates for Lanczos approximations to linear systems and rational matrix functions*, SIAM. J. Matrix Anal. & Appl., 34(3), 2013, 1046-1065

Relevant Projects:

1. **JARA-HPC:** Forschungszentrum Jülich and RWTH Aachen University combine their expertise in JARA-HPC (Jülich Aachen Research Alliance – Section High-Performance Computing): university departments, Collaborative Research Centres of the German Research

Foundation (DFG), a virtual Helmholtz institute, university courses, graduate school and elite training at the German Research School for Simulation Sciences. In the Aachen-Jülich region, university and non-university research is thus linked in a unique network.

2. **NIC:** Within the framework of its John von Neumann Institute for Computing (NIC), Jülich operates the largest and longest established German supercomputing centre together with its Helmholtz partner institutes DESY (German Electron Synchrotron Foundation) and GSI (Society for Heavy Ion Research).
3. **GCS:** In the Gauss Centre for Supercomputing (GCS) founded on the initiative of the German federal minister of education Annette Schavan in 2007, JSC cooperates with the two other national supercomputing centres in Stuttgart and Munich. GCS represents German interests on an international level.
4. **PRACE:** As one of the four hosting countries of the PRACE consortium (PRACE – Partnership for Advanced Computing in Europe), Jülich is working on specific plans for extending the European supercomputing infrastructure and making it the best in the world. The project intends to initiate long-term developments by preparatory investigations and developments for the generation after next of supercomputers.
5. **Exascale Labs:** The JSC hosts a number of Exascale Laboratories developed in collaboration with one or more HPC technology vendors, including the Exascale Innovation Center with IBM, the Exacluster laboratory with Partech and Intel, the NVIDIA application lab, and the POWER Acceleration and Design Center between NVIDIA and IBM. JSC leads European exascale initiatives, coordinating the DEEP and DEEP-ER projects and is a partner of the MontBlanc consortium.

Infrastructure:

- JSC offers computer resources of the highest performance class to its users. With JUQUEEN[1] (5008.86 TFlop/s) and JUROPA[2] (207 Tflop/s), it is one of the most powerful computer centres in Europe.
- JSC has established Exascale Labs (ExaCluster Laboratory, Exascale Innovation Centre, NVIDIA Application Lab, PADC)[3] with different vendors of high-performance computing systems or technology to enable novel co-design efforts.

3. The Barcelona Supercomputing Center

The Barcelona Supercomputing Center (BSC) was established in 2005 and is the Spanish national supercomputing facility and a hosting member of the PRACE distributed supercomputing infrastructure. The Center houses MareNostrum, one of the most powerful supercomputers in Europe. The mission of BSC is to research, develop and manage information technologies in order to facilitate scientific progress. BSC was a pioneer in combining HPC service provision, and R&D into both computer and computational science (life, earth and engineering sciences) under one roof. The centre fosters multidisciplinary scientific collaboration and innovation and currently has over 350 staff from 41 countries. In 2011, BSC was one of only eight Spanish research centres recognized by the national government as a "Severo Ochoa Centre of Excellence".

BSC has collaborated with industry since its creation, and has participated in projects with companies such as ARM, Bull and Airbus as well as numerous SMEs. BSC also participates in various bilateral joint research centers with companies such as IBM, Microsoft, Intel, NVIDIA and Spanish oil company Repsol. The centre has been extremely active in the EC Framework Programs and has participated in seventy-nine projects funded by it. BSC is a founding member

[1] http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html
[2] http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUROPA/JUROPA_node.html
[3] http://www.fz-juelich.de/ias/jsc/EN/Research/HPCTechnology/ExaScaleLabs/_node.html

of HiPEAC, the ETP4HPC and participates in the most relevant international road-mapping and discussion forums and has strong links to Latin America. Education and Training is a priority for the centre and many of BSCs researchers are also university lecturers. BSC offers courses as a PRACE Advanced Training Centre, and through the Spanish national supercomputing network (RES) among others.

Lead participants in the project:

Maria-Ribera Sancho (female) is a tenured professor at the Universitat Politècnica de Catalunya and the manager of Education and Training Team at Barcelona Supercomputing Centre. The team coordinates the Severo Ochoa Mobility Program, the BSC Research Seminar Series and the BSC International Doctoral Symposium. Dr Sancho has served as head of studies, vice-dean, and dean of the Barcelona School of Informatics (1998-2010). Her main research areas are conceptual modelling, information systems and software engineering and include learning analytics and adaptive learning. She's author of number of internationally published research papers and has participated in many EC funded projects. She also works with InLab http://inlab.fib.upc.edu/. She is the Spanish representative at the IFIP TC8 (Information Systems), Dean Country Ambassador at Deans 'European Academia Network-DEAN (2006-2010), President of the Spanish Council of Deans and Directors of Informatics (2006-2010) and a honorary member of this Council since 2010. She is member of the committee for the Barcelona Strategic Plan, of FIB Alumni, ATI and SISTEDES and of the INES platform. Dr Sancho is one of the organisers of the SC14 and 15 Workshop on Best Practices in HPC Training as well as a member of the organising committee of the ISC15 PRACE Training Day Workshop.

Nia Alexandrov (female) is the HPC Training Coordinator at BSC, Barcelona. She has over 14 years' experience as Postgraduate Studies Coordinator at the School of Systems Engineering and ACET (Advanced Computing and Emerging Technologies) Centre at the University of Reading and now at BSC. She coordinated multidisciplinary, joint and research based MSc Programs and taught on Post-Graduate level. Her research is in the area of collaborative and e-learning, with focus on curricula development, e-learning methodology and methodology for evaluation of on-line and blended learning. She was a member of the Career Space consortium and was involved with the Innovation Value Institute HE working group. She was researcher on a string of EC learning related projects and is the coordinator of PRACE Advanced Training Centre at BSC. Dr Alexandrov is a co-chair of the ISC15 PRACE Training Day Workshop and the BRIDGE Workshop series on ICCS conference (Bridging the Talent Gap with Computational Science Methods) as well as one of the organisers of the SC14 and 15 Workshop on Best Practices in HPC Training.

Francisco Javier Doblas-Reyes (male) is an ICREA Research Professor at BSC and Head of the Earth Sciences department at the BSC. He is a worldwide expert in the development of seasonal-to-decadal climate prediction systems. He is involved in the development of the EC-Earth ESM since its inception. He is an IPCC lead author (Fifth Assessment Report), serves in WCRP and WWRP scientific panels, has participated in a number of FP4 to FP7 projects and is author of more than 100 peer-reviewed papers, member of several international scientific committees and supervisor of three PhD students. He started working on climate variability at the Universidad Complutense de Madrid (Spain) in 1992, where he did his PhD. He then worked as a postdoc in Météo-France (Toulouse, France), at the Instituto Nacional de Técnica Aerospacial (Torrejón, Spain) and for ten years at the European Centre for Medium-Range Weather Forecasts (Reading, UK).

Oriol Jorba (male) leads the Atmospheric Composition group at the Earth Sciences department of the BSC. His research activities and interests have included high-resolution mesoscale meteorology and air quality, development of online meteorology-chemistry models, boundary layer studies, chemical mechanisms and environmental impact assessment. He held a research position at the University of California Irvine (USA) in 2011, and at the NASA Goddard Institute for Space Studies (USA) in 2013. He has co-authored more than 30 papers in international scientific journals (Atmospheric Environment, Atmospheric Chemistry and Physcis, Jorunal of Geophysical Research, others) and over 100 communications to international conferences. He has participated in several Spanish and European projects of the FP5 and FP7 Framework Programme (e.g., EARLINET, ACCENT, IS-ENES, FIELD-AC, IS-ENES2). He has been the principal investigator of the Spanish research project CGL2008- 02818, and coordinates the development of the multiscale chemical weather forecasting system NMMB/BSC-AQ. He is member of the management committee of 2 European COST Actions (ES1002, ES1004) as a Spanish representative, and of the Scientific Committee of the International Technical Meeting on Air Pollution Modelling and its Application. He has acted as reviewer of several international journals (Atmospheric Environment, Atmospheric Research; Geoscientific Model Development; Tethys; Water, Air and Soil Pollution).

Albert Soret (male) leads the Services group within the Earth Science department of the BSC. His research activities and interests have included: emission modelling, high resolution mesoscale meteorology and air quality, and environmental impact assessment. He has been involved in several national and international research projects, including the Spanish air quality-related CALIOPE Project, and the EC-FP7 projects Field_AC, IsENES and IsENES2. During this time, he has also been involved in several meteorological and air quality studies and collaborations, air quality medialization regarding particulate matter for the Iberian Peninsula, and in the improvement of the Saharan dust regional model to prevent dust intrusions in the southern Europe and the Canary Islands. Before that, he has worked in a number of different environmental agencies, and he is still involved in climate change discussion groups. He has authored more than 17 publications in scientific and technical journals as well as 20 international and national conferences.

Relevant Publications:

1. N. Alexandrov and V. Alexandrov, *"Computational Science Research Methods for Science Education at PG level"*, Procedia Computer Science (2014), (in press).
2. N. Alexandrov, R. Ramirez, and V. Alexandrov, *"Technological Advances in Interactive Collaborative Learning"*, Taylor and Francis Group LLC, (2013) ISBN: 978-1-4665-0208-6 (Hardback).
3. A. Badia and O. Jorba, *"Gas-phase evaluation of the online NMMB/BSC-CTM model over Europe for 2010 in the framework of the AQMEII-Phase2 project"* Atmospheric Environment (in press).
4. A. Soret, M. Guevara, and J. M. Baldasano, *"The potential impacts of electric vehicles on air quality in the urban areas of Barcelona and Madrid (Spain)"*, Atmospheric Environment **99**, 51-63 (2014).
5. M. Guevara, M. T. Pay, F. Martínez, A. Soret, H. D. van der Gon, and J. M. Baldasano, *"Inter-comparison between HERMESv2.0 and TNO-MACC-II emission data using the CALIOPE air quality system (Spain)"*, Atmospheric Environment **98**, 134-145 (2014).

Relevant projects:

1. PRACE Partnership for Advanced Computing, Implementation Phase Project 1, 2, 3, 4:
The Implementation Phase of PRACE receives funding from the EU's Seventh Framework

Program (FP7/2007-2013) under grant agreement RI-312763 and from the EU's Horizon 2020 research and innovation program (2014-2020) under grant agreement 653838.
2. IS-ENES2: is the second phase project of the distributed e-infrastructure of models, model data and metadata of the European Network for Earth System Modelling (ENES). The project is funded by the 7th Framework Programme (Grant Agreement number: 312979).
3. FAIRMODE-Forum for air quality modelling in Europe. The Forum for Air quality Modeling (FAIRMODE) was launched in 2007 as a joint response initiative of the European Environment Agency (EEA) and the European Commission Joint Research Centre (JRC). The forum is currently chaired by the Joint Research Centre.
4. MOOC: Introduction to Parallel Programming, project: 2014MOOCS00057, AGAUR funding program under the Resolution UNI/962/2005 (January–December 2015)
5. RISC A Network for Supporting the Coordination of Supercomputing Research Between Europe and Latin America, EC 7Th Framework Program, Grand Agreement 288883 c. 440 K Euros (October 2011- September 13)

Infrastructure:

- BSC hosts MareNostrum,[4] the most powerful supercomputer in Spain with the calculation capacity 94.21 Tflop/s.
- In collaboration with Intel, BSC hosts the Intel-BSC Exascale Lab which aims at further developing the functionality and utilization of the infrastructure, evaluating its potential and how it can target the Exascale needs.

Letters of support

We attach the following letters supporting the importance of the project from:

- IBM Cyprus
- NVIDIA Europe
- Medochemie LTD pharmaceutical industry
- Department of Meteorology, Cyprus

[4] http://www.bsc.es/marenostrum-support-services

IBM Italia S.p.A.
42-44 Griva Digeni Avenue, 1080 Lefkosia
P.O. Box 22019, 1516 Nicosia, Cyprus
Company registration number: AE 591
VAT registration number: 90000066 S
Tax id : 19118381 A

To Whom It May Concern

April 30th, 2015

Subject: **Letter of support for the Twining program in Computational Science entitled *Computational Science Twinning for Advancing Research*- coSTAR**

I am writing in my capacity as General Manager of IBM Cyprus. I would like to express my company's strong support for the proposed twining programme coSTAR.

IBM, as one of the leading vendors for High Performance Computing (HPC) solutions world-wide, is constantly seeking to advance training and research in the technology that is at the core of our business. The proposed programme will improve the research capacity in cutting edge sciences that increasing rely on HPC to be competitive. It will train local scientists and students delivering potential employees with the right skill set. Especially the focus on training in HPC is of high interest to us. IBM Cyprus supports programs to advance the local HPC expertise that will provide, in the long-run, the knowhow the company needs.

Apart from the advantages for IBM directly, we also appreciate the impact that this programme will have for Cyprus economy in general. HPC is becoming essential in many sectors and we welcome the specific training that combines HPC technologies, algorithmic development and cutting-edge scientific applications allowing Cyprus to join the European effort to reach exascale computing.

With my best regards,

Marios Kapiris
General manager
IBM Cyprus

April 27, 2015

Letter of support for the Twinning program in Computational Sciences entitled CoSTAR (Computational Science Twinning for Advancing Research)

To Whom It May Concern:

I am writing in my capacity as Director Business Development HPC EMEA. I would like to express our strong support for the proposed twinning program CoSTAR.

As one of the leading vendors for High Performance Computing (HPC) solutions world-wide, we are constantly seeking to advance training and research in the technology that is at the core of our business. The proposed program of activities within CoSTAR will further the development of the Cypriot research capacity in cutting edge sciences that increasing rely on HPC to be competitive. Furthermore, HPC is becoming essential in many sectors and the program will train local scientists and students, delivering potential employees with the right skill sets for these sectors in the region.

As members of the POWER Acceleration and Design Center (which is a joint effort of IBM, NVIDIA and Juelich Supercomputing Centre) we strongly support the participation of CaSToRC in the open information and training events that this partnership will generate. We welcome the envisioned training activities within CoSTAR that combine application and hardware development, allowing Cyprus to play a role in European emerging computational technology. We also appreciate the impact that such participation will have in driving the development of the Cyprus HPC ecosystem in general.

With my best regards,

Stefan Kraemer
Director Business Development HPC-EMEA
Professional Solutions Group

NVIDIA
Adenauer Str. 20 A4
52146 Würselen
Germany
Cell +49 (0)172 8328263
skraemer@nvidia.com
www.nvidia.com
http://eu.nvidia.com

MEDOCHEMIE

MEDOCHEMIE LTD
PHARMACEUTICAL INDUSTRY
Executive Chairman's Office

17th April 2015

Letter of support for the Twining program in Computational Science entitled
Computational Science Twinning for Advancing Research- coSTAR

To whom it may concern

As the founder and Executive Chairman of Medochemie, Cyprus, I am very pleased to write this letter in support of the proposed twining programme coSTAR. Medochemie is the leading pharmaceutical company in Cyprus interested in pursuing innovative methods in drug design.

Given the potential in using computational methods for drug design and discovery we are pleased to support initiatives that promote scientific knowhow in Cyprus in this direction. Medochemie strongly supports the proposed program as it will give local scientists the highest-level training and expand their research capabilities. This exchange program will improve their HPC knowledge in various aspects of quantum chemistry with potential applicability in drug design. The company sees very positively the training of scientists in computational science and would be interested in the engagement of scientists with such skills in the company.

Yours faithfully

Dr. Andreas Pittas
Founder and Executive Chairman,

Correspondence to:
MEDOCHEMIE LTD
P. O. Box 51409
CY-3505 Limassol
Cyprus (Europe)

Tel.: +357-25-867600, Fax: +357-25-560863
E-mail: office@medochemie.com
http://www.medochemie.com
Telex 2990 MEDO CY
Cables Medochemie Limassol

Central Office
Medochemie Building
Constantinoupoleos Str.,
3011 Limassol, Cyprus

International Offices
• Bulgaria • Czech Republic • Greece • Holland
• Lithuania • Romania • Russia • Singapore
• Slovakia • Thailand • Ukraine • Vietnam

REPUBLIC OF CYPRUS
MINISTRY OF AGRICULTURE,
RURAL DEVELOPMENT
AND ENVIRONMENT

DEPARTMENT OF METEOROLOGY
1418 NICOSIA, CYPRUS

Ref. No: 5.26.001

20 April, 2015

To Whom It May Concern

Subject: Letter of support for the Twinning program in Computational Science entitled CoSTAR (Computational Science Twinning for Advancing Research)

I am writing in my capacity as the Director of the Cyprus Department of Meteorology. I would like to express my strong support for the proposed twinning programme CoSTAR.

The Department of Meteorology under the Ministry of Agriculture, Rural Development and Environment, provides the national meteorology service of Cyprus. Its mission is to provide meteorological and climatological services to all economic and social sectors over Cyprus. The Department is engaged in numerical weather forecasting, research and climate studies, heavily relying on High Performance Computing (HPC) infrastructure and services. It cooperates closely with the Cyprus Institute Computational Science and Technology Research Center (CaSToRC) for the provision of computational resources, advanced user support and expertise.

The proposed programme will improve the computational competence and strengthen the research capacity in geophysical model development, code optimization and porting to new architectures and the management, analysis and visualization of atmospheric and climate model generated data. Apart from the advantages for the Meteorological Department directly, we also appreciate the impact that this programme will have for the Cyprus HPC ecosystem in general. HPC is becoming essential in many sectors and we welcome the specific training that combines application and hardware development allowing Cyprus to play a role in European efforts to remain competitive in future and emerging computational technology.

With my best regards,

Dr. Silas Michaelides
(Director)
Cyprus Department of
Meteorology

Department of Meteorology, 1418 Nicosia, Cyprus, Tel. +357 22802932 - Fax +357 22305500
E-mail: metservice@ms.moa.gov.cy - Website: http://www.moa.gov.cy/ms

4.2. Third parties involved in the project (including use of third party resources)

Please complete, for each participant, the following table (or simply state "No third parties involved", if applicable):

Does the participant plan to subcontract certain tasks (please note that core tasks of the action should not be sub-contracted)	N
If yes, please describe and justify the tasks to be subcontracted	
Does the participant envisage that part of its work is performed by linked third parties[1]	N
If yes, please describe the third party, the link of the participant to the third party, and describe and justify the foreseen tasks to be performed by the third party	
Does the participant envisage the use of contributions in kind provided by third parties (Articles 11 and 12 of the General Model Grant Agreement)	N
If yes, please describe the third party and their contributions	

Section 5: Ethics and security

This section is not covered by the page limit.

5.1 Ethics

Not applicable for this project

5.2 Security[2]

Please indicate if your project will involve:

- activities or results raising security issues: NO
- 'EU-classified information' as background or results: NO

Digitally signed by sealingservice.grants.ec.europa.eu
Date: 2015.05.07 18:17:52 CEST
Reason: Acknowledgment of Receipt

This electronic receipt is a digitally signed version of the document submitted by your organisation. Both the content of the document and a set of metadata have been digitally sealed.

This digital signature mechanism, using a public-private key pair mechanism, uniquely binds this eReceipt to the modules of the Participant Portal of the European Commission, to the transaction for which it was generated and ensures its full integrity. Therefore a complete digitally signed trail of the transaction is available both for your organisation and for the issuer of the eReceipt.

Any attempt to modify the content will lead to a break of the integrity of the electronic signature, which can be verified at any time by clicking on the eReceipt validation symbol.

More info about eReceipts can be found in the FAQ page of the Participant Portal. (http://ec.europa.eu/research/participants/portal/page/faq)