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Linking Scientific Computing in Europe and the Eastern  
Mediterranean – Phase 2**

**Grant Agreement Number: RI-261600**

**D4.4  
Final Report on Training Activities Performed**

*Final*

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## Project and Deliverable Information Sheet

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## List of Acronyms and Abbreviations

BA	Bibliotheca Alexandrina
CaSToRC	Computation-based Science and Technology Research Centre of the CyI
CPU	Central Processing Unit
CyI	The Cyprus Institute
ESRF	European Synchrotron Radiation Facility
FZJ	ForschungszentrumJülich (Germany)
GPU	Graphic Processing Unit
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HPCC	HPC Challenge benchmark, <a href="http://icl.cs.utk.edu/hpcc/">http://icl.cs.utk.edu/hpcc/</a>
JSC	Jülich Supercomputing Centre (FZJ, Germany)
LinkSCEEM	Linking Scientific Computing in Europe and the Eastern Mediterranean
LinkSCEEM-2	Linking Scientific Computing in Europe and the Eastern Mediterranean – Phase
MPI	Message Passing Interface
MPG	Max Planck Gesellschaft
NARSS	National Authority for Remote Sensing & Space Sciences
RTI	Reflectance Transformation Imaging
SESAME	Synchrotron-light for Experimental Science and Applications in the Middle East
UNITE	UNiform Integrated Tool Environment
WP	Work Package

## Executive Summary

WP4 implements a series of training activities focusing on developing a tiered HPC training program to support new and existing users from the Eastern Mediterranean region and on providing an online training portal. WP4 tasks also include the implementation of a consulting service to provide the necessary advice on compute intensive methodologies to users and the monitoring of the evolving needs of users to appropriately adapt the HPC training programs offered by the LinkSCEEM-2 project. The present document reports on the activities carried out within the framework of WP4 during the fourth year of the LinkSCEEM-2 project.

## 1 Introduction

The main goal of WP4 is to provide training to researchers from the Eastern Mediterranean, to promote HPC and to provide consultation service to those in need of intensive computing services. This goal is served through the following specific objectives:

- Continued and improved training programs for general cross-disciplinary training and thematic training in climate modelling, cultural heritage research and synchrotron radiation data analysis.
- Provided training for technical personnel from CaSToRC, BA, NARSS.

The present document reports on the activities carried out within the framework of WP4 during the fourth year and the extension period of the LinkSCEEM-2 project. A detailed account on training events is presented.

### 1.1 WP4 partners

The WP4 partners are shown below in the table. NARSS is leading the WP. There are a total of 40 person months expected in this package over the 4 years of the project.

**Table 1: WP 4 load share**

<b>Participant</b>	<b>Person Months</b>
CyI-CaSToRC	12
NARSS	10
BA	4
JUELICH	3
UNIVERSITY OF ILLINOIS	3
SESAME	2
ESRF	2
MPG	4
Total	40

## 1.2 Summary of Activities in final reporting period

During the 4th year and the project extension of LinkSCEEM-2 numerous training events were held within the framework of WP4. These are summarized in the table below.

**Table 2: Training events performed during year four**

Organised training events during 4th Year	Location	Date
3 <sup>rd</sup> LinkSCEEM-SESAME Summer School	Allan, Jordan	08-10/09/2013
LinkSCEEM EasyBuild training	Nicosia, Cyprus	22-24/10/2013
2014 PRACE/LinkSCEEM Winter School	Tel Aviv, Israel	10-13/02/2014
RTI & Cultural Heritage Workshop	Nicosia, Cyprus	03-06/06/2014
4th LinkSCEEM General User Meeting June 2014	Nicosia, Cyprus	10-13/06/2014
4 <sup>th</sup> SESAME-LinkSCEEM Summer School	Amman, Jordan	15-07/06/2014
Advanced analysis for climate change impact assessment	Amman, Jordan	08-10/07/2014
LinkSCEEM HPC Roadshow 2014	Greece and Egypt	03-07/2014
LinkSCEEM/Cy-Tera HPC Administrator Workshop	Cyprus	19-21/01/2015
LinkSCEEM HPC Roadshow 2015	Greece, Jordan, Egypt	03-19/02/2015

## 2 Adaptation of Training Programs (Task 4.1)

During the final period of the project the activities on the training programs so as to reflect to the users training needs have continued. The focus was mainly given on the implementation of the Supercomputing Training Portal.

The portal recommends content within categories and provides an environment to browse the content while remaining within the website. Through the portal access is given to Euclid, the LinkSCEEM training cluster for the purpose of engaging in hands-on HPC education and training.

The Supercomputing Training Portal is accessible via the following link:

[supercomputing.cyi.ac.cy](http://supercomputing.cyi.ac.cy)

The portal was made available during the 4<sup>th</sup> year of the project. It was used by the attendees of the training events as their mean to connect to Euclid for the hands-on sessions.

Categories were organized in collaboration with other work packages, such as WP6 and WP9. The current status of the Supercomputing Training Portal is shown below. Significant amount of content was added during the past 6 months.

The workpackage has reviewed suitable ways of structuring and presenting training content on the training portal. The main content categories have been agreed and were implemented. A scheme similar to the training roadmap on [www.hpcuniversity.org](http://www.hpcuniversity.org) was created to guide users through the content. In addition, the first training material with embedded tutorials was implemented. The content was captured during the 4th LinkSCEEM General User Meeting.

**SUPERCOMPUTING Training Portal**

Log in Register

Practical HPC Development Improvement Visualisation Contact Us

### Using the Portal Features

Category: Portal basics

Essentially the portal consists of two main features:

- HPC training content organised according to specific categories
- Access to an educational HPC cluster for the purpose of engaging in hands-on HPC education and training

Luckily it's much more interesting than that sounds! We've tried to create a portal where you can use the highest quality training material and do hands on examples with the lowest possible barriers. Here we explain in more detail how this is achieved.

Read more: Using the Portal Features

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### Supercomputer Interaction

Category: Practical HPC

This content is to help guide people who have never used a supercomputer before and can explain the very basics of what parallel computing is, basic linux commands and how to log on (and use) the educational supercomputer.

Read more: Supercomputer Interaction

### Programming

Category: Development

Even if you only want to make small modifications to an existing application, you will still have to have some grasp of a programming language so you have a basic understanding of what is happening in the code. The core concepts of many programming language overlap so once you've learned to use one language, learning to understand and modify another is not actually that hard.

If you are going to start on a computing project you definitely need to learn a programming language. For supercomputing environments, common languages have been C and Fortran because they usually give the best performance. However, the concepts and increased flexibility of modern computer languages mean they are becoming more and more common...so if you are really starting from scratch I'd suggest you use C++!

Read more: Programming

### OpenMP

Category: Development

OpenMP (Open Multiprocessing) uses a portable, scalable model that gives programmers a simple and flexible interface for developing parallel applications for platforms ranging from the standard desktop computer to the supercomputer.

It is an API that supports multi-platform shared memory multiprocessing programming in C, C++, and Fortran, on most processor architectures and operating systems.

Because it is available on many platforms, modifications you make to your program that help it to run efficiently on one system should be useful on most other platforms too.

Today, there is no OpenMP support for accelerators (like a GPU). It is intended to merge the OpenACC API with the OpenMP specification to create a common specification which extends OpenMP to support accelerators in a future release of OpenMP.

Read more: OpenMP

Figure 1: Supercomputing Training Portal

More details about the Supercomputing Training Portal, its functionalities and content are given in deliverable D4.6.

### **3 Technical Personnel Training (Task 4.2)**

This task focuses on the training of personnel from CaSToRC, BA and NARSS at any of the three sites and at FZJ-JSC. The training of the personnel is focused on the management of the hardware systems available at the three sites and on setting up HPC system monitoring tools, management of storage of large data sets and maintenance of software and tools among others. During the fourth year of the project the following specialised training activities took place.

#### **3.1 LinkSCEEM EasyBuild training (Nicosia, Cyprus, October 22-24, 2013)**

EasyBuild is a software build and installation framework written in Python that allows users to install software in a structured, repeatable and robust way (<http://hpcugent.github.io/easybuild/>). Once setup for a particular application, Easybuild offers very simple procedures for users to compile and run complex applications. This is very useful, especially in inexperienced user communities.

Continuing last year's EasyBuild training event, the EasyBuild developers returned to Cyprus for another 3-day training workshop. Purpose of the workshop was to train administrators of regional HPC centres on EasyBuild so that modules for popular regional applications can be created. Invitations were sent to System Administrators in Israel, Egypt, Saudi Arabia and Cyprus. Administrators from Israel, Egypt and Cyprus joined the training. Also, there was participation from the UNITE team of JSC resulting to a very important outcome; the addition of the UNITE performance analysis tools in the EasyBuild framework. The workshop was planned to continue its activity in JSC during February 2014. The agenda of the workshop can be found in Appendix A.

#### **3.2 Training of technical personnel at FZJ-JSC (Julich, Germany, February 19-21 and 2-5 June, 2014)**

During year 4 the CaSToRC technical personnel has visited JSC twice for training purposes.

The first visit was in February 2014, 19th-21st, for another EasyBuild workshop, organised by the UNITE team of JSC. The workshop participants have continued their work on EasyBuild according to the needs of their sites. During the visit, the CaSToRC personnel had the chance to meet with many groups of the operations team at JSC and have discussions with them on the activities performed by the technical personnel of LinkSCEEM.

From the 2nd to the 5th of June 2014, the CaSToRC technical personnel visited JSC to work on the potential of having an open source resource manager on Cy-Tera called SLURM. The CaSToRC team was working closely with the experts of batch systems at JSC, trying to mirror in SLURM all functionalities and policies that are currently implemented in Torque/MOAB.

#### **3.3 LinkSCEEM/Cy-Tera HPC Administrator Workshop (Nicosia, Cyprus, January 19-21, 2015)**

During the extension period of the project, LinkSCEEM and Cy-Tera projects jointly organised a workshop for HPC system administrators at the Cyprus Institute in Nicosia, Cyprus. The program was balanced between theoretical and hands-on training sessions to



enable deep understanding of the concepts. For the hands-on sessions participants were given access to Euclid, the training cluster of the LinkSCEEM project, where they had the chance to carry out the exercises and practice what they have learned.

The main goal of the workshop was to present useful tools and best practices for administrating HPC systems. Thus, the program included topics for software installation, benchmarking, monitoring and also presentations from experts in the field that shared their experience and knowledge with the trainees.

The trainers for the workshop came from Bull (France), JSC (Germany) and NCSA (USA). Attendance to the workshop was by invitation only. HPC system administrators from Cyprus, Greece, Lebanon, Israel and Egypt attended the workshop. The agenda of the event can be found in Appendix A.



**Figure 2: LinkSCEEM/Cy-Tera HPC Administrator Workshop**

## 4 Basic and Advanced User Training Programs (Task 4.3 and 4.4)

The LinkSCEEM training program continued throughout the 4th year and the extension of the project. The training program focused on two series of regional roadshows (2014 and 2015) with basic training to enable new users to access the systems. In addition 2 large cross-sectional training workshops were held with general HPC training in parallel programming techniques. This was supplemented with thematic workshops focusing on specific regional user communities.

### 4.1 LinkSCEEM regional roadshow

Two successful series of regional Roadshow events were held in 2014 and 2015. A detailed report on the events is given in deliverable D2.4. Only the training aspects are briefly presented here.

A total of 6 events were held in Greece and Egypt in 2014 and a total of 9 events were held in Greece, Egypt and Jordan in 2015. Another roadshow event was planned in February 2015 at Koc University in Istanbul, Turkey. Unfortunately, the event was cancelled one day before the scheduled date because Koc University remained closed due to severe weather conditions.

The biggest part of the one day events was dedicated to information about the LinkSCEEM project and how to access the LinkSCEEM resources. Additionally, a big emphasis was given on the LinkSCEEM training activities focusing on the LinkSCEEM supercomputing training portal. The events concluded with hands-on training sessions on the following core skills:

- Key generation for access to machines
- Access to machines
- Modules and compilers
- Scripts
- Basic application examples

All participants were working on Euclid, through the supercomputing training portal. Access was given for 6 months to encourage following up the training.

### 4.2 Training during the cross-sectional workshops

A detailed report on the cross-sectional workshops is given in deliverable D2.4. Two large cross-sectional workshops were held in the fourth year: the *PRACE/LinkSCEEM winter school* (Tel-Aviv, Israel, 10-13/02/2014 in collaboration with PRACE) and the *4th LinkSCEEM General User meeting* (Nicosia, Cyprus, 10-13/06/2014). The focus of these two workshops was the provision of training on programming skills for High Performance Computing.

#### *PRACE/LinkSCEEM winter school*

The program was split into two main parts: Part I was a half day mini-workshop entitled "The Future of HPC: Israeli Innovation", where Israeli companies and researchers who are developing the future HPC technologies for the next 5 years were presented. Part II was an introductory workshop on how to use PRACE/LinkSCEEM resources. Part II included hands-on sessions, limited to 60 people. The 3-day workshop of Part II included the following training sessions:

- Parallel Programming with MPI
- Advanced MPI

- Parallel Programming with OpenMP
- Hybrid (MPI + OpenMP) Programming
- Use of Maths and Scientific Libraries
- Profiling
- Optimization and Benchmarking
- Job submission scripts – Accounting Tools
- CUDA Programming

#### *4th LinkSCEEM General User meeting*

The workshop was split into two parts. During the first two days of the event the participants received training on the following topics from the Software Carpentry (<http://software-carpentry.org/>) team:

- Task Automation with the Unix shell
- Version Control with Git
- Building Programs with Python
- Task Automation with make

The third day was dedicated to OpenMP programming. Introductory and advanced OpenMP concepts were introduced, along with hands on exercises. For this, LinkSCEEM funded a specialized trainer from Fermi lab, US, to join the workshop. Finally, the fourth day of the event was dedicated to more advanced parallel programming focusing on Accelerator Programming with Compiler Directives and more precisely OpenMP 4.0 for accelerators and OpenACC directives for GPU programming.



Figure 3: 4th LinkSCEEM General User Meeting, Nicosia, Cyprus

### 4.3 Thematic workshops

A detailed report on the thematic workshops is given in deliverable D2.4. A total of 4 thematic workshops were held in the fourth year of the project. A summary of the training aspects for each workshop is outlined below.

*3rd SESAME-LinkSCEEM summer school*

During the first day of the school the participants received general introduction about HPC and its applications on the Synchrotron Radiation field. In the following 2 days each participant had to select one of the two parallel training sessions: Density Functional Theory and HPC for Bioinformatics. The first session included training on Density Functional Theory implementation using Quantum Espresso and ABINIT followed by hands-on practical sessions. The second session included training on tomography data collection and processing and also XANES and EXAFS data analysis using IFEFFIT software.

*RTI & Cultural Heritage Workshop*

The workshop brought together experts on the field of RTI and cultural heritage from Europe, US and the Eastern Mediterranean region. The program was balanced between sessions and discussions focusing on the challenges and opportunities for the application of RTI to the academic research in general and on the current state and future potential of RTI and its applications on cultural heritage. The program also included sessions with information on various funding instruments and discussions on future funding opportunities.



**Figure 4: Reflectance Transformation Imaging (RTI) & Cultural Heritage Workshop**

*4<sup>th</sup> SESAME-LinkSCEEM Summer School*

The first day of the event was dedicated to Synchrotron Radiation training. An introduction to the computational aspects of SR data analysis was given. Additionally, trainers from SESAME and ESRF presented the pyFAI software for fast SAXS/WAXS/XRPD data processing and hands-on training session on the specific software followed. The last two days of the event, covered the same topics that were covered during the 4<sup>th</sup> LinkSCEEM General User Meeting by the Software Carpentry instructors:

- Task Automation with the Unix shell
- Version Control with Git
- Building Programs with Python
- Task Automation with make

*Advanced analysis for climate change impact assessment*

The fourth year LinkSCEEM Climate workshop was held in Jordan as part of a 10-day training course called “Advanced analysis for climate change impact assessment”. The training course was held from the 1<sup>st</sup> to the 10<sup>th</sup> of July 2014, where the last three days, from the 8<sup>th</sup> to the 10<sup>th</sup> of July 2014 were dedicated to LinkSCEEM. During the first LinkSCEEM day, a session similar to the Roadshow sessions was given with an introduction to the LinkSCEEM project, details on how to access the LinkSCEEM resources and hands-on core skills training exercises on Euclid, the LinkSCEEM training cluster. The last two days were dedicated to climate related presentations by scientists from CaSToRC-CyI and MPG. The following topics were presented:

- Model projected heat and air quality extremes in the eastern Mediterranean and the Middle East
- Heat waves in the Middle East
- Extreme precipitation events in the Middle East
- Practical on climate change impact assessment case studies to continue

## 5 Consultancy Systems (Task 4.5)

The consultancy service will be in charge of sustaining the efforts of LinkSCEEM-2 by providing technical assistance to researchers in need of HPC and advice on computing methodologies, and by maintaining the network of specialists in the field to address future technical problems. Consultancy services are being built via the collaboration with WP6 and WP9 Work Packages of the LinkSCEEM-2 project.

The first consultancy activity in year 4 was performed after the EasyBuild workshop where the CyI operations team was in contact with an administrator at the Faculty of Computer and Information of Cairo University who attended the workshop for assisting in setting up their cluster. The cluster was using Rocks Cluster Distribution and the CyI team started investigating on what kind of help could be provided. After having a few discussions, communication were unfortunately inadequate due to the current political situation in Egypt, so not enough progress has occurred. Following from initial discussions, consulting on the reuse of the IMAN1 cluster, and on the procurement of a new system was given. SESAME is now proceeding with an upgrade.

Assistance was also provided to the Faculty of Engineering of Cairo University for the administration of their cluster. The members of the team who is administering the cluster have visited the Cyprus Institute for a short period of time and the CyI Operations team has had meetings with them.

Additionally, the CyI operations team had a number of Skype calls with the technical team at BA to consult on the tender procedure they needed to follow for their new cluster focusing on what the acceptance tests from the vendor should include. Similar discussions have been made with the technical team responsible for IMAN1 first supercomputer in Jordan. Furthermore, the CyI operations team had a discussion with the Egypt Nanotechnology Centre at Cairo University to advice on the infrastructure needed for the installation of their new cluster.

Help for specific software builds for the University of Jordan (WIEN2K) was provided through face-to-face meetings during a workshop and follow-on video calls.

Consulting on cluster room requirements and infrastructure for a medium size cluster at the Egypt Nanotechnology Center at Cairo University was provided remotely.

Finally, the CyI operations team has visited three university classes which got Educational Access on Euclid, giving a hands-on session on how to using the system and throughout their access on the system they have been given adequate support and guidance to perform their projects.