HP-SEE User Forum 2012, Belgrade

LinkSCEEM-2: Development of an HPC ecoSystem in the Eastern Mediterranean

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Scientific Coordinator for CaSToRC Research

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CaSToRC

Content

- **The Cyprus Institute – Who we are**

- **HPC at The Cyprus Institute**

- **LinkSCEEM – building the community**

- **Summary**

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- **The Cyprus Institute – Who we are**

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- **Summary**

The Cyprus Institute

An international research establishment, partnered with leading Institutions in the world, pursuing regional problems of global significance in the areas of:

- **Computation – Based Science and Technology – High Performance Computing**

- **Energy, Environment/Climate and Water**

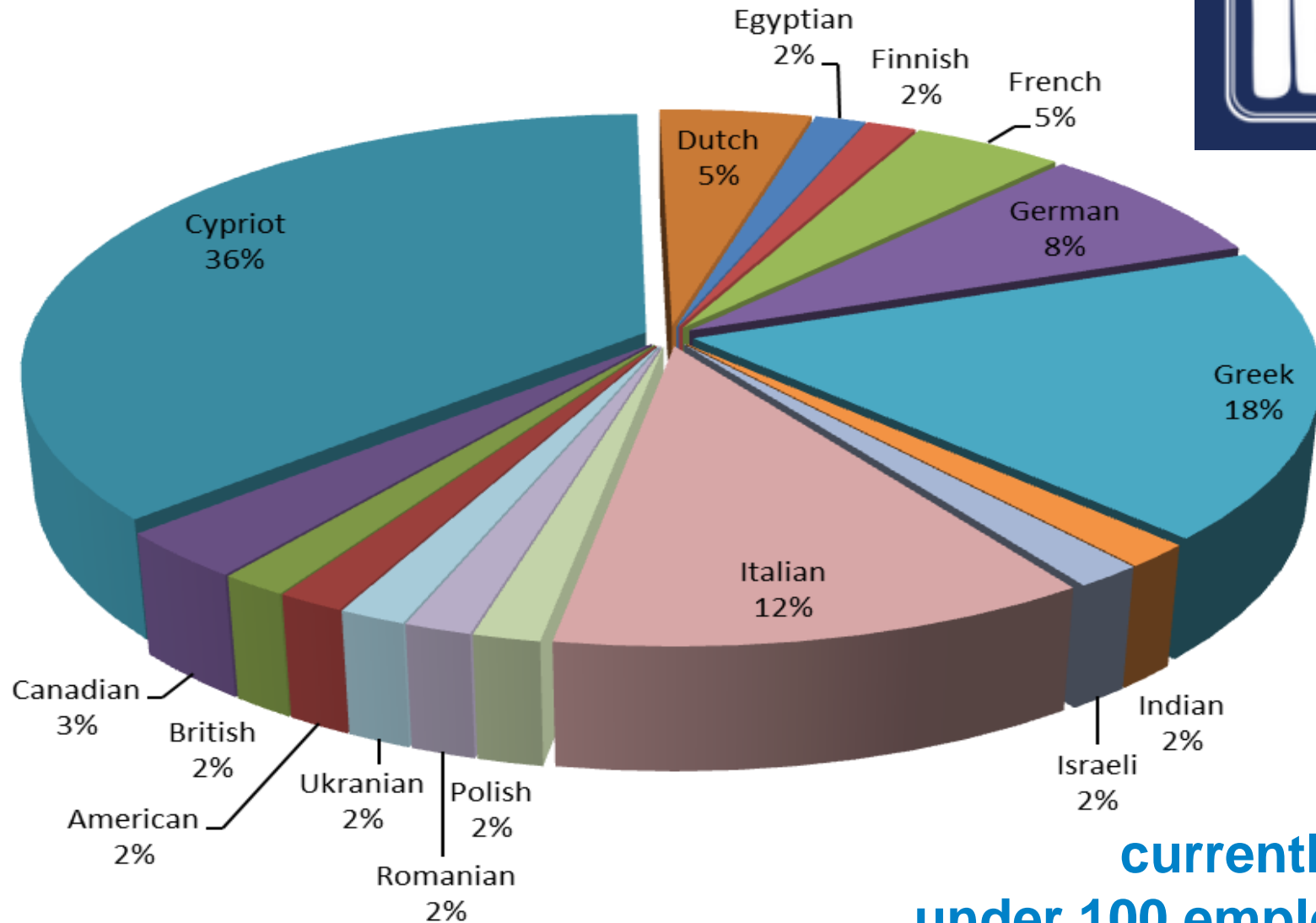- **Science and Technology in Archaeology & Culture**

The Cyprus Institute

The Cyprus Institute
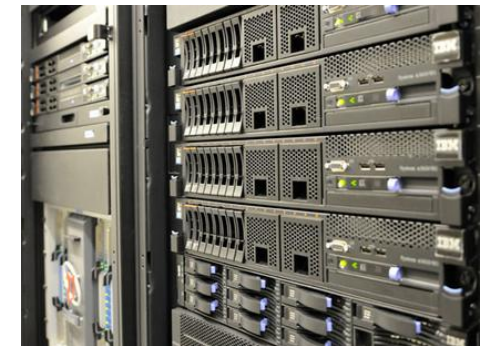
Nationality - Research staff

- Egyptian 2%
- Finnish 2%
- French 5%
- German 8%
- Greek 18%
- Italian 12%
- Indian 2%
- Israeli 2%
- Dutch 5%
- Cypriot 36%
- Canadian 3%
- British 2%
- American 2%
- Ukranian 2%
- Polish 2%
- Romanian 2%

currently just under 100 employees

The Cyprus Institute

- **Energy, Environment and Water Research Center (EEWRC) – opened in 2007**

- **Science and Technology in Archaeology Research Center (STARC) – opened in 2009**

- **Computation-based Science and Technology Research Center (CaSToRC) – opened in 2009**

The Cyprus Institute

STRATEGIC PARTNERSHIPS:

- **Centre de Recherche et de Restauration des Musées de France (C2RMF)**

- **Massachusetts Institute of Technology (MIT)**

- **Max Planck Society**

- **NCSA and University of Illinois at Urbana-Champaign (UIUC)**

- **University of California, Davis**

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- **Summary**

Computation-based Science and Technology Research Center (CaSToRC)

- To create a research program in computational science, engineering and underlying areas of scientific computing

- Development of and education in computation-based science and technology in Cyprus and the Eastern Mediterranean region

- To provide adequate computing resources to enable Cyprus and the Eastern Mediterranean research community to pursue forefront computing-related research

- To support the research missions of the other CyI Research Centers

Cy-Tera HPC facility

- **Cy-Tera (116 nodes: 98 CPU nodes, 18 GPU nodes)**
  - Hybrid CPU/GPU Linux Cluster Theoretical Peak Performance (TPP) 30.5Tflops

- **Euclid (6 GPU nodes)**

- **Prometheus (8 GPU nodes)**

- **Planck (24 CPU nodes)**

Cy-Tera Strategic Infrastructure Project

- **A new research unit to host a HPC infrastructure**
  - Create infrastructure to host a HPC unit
  - Procure HPC hardware and establish operations for such system
  - Initiate research on the system
- **RPF funded project**
  - The Project Cy-Tera (ΝΕΑ ΥΠΟΔΟΜΗ/ΣΤΡΑΤΗ/0308/31) is co-financed by the European Regional Development Fund and the Republic of Cyprus through the Research Promotion Foundation

ΚΥΠΡΙΑΚΗ ΔΗΜΟΚΡΑΤΙΑ

ΔΙΑΡΘΡΩΤΙΚΑ ΤΑΜΕΙΑ
της Ευρωπαϊκής Ένωσης στην Κύπρο
οι ιδέες μας, πράξη και ανάπτυξη

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- **Summary**

Development of a HPC ecoSystem in Cyprus and the Eastern Mediterranean
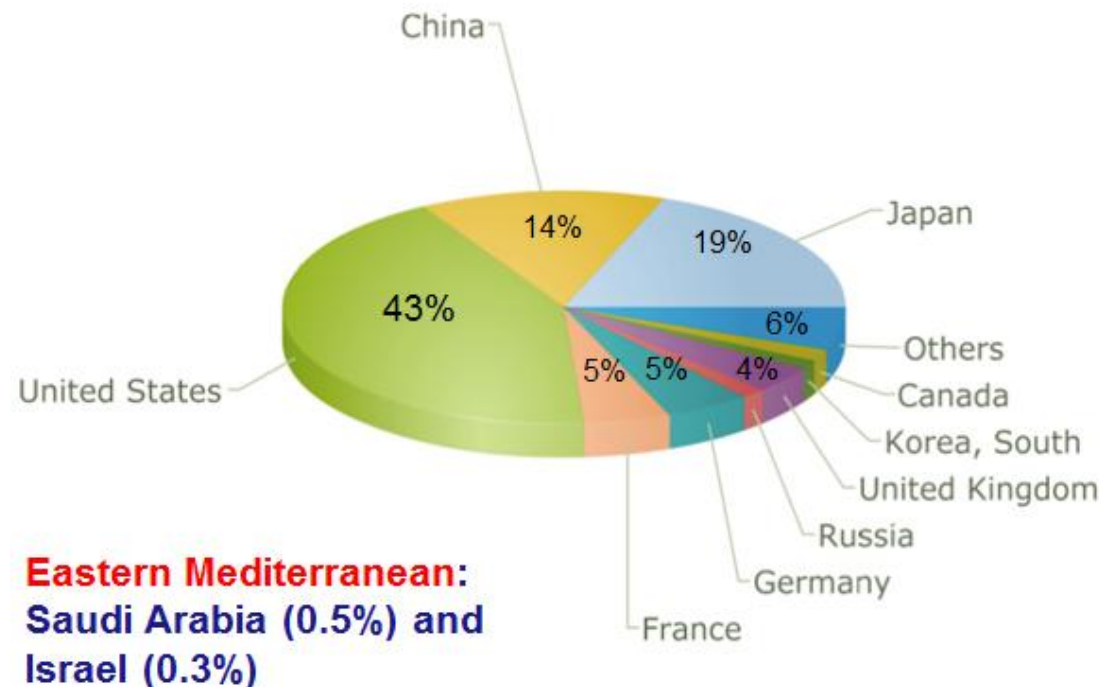

HPC infrastructure

HPC user

HPC user community

LinkSCEEM-1 Assessment stage

- **LinkSCEEM-1 project run from 2008-2009**
  - assessment of HPC resources and users in the Eastern Mediterranean
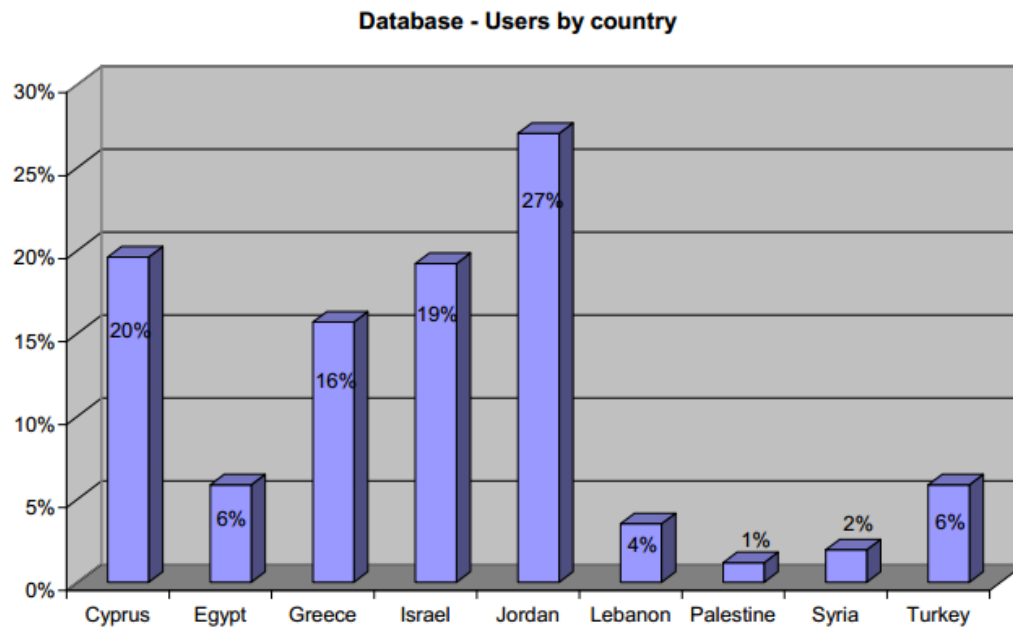
  - lack HPC resources
  - lack of connectivity

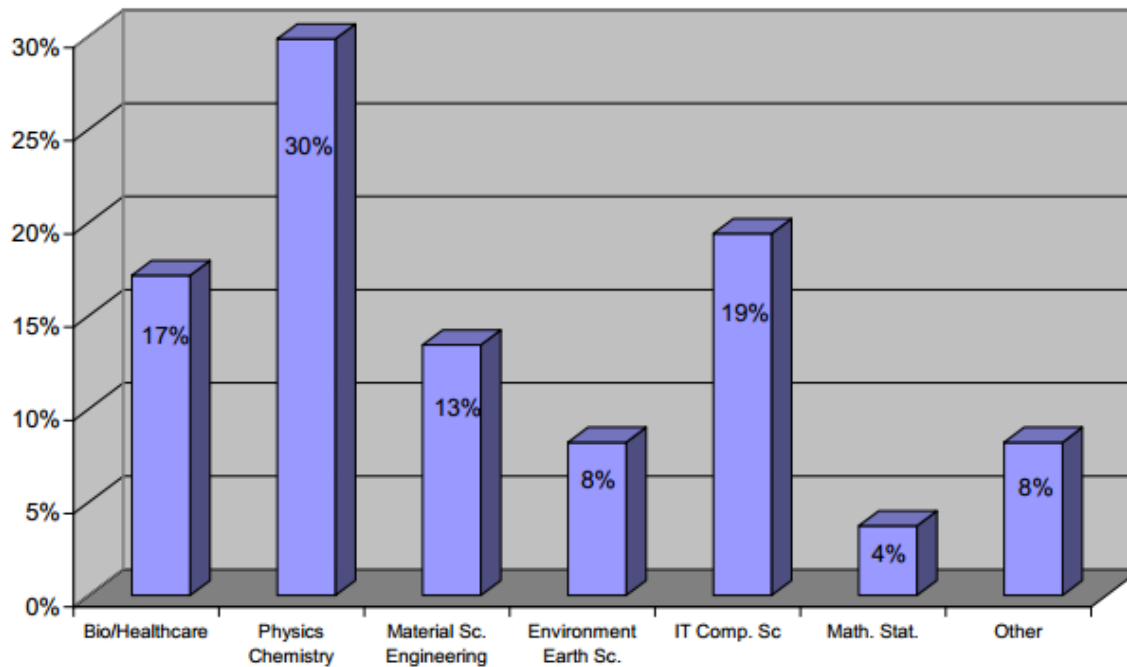countries by HPC resources (status Nov 2011)

China

United States 43%

14%

Japan 19%

6%

Others
Canada
Korea, South
United Kingdom
Russia
Germany
France

5% 5% 4%

Eastern Mediterranean:
Saudi Arabia (0.5%) and
Israel (0.3%)

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LinkSCEEM-1 Assessment stage

- **LinkSCEEM-1 project run from 2008-2009**
  - there are users in the region

Database - Users by country

CaSToRC database 2009
(347 contacts)

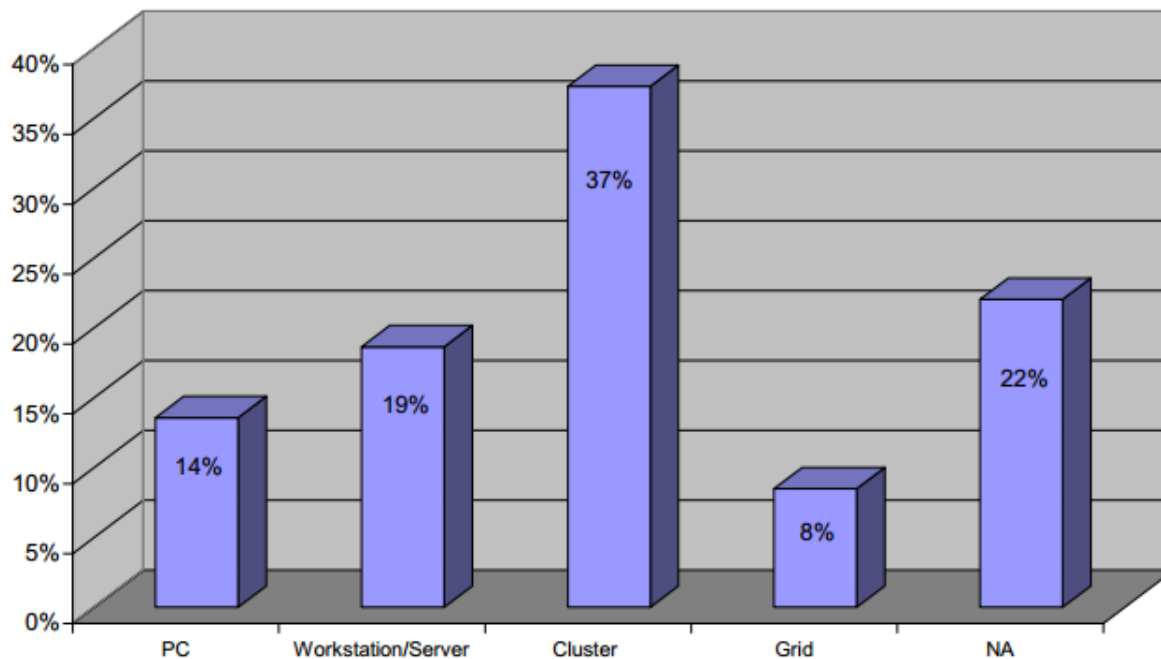# LinkSCEEM-1 Assessment stage

- **LinkSCEEM-1 project run from 2008-2009**
  - there are users in the region

CaSToRC database 2009
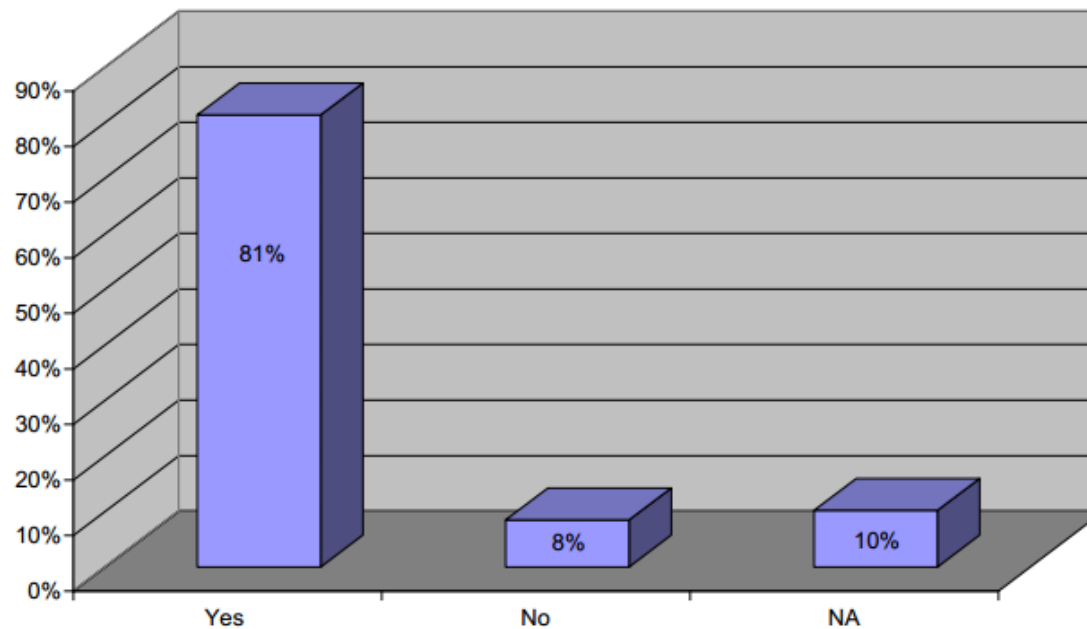(347 contacts)

LinkSCEEM-1 Assessment stage

- **LinkSCEEM-1 project run from 2008-2009**
  - there are users in the region

Available resources
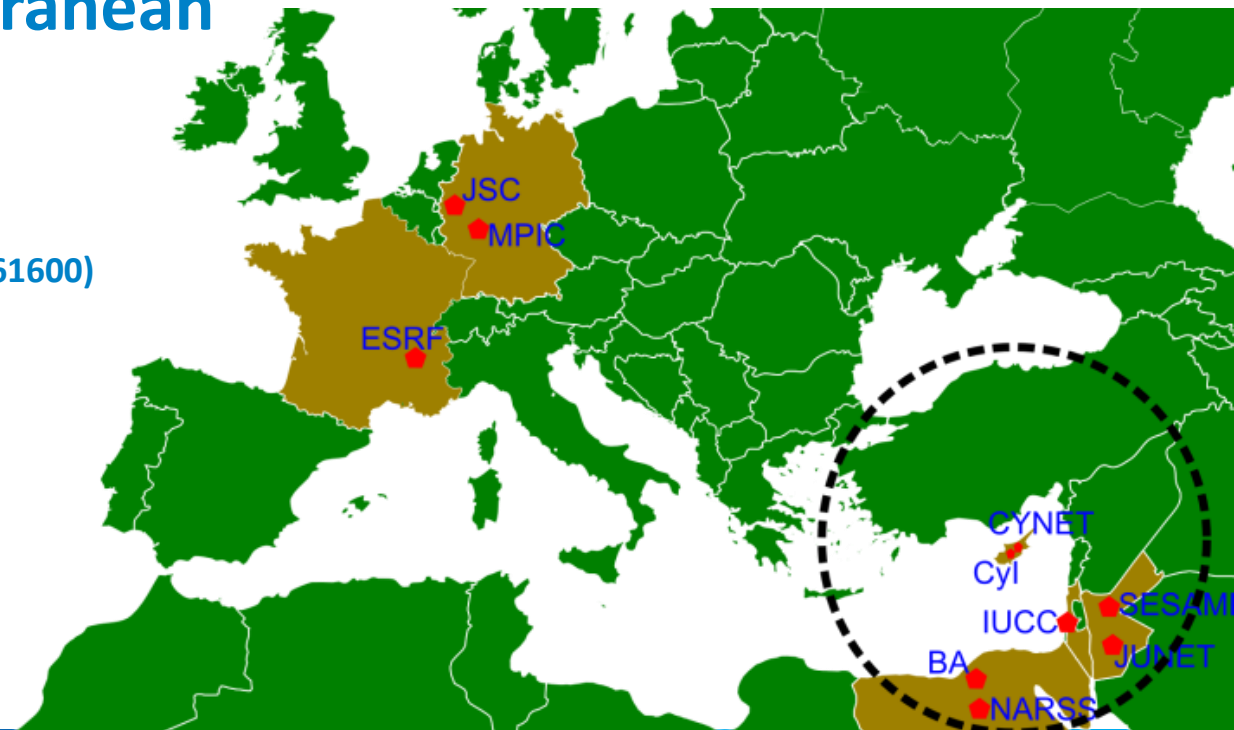(LinkSCEEM-1 survey 59
participants)

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LinkSCEEM-1 Assessment stage

- **LinkSCEEM-1 project run from 2008-2009**
  - there are users in the region

Need for additional resources
(LinkSCEEM-1 survey 59
participants)

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LinkSCEEM-1 Assessment stage

- **The assessment of the region highlighted here are users in the region, but**

  - more HPC resources needed

  - more raining needed

  - collaboration in the region needs to intensify

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Establish a HPC EcoSystem in the Eastern Mediterranean – LinkSCEEM-2

- **Enlarging the European Research Area**

- **Enabling science in the Eastern Mediterranean**

- **EU-funded FP7 project**
  (under grant agreement no RI-261600)

Project consortium

- **Regional research institutions and international centres of excellence in high performance computing (HPC)**
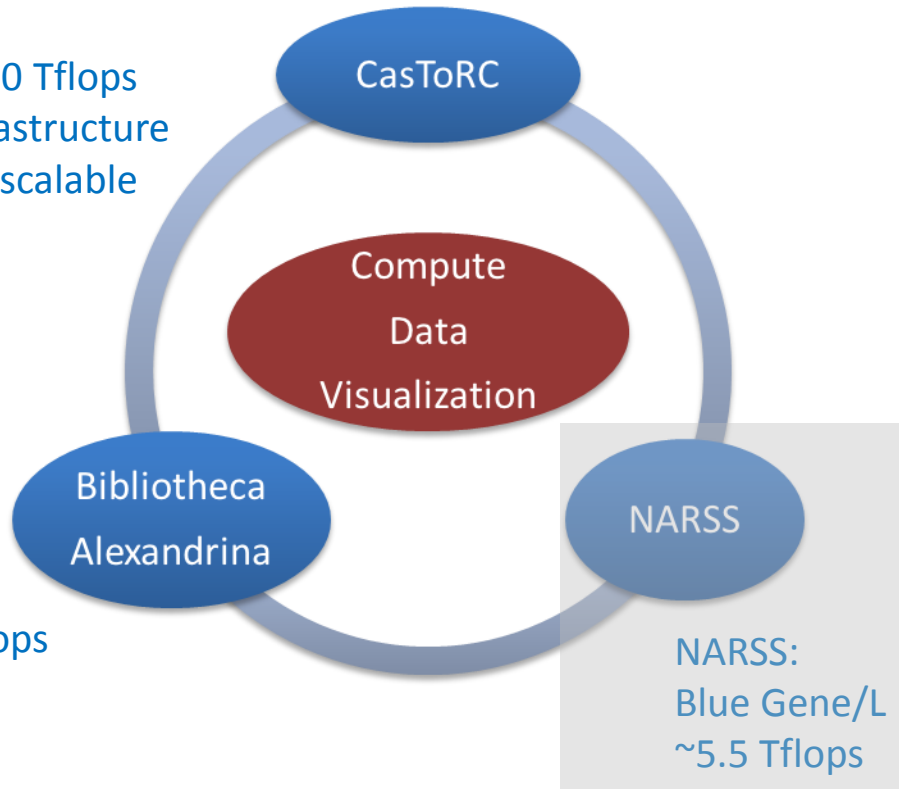
Project objectives

- **Integrate regional computational resources**

- **Create user support and training programs**

- **Enable research of particular relevance to the region (Climate, Cultural heritage, Synchrotron)**

- **Contribute to the upgrade of the regional network connectivity**

- **Build strong links to the European Research Area in accord with the European Neighbourhood Policy**
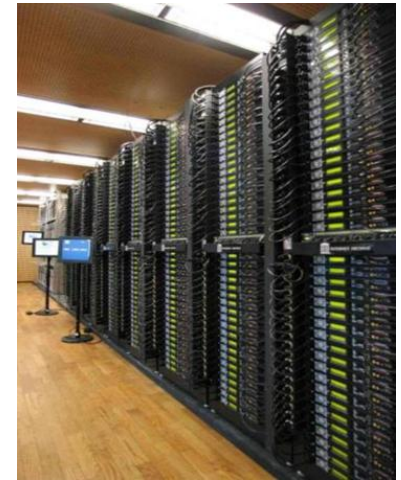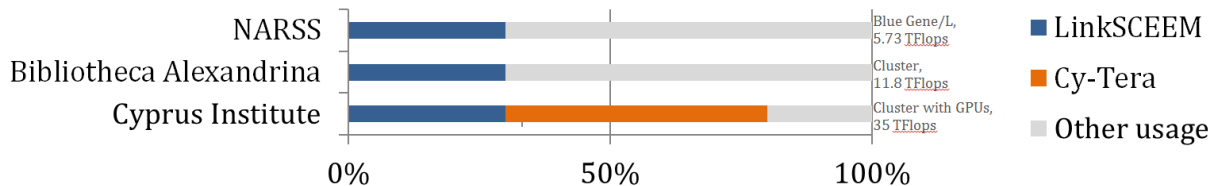
HPC facilities within LinkSCEEM

CaSToRC
- Cy-Tera machine, ~30 Tflops
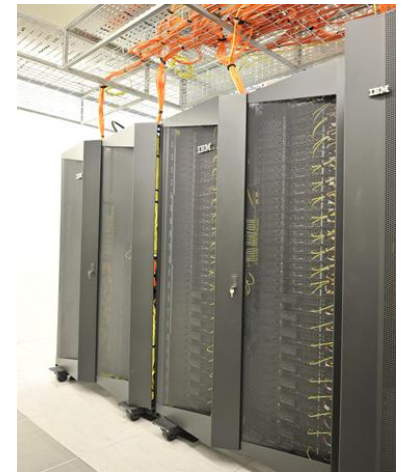- 3D visualization infrastructure
- Data storage 300TB scalable to 1PB

The BA archive system of 43 racks

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Compute
Data
Visualization

Bibliotheca Alexandrina

NARSS

Bibliotheca Alexandria:
- SUNcluster of ~12 Tflops
- Storage of 1.6 PB

NARSS:
Blue Gene/L
~5.5 Tflops

NARSS			Blue Gene/L, 5.73 TFlops
Bibliotheca Alexandrina			Cluster, 11.8 TFlops
Cyprus Institute			Cluster with GPUs, 35 TFlops

0%   50%   100%

- LinkSCEEM
- Cy-Tera
- Other usage

The Cy-Tera machine at CaSToRC

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HPC facilities within LinkSCEEM

- **Implemented HPC Baseline Configuration across sites**
  - Users should have a consistent documented environment across HPC sites
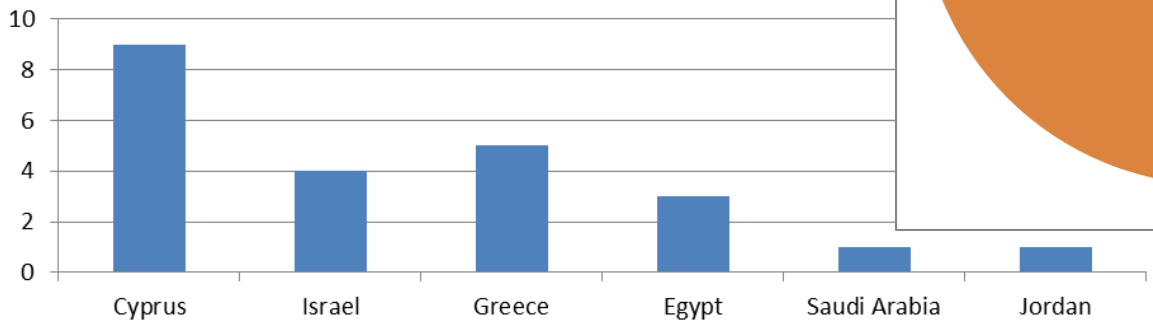 - Technical personnel maintain systems according to certain policies
- **Joint calls of participating HPC centres**

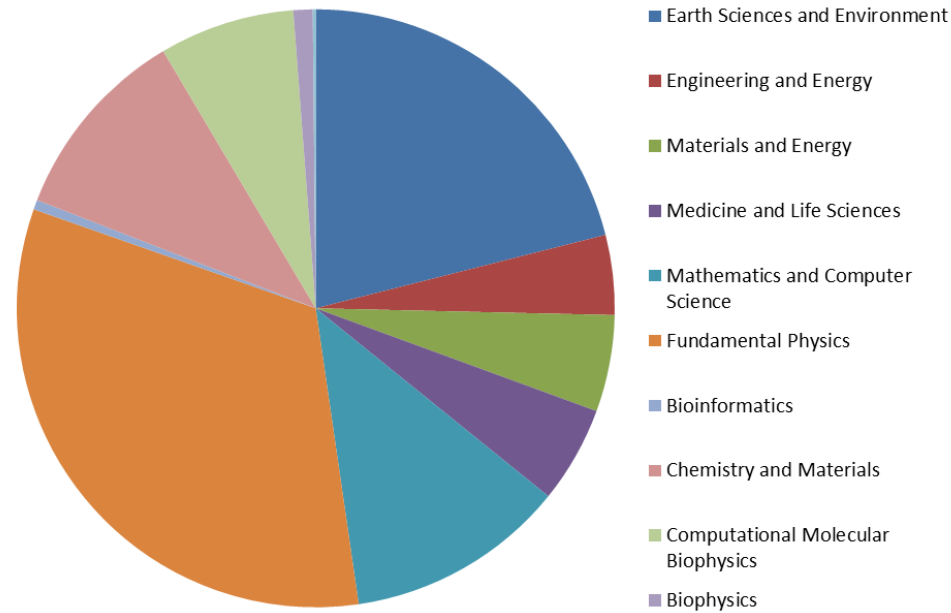|	Participating Shared Resource Centers are BA, Cyl, NARSS			
Policy tag #	Policy Topics	BA	Cyl	NARSS
LS2_05-01	Multiple-Version Software	✅	✅	👍
LS2_05-05	Queue Names	✅	✅	
LS2_05-06	Login Shells	✅	✅	👍
LS2_06-01	Open Source Math Libraries	✅	👍	👍
LS2_06-04	Editors and Scripting Tools	✅	✅	👍
LS2_06-05	Set of Debuggers	✅	✅	
LS2_06-15	Sample Code Repository	✅	✅	👍
LS2_06-17	Multiple-Version Software Access via Modules	✅	✅	👍
LS2_06-19	Open Source Utilities	✅	✅	👍
LS2_07-02	Open Source Performance and Profiling Tools	✅	✅	👍
LS2_07-03	Common Set of Open Source Compilers	✅	✅	👍
LS2_10-01	New/Returning User Welcome Letter	✅	✅	👍
LS2_10-02	Common Open Source High Productivity Languages	👍	👍	👍
LS2_11-99	GPU Productivity Environment	N/A	👍	N/A
LS2_11-98	Common Set of Environment Variables	✅	✅	
LS2_11-97	Climate Science Productivity Environment		👍	
LS2_11-96	Common Set of Commercial Compilers	✅	✅	
LS2_11-95	Molecular Dynamics Productivity Environment		👍	

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HPC facilities within LinkSCEEM

- **First LinkSCEEM production access since May 2012**

Distribution of CPU resources by field

- Earth Sciences and Environment
- Engineering and Energy
- Materials and Energy
- Medicine and Life Sciences
- Mathematics and Computer Science
- Fundamental Physics
- Bioinformatics
- Chemistry and Materials
- Computational Molecular Biophysics
- Biophysics

Number of submissions by country

Country	Submissions
Cyprus	9
Israel	4
Greece	5
Egypt	3
Saudi Arabia	1
Jordan	1

User Support and Training

- **User support/training**
  - User support services (helpdesk)
  - Online services (website, training portal)

- **9 annual training events**
  - Four 1-day user meetings
  - One 3-day general user meeting
  - One 3-day advanced cross-sectional workshop
  - Three 3-day thematic workshops

User support webpage

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User Support and Training

- **Extensive online documentation for users**
  - welcome packs
  - information on software, queuing etc.
- **Training portal (http://linksceem.eu/ATutor)**
  - online training courses in topics relevant to HPC

Course

1.1 Parallel Computing Explained
Category: Parallel Computing

2.1 Introduction to MPI
Category: HPC Programming

2.2 Introduction to OpenMP
Category: HPC Programming

2.3 Debugging Serial and Parallel Codes
Category: HPC Programming

2.4 Multilevel Parallel Programming
Category: HPC Programming

2.5 Intermediate MPI
Category: HPC Programming

3.1 Parallel Numerical Libraries
Category: HPC Applications and Libraries

4.1 Introduction to Performance Tools
Category: HPC Performance Tuning

4.2 Performance Tuning for Clusters
Category: HPC Performance Tuning

4.3 Introduction to Multi-core Performance
Category: HPC Performance Tuning

5.1 Introduction to Visualization
Category: Data and Scientific Visualisation

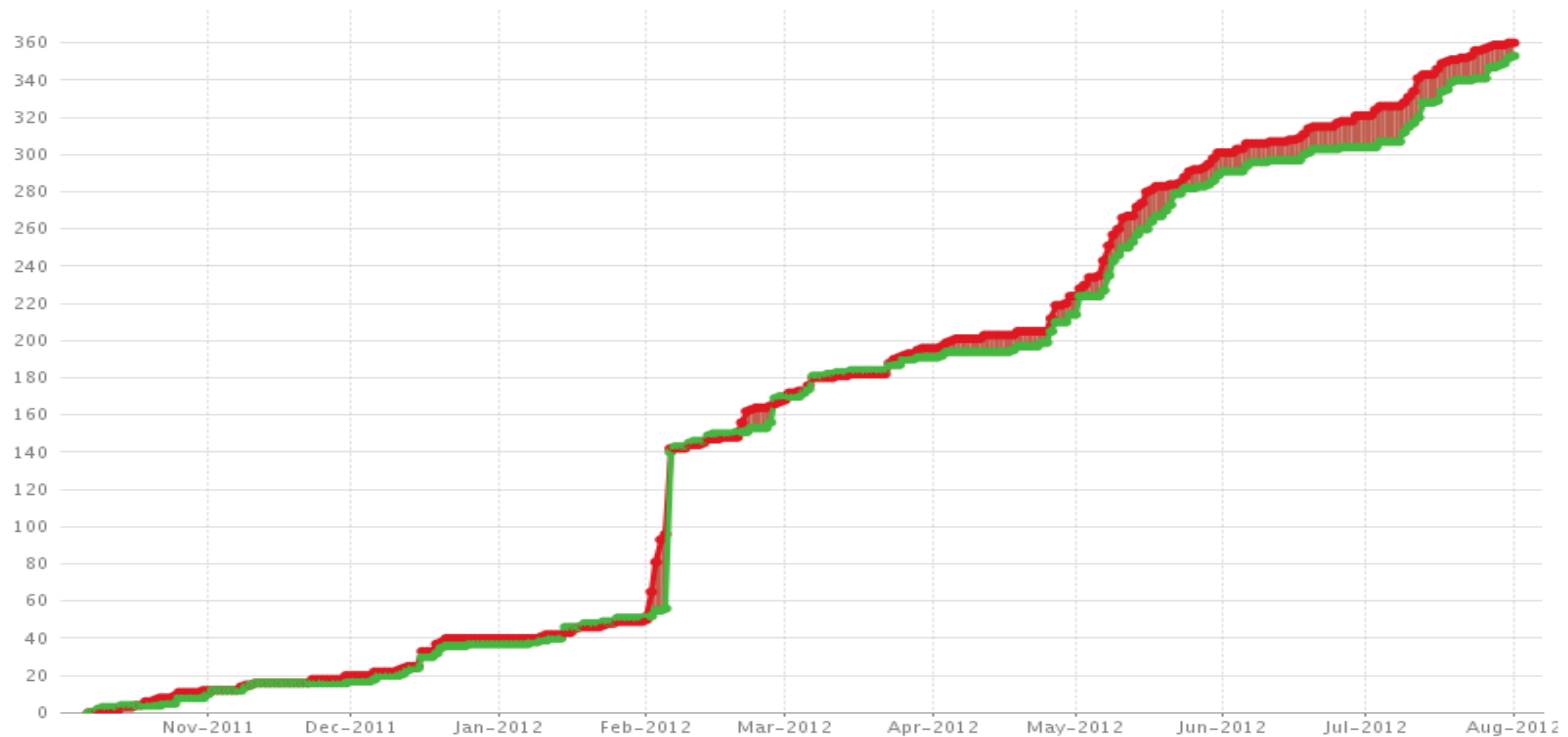5.2 Tuning Applications for High Performance Networks
Category: Data and Scientific Visualisation

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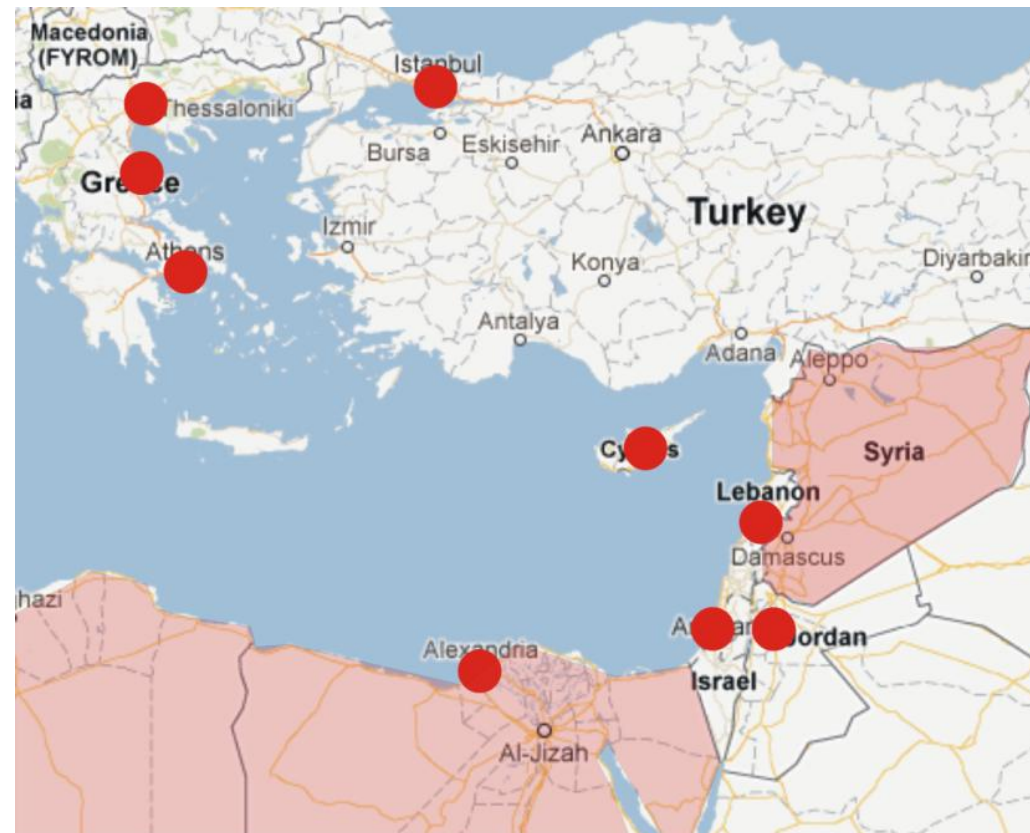# User Support and Training

- **User helpdesk**

User enquiries over the last 300 days (red: requests, green: requests resolved)

User Support and Training

- **presence in a difficult region**
  - 8 one day user meetings
  - 2 general User meetings (3 days)
  - 2 cross sectional work shops (3 days)
  - 6 thematic workshops (3 days)
  - participation in numerous community events
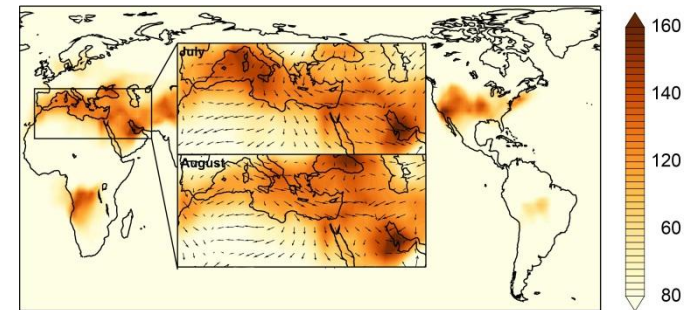
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Project Research Themes

- **Cross sectional research**
  - performance analysis and optimisation for community codes

- **Climate**
  - development of atmospheric chemistry climate models to study the Eastern Mediterranean region

- **Digital cultural heritage**
  - imaging and image processing of regional artifacts

- **Synchrotron radiation data analysis**
  - synchrotron data analysis and simulation on GPU systems

Polynomial Texture Mapping of a copy of an ancient coin from Petra, Jordan, depicting Alexander the Great or one of his successors

Mediterranean and Middle East hot spot of ozone air pollution

Project Research Themes

- **Achievements during the first 2 years**
  - Compliance matrix for participating HPC centres (set of scientific and mathematical libraries)
  - Introduction of UNICORE for workflows and access (on-going)
  - Performance analysis of community codes using Scalasca
  - Porting of community codes for GPU's
  - Porting and optimising the global ECHAM/MESSy Atmospheric Chemistry (EMAC) climate model to the CaSToRC and BA
  - Algorithmic improvements of the EMAC radiation code
  - Development of data repository for Cultural Heritage and Climate studies (Medici)

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Summary

- **A clear need for development of a HPC user community was identified in the region**

- **LinkSCEEM projects address these needs by**
  - providing HPC resources to the region
  - training the user community
  - transferring knowledge form experienced organisations
  - initiating and supporting HPC related research of regional relevance

Establishing a sustainable user community is a long term effort ...

Summary

... and LinkSCEEM helps to pave the way

Join the community!

- **our online material is for free and for everyone (regardless where you are)**

www.linksceem.eu

Linked in **LinkSCEEM group**

Thank you

www.cyi.ac.cy

www.linksceem.eu

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