Synchrotron-light for Experimental Science and Application in the Middle East

SESAME and LinkSCEEM Project

By SESAME Scientific Group

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LinkSCEEM-2

- **Linking Scientific Computing in Europe and the Eastern Mediterranean-Phase 2**
  - 48 month project
  - Funded by the EU FP7 Research Infrastructures support program
- **Follow-up and implementation of LinkSCEEM findings**
- **Main goal: Develop a High Performance Computing (HPC) eco-system in the Eastern Mediterranean region by integrating regional compute, data and visualization resources.**

Objectives

- **Optimally integrate regional computational resources utilizing expertise from established lead HPC centers**
  - develop and share best practices for managing integrated resources
- **Create user support and training programs, and an active networking process to engage research communities and enable scientists in the region to utilize HPC**
- **Enable research of particular relevance to the region in climate science, cultural heritage and synchrotron applications**

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LinkSCEEM-2 Partners

LinkSCEEM-2 Partners List

- The Cyprus Institute – CaSToRC
- National Authority for Remote Sensing and Space Sciences
- Bibliotheca Alexandrina
- Juelich Supercomputing Center
- National Center for Supercomputing Applications – University of Illinois
- ***S***ynchrotron-light for ***E***xperimental ***S***cience and ***A***pplication in the ***M***iddle ***E***ast (SESAME)
- Installation Europenne de Rayonnement Synchrotron (IERS) - ESRF
- Max Planck Institute
- KEAD (Cyprus Research and Academic Network)
- Jordanian Universities Network
- Inter University Computation Centre (IUCC)

What Is HPC?

- **Definition:** High-performance computing (HPC) is the use of parallel processing for running advanced application programs efficiently, reliably and quickly. The term applies especially to systems that function above a teraflop or 10^{12} floating-point operations per second. The term HPC is occasionally used as a synonym for supercomputing.

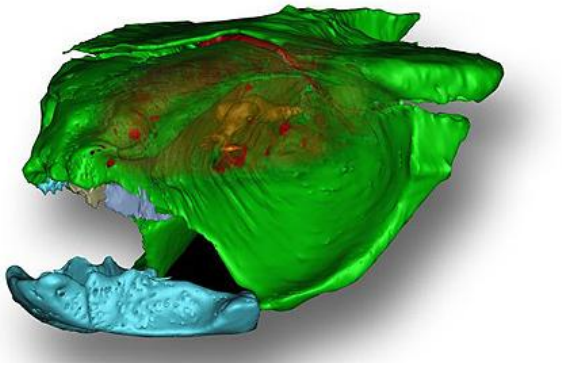
- **HPC Goal:** Reduce execution time - accommodate larger and more complicated problems.

HPC Users

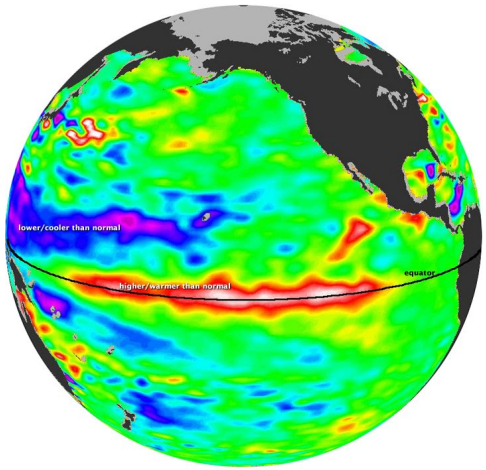
- The most common users of HPC systems are scientific researchers, engineers and academic institutions.
- Some government agencies, particularly the military, also rely on HPC for complex applications.
- High-performance systems often use custom-made components in addition to so-called commodity components. As demand for processing power and speed grows, HPC will likely interest businesses of all sizes, particularly for transaction processing and data warehouses.
- An occasional techno-fiends might use an HPC system to satisfy an exceptional desire for advanced technology.

HPC Solutions

- **Synchrotron applications**
  - Decrease the latency for data processing to allow significantly faster data analysis and simulation through the usage of GPUs

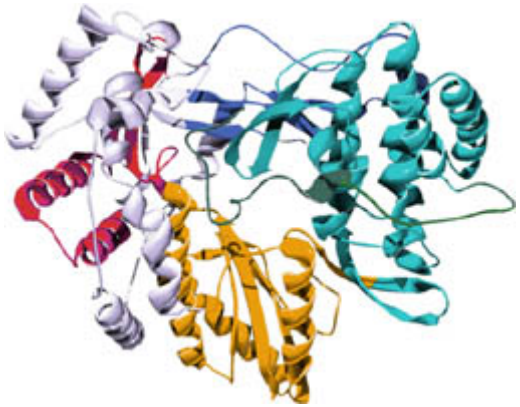


- **Climate Science**
  - Global climate change is a contentious topic these days, in large part due to the extreme complexity of the problem. As computational models improve, we may be better informed in our policy decisions, and able to act in a more unified manner.



HPC Solutions

- **Biochemistry**
  - Protein-folding attempts to determine the overall shape of a protein based on the sequence of amino acids; the effort may lead to better understanding of biological processes, and new medicines.



- **Chemistry**
  - Materials research helps to identify new materials, such as high-temperature superconductors, affordable electrodes for fuel cells, efficient catalysts, new methods of energy storage, etc.

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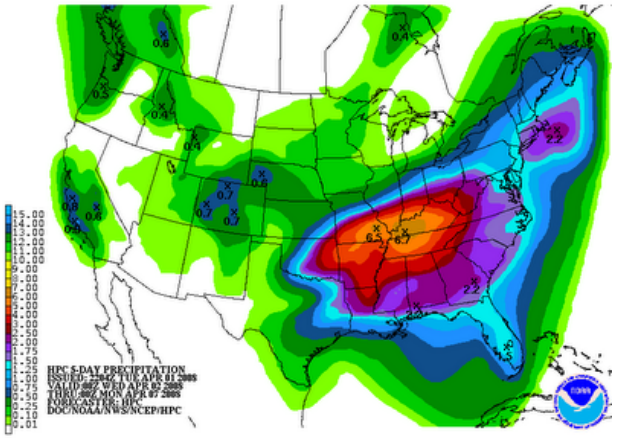
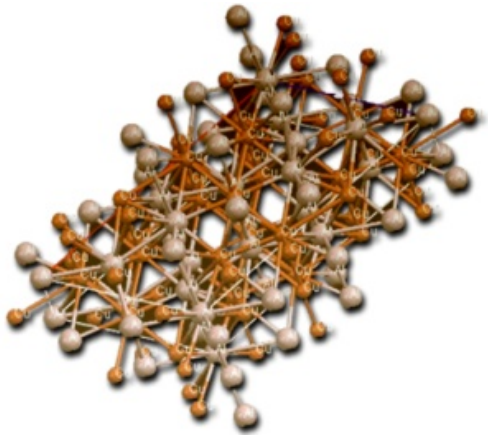
HPC Solutions

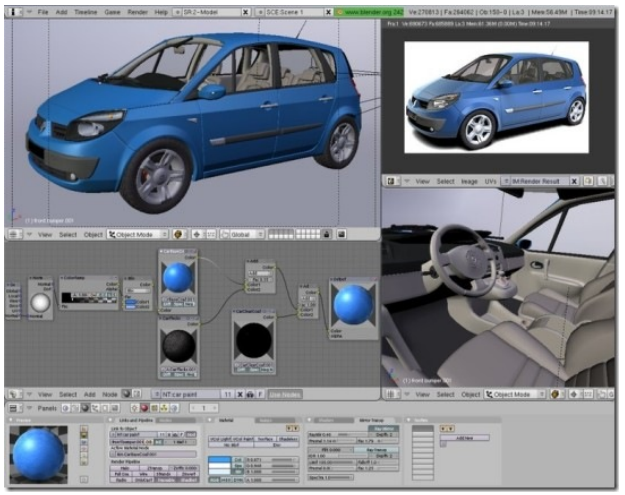
- **Environment Modeling**
  - The simulation of earthquakes can be startlingly complex. These simulations can be used to predict which areas are likely to experience a large earthquake, and what the conditions will be. This work helps inform building codes, development planning, and emergency action plans.
- **Material Science**
  - Characterization of the electronic, structural and dynamic properties of small, extended and massive atomic/molecular systems.
  - Applying the quantum/classical modeling and simulations in order to understand and to predict properties of micro-, nano- and macroscopic systems.

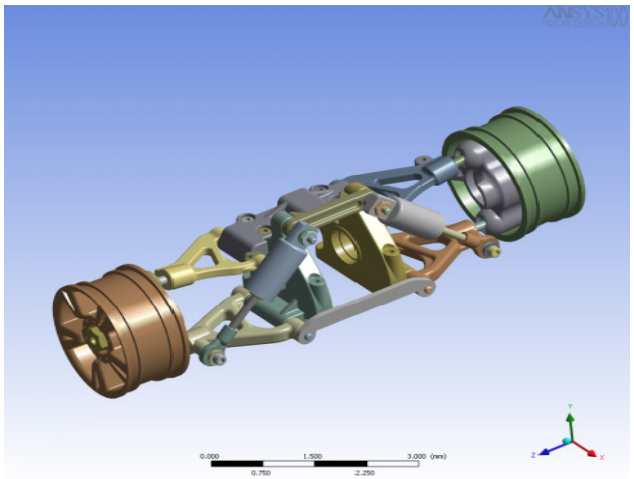




HPC Solutions

- **Industry**
  - Products: Prototyping is often an expensive and time-consuming process. Computer modeling can reduce the time and cost of physical prototyping and make optimization much easier.
  - Services: Many corporations handle large amounts of data, and deal with complex routings or decisions. Insurers, for instance, use models to calculate risk, while the oil/ gas industry uses seismographic data to determine where oil and gas fields are located underground. Wal-Mart optimizes supply chains, and Fed-Ex monitors and routes packages. The financial sector uses models to spot trends and calculate risks.



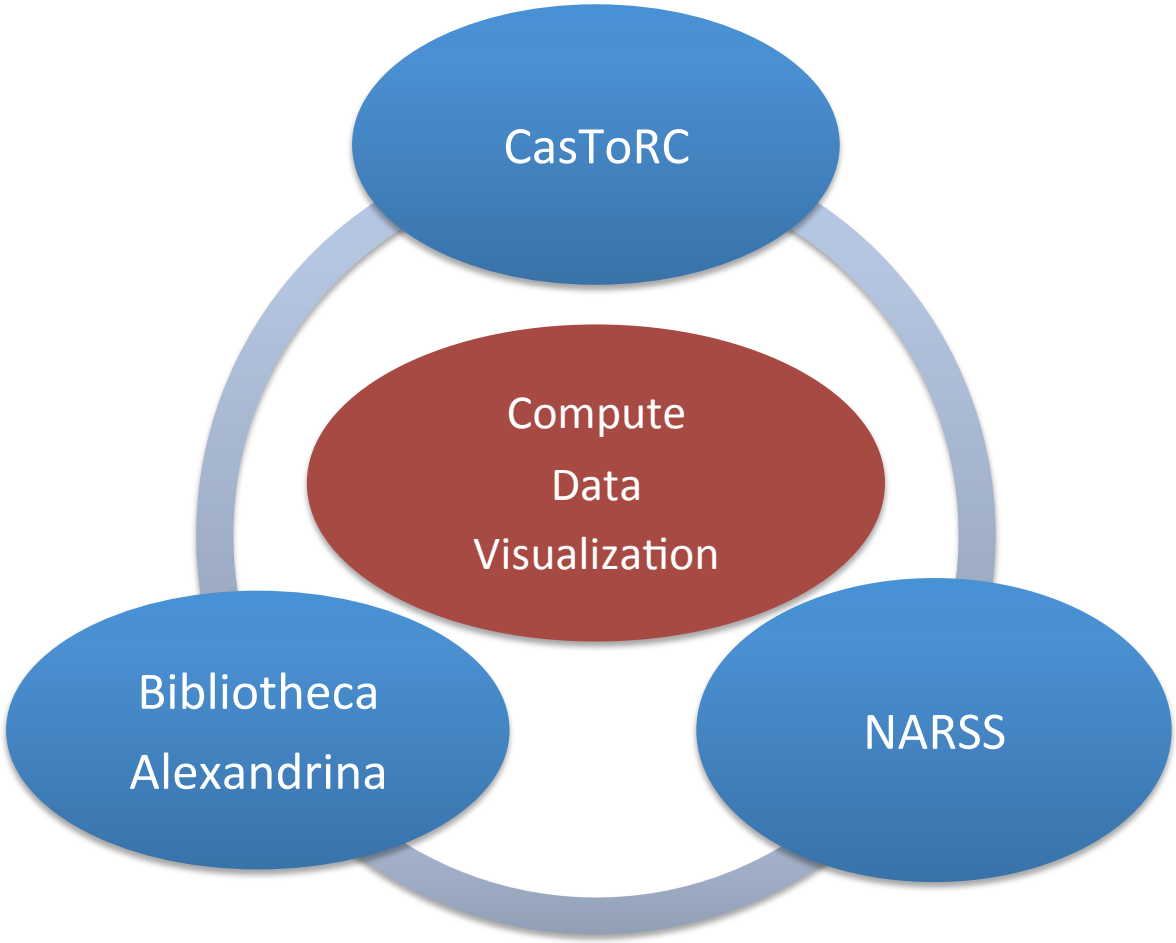


LinkSCEEM HPC Resources

LinkSCEEM-2 partners have three High Performance Computing (HPC) centers from the Eastern Mediterranean region:

- Computation based Science and Technology Research Center – Cyprus
- National Authority for Remote Sensing and Space Sciences (NARSS) – Egypt
- Bibliotheca Alexandrina - Egypt

Integration of HPC Resources



LinkSCEEM HPC Resources

- **Computation based Science and Technology Research Center (CaSToRC)– Cyprus**

  - CaSToRC (arch: x86_64 w. Tesla GPUs) system used for:
    - climate modeling
    - Astrophysics
    - high energy and plasma physics.
    - materials science
    - Chemistry
    - 3D visualization
    - Biology
    - financial and economic modeling.

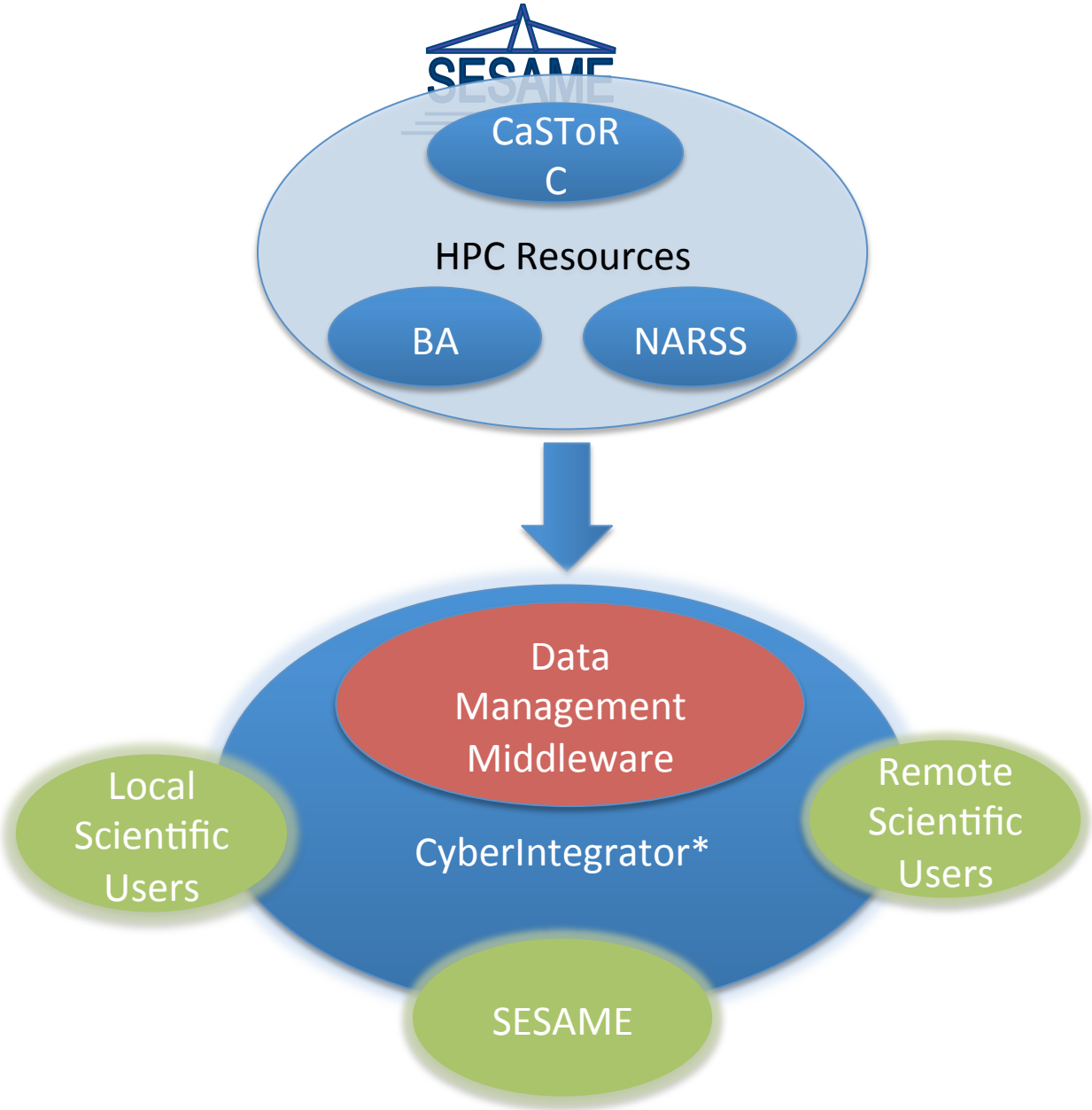
LinkSCEEM HPC Resources

- **National Authority for Remote Sensing and Space Sciences (NARSS) – Egypt**
  - NARSS (arch: BlueGene/L, PowerPC) system used for:
    - Geological applications and Mineral Resources
    - Agricultural Applications
    - Soil, and Marine sciences
    - Engineering Applications and Water Resources
    - Environmental Studies and Land use;
    - Data Reception Analysis and Receiving Station Affairs
    - Aerial Photography and Aviation;
    - Space Sciences and Strategic Studies
    - Scientific Training and Continuous Studies

LinkSCEEM HPC Resources

- Bibliotheca Alexandrina (BA)- Egypt

- BA (arch: x86_64) system used for:
  - 3D computer graphics
  - cultural heritage
  - analysis of the visualized data
  - Medical Visualization
  - Software developments.



* System developed at NCSA

Coordination Activities

- **Networking of User Communities**
  - Organization of general and thematic user meetings
  - Online communications and knowledge tools
  - Industrial networking program
  - Coordination with EU projects with overlapping goals
- **Management of Access to Resources**
  - Implement a peer review process for compute resources visualization systems and data repositories

Coordination Activities (cont.)

- **Training**
  - Develop a tiered and adaptive HPC training program
  - Provide a consultancy service
- **Dissemination and Outreach**
  - Organize a Computational Science International Conference, create awareness through outreach programs
  - Investigate sustainability of e-Infrastructure

Service Activities

- **User Support**
  - Tiered user support through help-desk, updated documentation material, user meetings and a performance consulting mechanism.
- **Network Connectivity**
  - Improve regional network connectivity by upgrading link between Cyprus and Jordan
- **Integration of Resources**
  - Develop software infrastructure for data management, linking software applications with hardware resources and providing a scientific workflow application.

Research Activities

- **Cross-disciplinary activities**
  - Facilitate the optimization of parallel applications on HPC through development of performance analysis tools
  - Adapt data management tools to specific data sets (i.e. climate, cultural heritage and synchrotron)
- **Thematic Research**
  - Climate Research
  - Cultural Heritage Research
  - Synchrotron Data Analysis and Modeling

Vision for the Future

- **Reinforce CaSToRC as an HPC regional partner facility**
  - offering resources to scientific communities in the region
  - promoting research and educational collaboration activities
- **Sustain efforts to promote HPC usage and create a virtual research community**
- **Focus on the exploration of activities that will enable the long-term sustainability of the LinkSCEEM-2 e-Infrastructure and community**

LinkSCEEM-SESAME

SESAME is a partner in the LinkSCEEM-2 Project across different WPs:

WP #	Short Name	Personnel / Month
WP2	Networking	2
WP4	Training	2
WP5	**Dissemination & Outreach**	**5 (Leader)**
WP6	User Support	1
WP8	Integration of resources	2
WP9	Cross disciplinary research	2
WP12	Synchrotron Radiation Research	7

International HPC Conference

News and Updates:

In collaboration with PRACE and LinkSCEEM, the international conference will be held in Cyprus **5 – 8 November, 2013.**

The Scientific and Local Organization Committees are defined.

CyI will take the lead with NCSA/SESAME for organizing the International HPC conference:

- **CyI and SESAME local organizing committee:**
  1. Stelios Erotokritou (CyI)
  2. Thekla Loizou (CyI)
  3. Jens Wiegand (CyI)
  4. Eleftherios Eleftheriou (CyI)
  5. Salman Matalgah (SESAME)
  6. Mostafa Zoubi(SESAME)
  7. Hafeez Hoorani (SESAME)
- **Scientific Program committee:**
  1. Hafeez Hoorani (SESAME)
  2. Jens Wiegand (Cyprus Institute)
  3. Tom Dunning (NCSA)

LinkSCEEM Website

- The new LinkSCEEM-2 website has been published in September, 2011 (www.linksceem.eu).
- After that, regular updates on the project website have been taken such as project reports, announcement of events, project news, etc.
- SESAME has prepared tutorials on how to deal with LinkSCEEM website for LinkSCEEM staff that to add \edit events, news articles, menus, etc.
- LinkSCEEM-2 website acts as a central user portal for access to user information. Moreover, it lists up-to-date information on future events for both:
  - LinkSCEEM events :

  (http://linksceem.eu/ls2/news-and-activities/events/events/events.html)
  - Other related events which appear as external links to other conferences and training events in the same fields: (Done yearly)

  (http://linksceem.eu/ls2/news-and-activities/events/hpc-upcoming-events/cat.listevents/2012/07/14/-.html).

Thank you….