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

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**D4.2
Year-2 Report on Training Activities Performed**

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List of Acronyms and Abbreviations

CaSToRC	Computation-based Science and Technology Research Centre of the CyI
CPU	Central Processing Unit
CyI	The Cyprus Institute
EC	European Community
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, http://icl.cs.utk.edu/hpcc/
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 2

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 second 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 (during the second year):

- Continued and improved training programs for general cross-disciplinary training and thematic training in climate modelling, cultural heritage research and synchrotron radiation data analysis.
 - During the first year we successfully completed the goal for the general cross-disciplinary training and the thematic training in synchrotron radiation.
 - During the second year we concluded the remaining thematic training (climate related research and cultural heritage) and are on track with the second year training programs for climate related research, cultural heritage and synchrotron radiation.
 - During the second year we held the general cross-disciplinary training and first MEWEMS training program for women in the Eastern Mediterranean.
- Provided training for technical personnel from CaSToRC, BA, NARSS at CaSToRC that may aggregate to the project.
- Provided basic user training (cross-disciplinary) to a wide spectrum of the computational science community.
 - Training was in GPGPU, MPI, parallel programming, computational fluid dynamics, molecular dynamics and other topics.

According to the LinkSCEEM-2 program WP4 is involved in the organization of several events to be held each year. Specifically:

- One 3-day general user meeting
- One 3-day advanced cross-sectional workshop
- Three 3-day thematic workshops (one in each thematic area)

The present document reports on the activities carried out within the framework of WP4 during the second year of the LinkSCEEM-2 project. A detailed account on training events is presented. Each of the following sections focuses on the activities of a specific WP4 task. Specifically, section 2 describes Adaptation of Training Programs (Task 4.1), section 3 presents the progress in technical personnel training (Task 4.2) while section 4 presents progress in basic user training programs (Task 4.3), and section 5 highlights the progress on the remaining tasks 4.4 and 4.5.

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

Participant	Person Months
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 Second Year

During the 2nd year of LinkSCEEM-2 several tasks were performed within the framework of WP4. These are summarized in the table below.

Table 2 Subtasks performed during year one

Subtasks Performed During 1st Year	Performed during quarter
Maintenance of of training portal for trainees and workshop fellows	Q5
Hosting of the first thematic workshop on climate-related research at the Cyprus Institute, October 11-13, 2011	Q5
Successful hosting of winter school and technical training for personnel from CaSToRC, the Bibliotheca Alexandrina, NARSS <ul style="list-style-type: none"> • During Cyl winter school (Nicosia, Cyprus, February 6-8, 2012) 	Q6
Successful hosting of 1st cultural heritage thematic workshop (Nicosia, Cyprus, May 9-11, 2012)	Q7
Advanced User Training Programs <ul style="list-style-type: none"> • 3 day General user meeting (Nicosia, Cyprus, June 25-27, 2012) • 1st MEWEMS 3 day training for women from the Eastern Mediterranean (Nicosia, Cyprus, June 25-27, 2012) 	Q8

Subtasks Performed During 1st Year	Performed during quarter
Basic User Training Programs <ul style="list-style-type: none"> ● One day user meeting in Jordan, June 12th 2012. ● One day user meeting in Greece, June 15th 2012. ● One day user meeting in Israel, July 3rd 2012. ● One day user meeting in Egypt, July 11th 2012. 	Q8
Advanced User Training Programs <ul style="list-style-type: none"> ● Preparation of 2nd climate modeling workshop in Nicosia, Cyprus (Expected in October 2012) ● Preparation of 2nd Synchrotron Radiation Research Thematic Training Workshop , in Allam, Jordan (Expected in October 2012) ● Preparation of 2nd cultural heritage workshop, in Alexandria, Egypt (Expected in September 2012) 	Expected during Q9 (3 rd year)

2 Adaptation of Training Programs (Task 4.1)

During the second year the online training portal created by JSC was hosted at <http://www.linksceem.eu/ATutor>. The portal has 13 tutorials that cover a wide range of topics relevant to HPC in general and LinkSCEEM-2 users in particular.

No additional tutorials were added during the second year since all of the major topics were covered in the 1st year and only basic maintenance for the site was performed. Some discussions were considered to improve the portal by including some video material, and some enhanced teaching aids. This would significantly increase the required storage and might require structural changes to the portal. A feasibility analysis currently investigates, if this can be achieved within the LinkSCEEM-2 project. It was also decided to add new material from the thematic workshops on the LinkSCEEM website both in pdf and possibly in video if the files were of reasonable size.

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 first year of the project one workshop took place.

3.1 Training Technical Personnel Workshop (Nicosia, Cyprus, February 6-8, 2012)

The training for technical personnel was performed in parallel with the Winter school at Nicosia (more details in next section). After the winter school was concluded, technical fellows from CasTorC, BA and NARSS were trained on using Medici. The training was performed by members from NCSA.

4 Basic User Training Programs (Task 4.3)

For the purposes of this task the trainees are provided with basic training in using HPC for computational science. The initial set of topics covered by the training material have been defined in WP4: Task 4.1, described in section 2.1 of the present report. Below is a description of the events organized in Year-1 for basic user training.

4.1 One Day User Meetings

During the second year there will be 4 one day user meetings in coordination with WP2 and WP6. These events will take place in

- One day user meeting in Jordan, June 12th 2012.
- One day user meeting in Greece, June 15th 2012.
- One day user meeting in Israel, July 3rd 2012.
- One day user meeting in Egypt, July 11th 2012.

The user meeting will:

1. Provide a general introduction to LinkSCEEM and its resources.

2. Give an overview of available HPC systems and software available within LinkSCEEM.
3. Describe the training program of LinkSCEEM and the various LinkSCEEM training events.
4. Explain how people can access the HPC resources available through LinkSCEEM for the purpose of their scientific research projects.
5. The user meeting will also include a hands-on session where participants of the user meeting will be guided through the various steps which are required to access and submit jobs to a LinkSCEEM HPC resource. This will include the generation of ssh keys, compilation and submission of jobs – all of which will be accompanied with relevant hands-on practical examples.

The suggested program for the one day user meetings is shown below:

Time	Event
09:00 - 09:10	Introduction from the hosting side
09:10 - 09:30	Introduction to LinkSCEEM and its resources
09:30 - 09:50	Overview of available HPC systems and software
09:50 - 10:10	Training Program
10:10 - 10:30	Access to resources
10:30 - 11:00	Coffee/Tea Break
11:00 - 13:00	Core Skills: Unix accounts, compilation, make, job submission

5 Advanced User Training Programs (Task 4.4)

LinkSCEEM-2 advanced user training programs include both cross-disciplinary topics of general interest to the HPC community and thematic training on cultural heritage, climate studies and synchrotron radiation techniques, software tools and applications. According to the WP4 description one advanced training workshop of general nature and three specialized thematic workshops are planned to take place during each year of the project.

Activities during the second year included the general user meeting (February 2012), advanced cross sectional workshop (June 2012) and two thematic workshops on climate modelling (October 2011) and cultural heritage (May 2012). The first MEWEMS training was held in parallel with the advanced cross sectional workshop (June 2012). During the second year the following topics were covered (in brief):

1. GPGPU programming
2. Parallelization using #pragma programming
3. MPI
4. Partition theory
5. Computational fluid dynamics (CFD) using open source codes
6. Molecular dynamics and computational biology using open source codes
7. 3D imaging and modelling for cultural heritage
8. Climate modelling and atmospheric physics

Specific activities for the third and fourth year will cover:

1. General GPU programming
2. More parallel programming techniques
3. More diverse HPC use and applications such as CFD, computational biology and molecular dynamics
4. Advanced interactive workshops on digitization and cultural heritage data acquisition techniques, rendering and data visualization, on synchrotron radiation data analysis applications and climate modelling codes.

5.1 First Workshop on Climate-Related Research (Nicosia, Cyprus, October 11-13)

The number of attendees at this event was 17. The school was held from 11 to 13 October 2011 at the premises of the Cyprus Institute in Nicosia, Cyprus. The objective of the workshop was to provide highly motivated trainees interested in fields of climate modeling and high performance computing the fundamental skills in climate research and numerical modeling. The program covered topics in basic atmospheric physics and dynamics, coupling of complex sea-air regimes, numerical modeling of atmospheric flows and regional climate modeling. The workshop sessions included

- Atmospheric Science and Global Change.
- Numerical Modeling of Atmospheric Flows.
- Coupled Atmosphere-Ocean Modeling.
- Regional Atmospheric Dynamics.
- Regional Climate Change Modeling.

5.2 Advanced Cross-sectional Workshop (Nicosia, Cyprus, February 6-9, 2012)

The workshop was held at The Cyprus Institute between 6-9 February, 2012. A total of 54 participants from various countries attended the workshop . The workshop was composed of four different Special Interest Groups which ran in parallel across the 6th and 7th of February. These were the following:

- Computational fluid dynamics (featured software: OpenFOAM)
- Graph partitioning (featured software: metis/parmetis)
- Molecular Dynamics (featured software: GROMACS)
- Computational Biology & Bioinformatics (MrBayes & RAxML)

A further two different Special Interest Groups also run in parallel on the 8th of February. These were the following:

- GPU Kernel development for application porting (featured software: CUDA / OpenCL)

- Scalasca Introduction

Further to this, there was also a one hour session on “Parallel Programming with #pragmas” with the main language OpenMP. The workshop ran smoothly and received very good and positive feedback from the attendees.

5.3 Thematic Workshop in Cultural Heritage (Nicosia, Cyprus, May 9-11, 2012)

The workshop was held at The Cyprus Institute between the 9-11 of May, 2012. A total of 30 participants from various countries attended the workshop. The event was co-organised with V-Must NoE project; CARARE and Linked Heritage projects were presented as well, TIEM activities were part of the teaching material.

The program was balanced between theoretical aspects and field / laboratory practice on most innovative digital and imaging technologies and methodologies applied to Cultural Heritage research. They covered the entire research pipeline of data acquisition, archiving, processing and publication. Here is brief description of the contents:

- An introduction to the topic of the workshop and the new trends in Digital Cultural Heritage.
- Critical review of the most innovative applications of Augmented Reality and Virtual Reality in the Cultural Heritage field.
- Introduction to the concept of digital ancient landscapes and digital museology, through the new field of virtual museums.
- Introduction to photogrammetry and how it is applied in 3D documentation of tangible Cultural Heritage.
- History of stereoscopy and its applications in Cultural Heritage, introducing to the participants the visualization facilities of the Institute.
- Introduction on the use of laser scanners and photogrammetric 3D imaging in the field, 3D documenting an archaeological excavation and finds.
- Introduction to Meshlab, a major open-source software for processing 3D data.
- Introduction of the concepts of metadata, mapping tools and Europeana.
- Introduction of Medici, an online accessible digital repository for Cultural Heritage.
- Introduction to concepts of interfaces design, human-computer interaction and access to digital repositories of knowledge.

The workshop was in cooperation with WP2. WP4 covered the expenses for the trainers and some of the other expenses (fraction of lunch cost, dinner breaks and transportation) WP2 covered the remaining expenses and expenses for the trainees.

5.4 3 Day General User Meeting and MEWEMS Training (Nicosia, Cyprus, June 25-27, 2012)

The event was organized by CyI, NARSS, and JSC. The event was originally scheduled to take place in Egypt and hosted by NARSS. However, during the same period there were the run off elections in Egypt and it was expected to be quite risky to hold an event in Egypt during that period. The organizing committee and WP4 members decided it would be best to host the event in Cyprus one more time. The school was organized at the Athalassa campus of the former Higher Technical Institute at the entrance of Nicosia. The number of participants in this event were 44.

Since the event also hosted the first MEWEMS meeting, it is coordinated as well with WP5. The budget for the training, trainers and fellows for the general user meeting were from the

WP4 and WP2 budget, whereas the budget for the female participants accepted as fellows in the MEWEMS meeting was from the WP5 budget. Adding both events together enabled us to share the cost of trainers and also tailor the money for the fellows coming in from different regions of the Mediterranean to cover the increasing cost of travel from some countries.

The program was designed to introduce trainees to #pragma based programming. These are parallel programming paradigms that allow for inexperienced parallel programmers to start parallelizing their serial code in a fast and easy manner. This method enables the code to be parallelized progressively meaning that part of the code can be parallelized, run on a parallel machine before having to alter and parallelize all of the remaining code. This allows for easier performance gain analysis of the partial code parallelization which occurs.

Feedback on the organization of the school was in general very good and positive. Specifically, 93% said that the venue of the workshop was excellent/good, 97% found the overall organization excellent/good and 94% said that the information about the workshop was excellent/good.

With respect to the training offered, 91% of the participants found the topics of the school to be relevant to their research. Furthermore, 87% found that the pace of teaching was adequate, 94% that the material presented was appropriate and 97% found that the material in the workshop was related to the announcements and schedule.

5.5 Thematic Workshop in Cultural Heritage Alexandria, September 24-26, 2012)

Preparation for this workshop is currently underway. This workshop will be held at BA in Alexandria, Egypt, and will be held in cooperation with WP2. Following the successful collaboration with V-MUST during the 1st Cultural Heritage workshop, this event will again be co-hosted by V-MUST. In addition to technological aspects of digital cultural heritage, the workshop will also focus on visualisation aspects as well as connecting technology to institutional stake holders like curators.

5.6 Second Workshop on Climate-Related Research (CyI, October 09–11, 2012)

The second thematic workshop on climate-related research is being arranged by CyI and MPG. It will be held from 09 to 11 October 2012 at the Cyprus Institute. The meeting targets young researchers from the region and will comprise lectures and demonstrations on

- The LinkSCEEM-2 project
- Introductory Atmospheric Chemistry
- History of the Atmosphere
- The Troposphere
- The Stratosphere
- Aerosols
- Chemistry Climate Modeling

5.7 Synchrotron Radiation Research Thematic Training Workshop - Second LinkSCEEM summer school

The main objectives of the SESAME – LinkSCEEM Summer School is to motivate the scientists in the Middle-East region with topics related to Synchrotron Radiation (SR) and High Performance Computing (HPC) and the applications of these topics in their respective

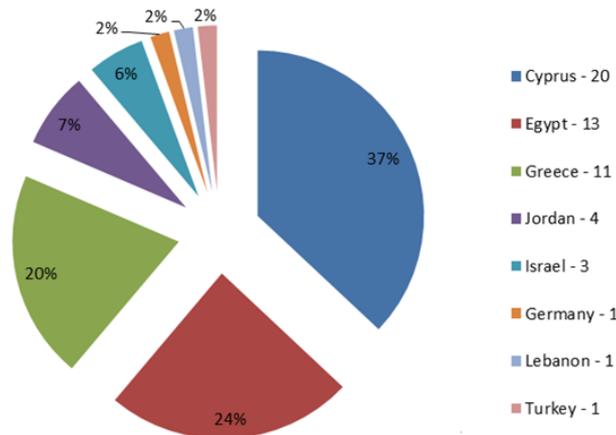
field of research. On the other hand, this activity will give an opportunity to participants to present their research and projects to school trainers and trainees. Moreover, the school will help to establish a potential user's base of the HPC users in SR research domains within the SESAME region.

5.8 Demographics of Different Workshops

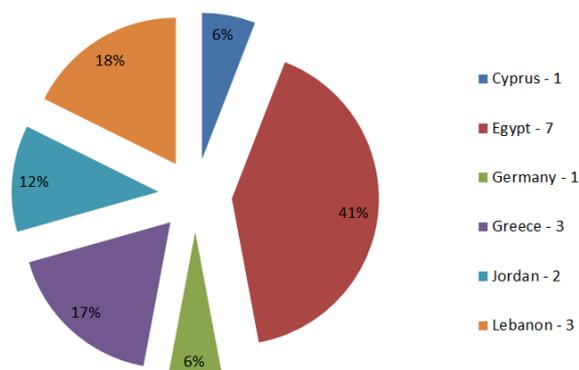
The following table shows the total number of participants in all the events so far. The figures show the breakdown across the partners and some Eastern Mediterranean countries.

Event	Number of Participants
First Workshop on Climate-Related Research, Nicosia, Cyprus 11–13 October 2011	17
Cyprus Advanced HPC Workshop Winter 2012 Nicosia, Cyprus 6-8 February 2012	54
1st Cultural Heritage Thematic Workshop	30
3 Day General User Meeting and MEWEMS Workshop (June 25th-27th)	44

Cyprus Advanced HPC Workshop - Winter 2012
Proportion of Participants per country



LinkSCEEM2 - Climate Modeling Thematic Workshop
Proportion of Participants per country



5.9 Summary of User Feedback

In general, all 3 day meetings were a success as seen from the detailed meeting reports that are included on the eniac website. During the 1st winter and summer workshops more effort was placed on teaching computer HPC skills. The users in general accepted the material and recommended that the training would continue for longer periods. The thematic specialized workshops held (Synchrotron Radiation and Climate) also met equal success in their research oriented goals. These workshops were more focused on delivering physics and less on the HPC side. During the 2nd year the specialized thematic workshops were focused more on the HPC needs to address the physics problems. The last winter workshop held in Nicosia during February 2012 addressed application and real industry needs. The feedback from the fellows attending the meeting was extremely positive and the training were able to fulfill two basic gaps: (a) need of HPC for specialized fields such as computational fluid dynamics, and (b) educating users how to use some of the parallel open source resources.

Follow Up Recommendation

For all previous workshops/winter/summer schools, there has been limited follow up from LinkSCEEM2 partners with trainees and fellows. Such follow up is needed for several reasons:

- A means to measure success of individuals using HPC later.
- A means to measure overall success of LinkSCEEM-2
- A means to advertise on the LinkSCEEM-2 website, stories of success
- A means to further promote the use of HPC by guiding fellows to use the available resources at NARSS, BA and CYI.

WP4 will extend it's focus to include training impact measures for the second half of the project.

- One negative comment that came up from a couple of participants was related to the amount of funding, mentioning that it was not satisfactory.

Because of this comment the approach to trainee funding was modified such as to take into account varying flight costs for individual countries. This was actually implemented in the last 3 day general meeting and MEWEMS workshop and most attendees gave positive feedback on the provided funding.

6 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.

During the second year there were initial discussions on how this service should be launched and on the level of service that will be offered. Several comments came out of these discussions:

1. Will the service be offered for start ups in the field of HPC. Here we are considering technical support on both hardware and software. What equipment should someone purchase? What are the software needs and so on.
 - Decided not to pursue this service.
2. Will the service provide technical assistance to current system administrators? A suggested form of this technical assistance is a tech forum hosted on the LinkSCEEM website.
 - Decided to pursue this service.
3. Will the service provide thematic assistance for the three scientific themes. What level of scientific help is offered or is it software help only?
 - Decided not to pursue this service since the demand of personnel is prohibitive and availability of all the technical staff is not feasible.
4. Will there be a dedicated answering service, or an email response system?
 - Yes, there will be a system that has been tested at CyI during the first year that issues tickets (emails to technical staff) that can answer the questions.

Some of the issues were discussed in the first and second quarter of the second year. However, no progress was made to materialize the consultancy system because of staff changes and the general work load related to start of the first LinkSCEEM production access. There will be more emphasis on this during the 3rd year of the project.