JÜLICH
FORSCHUNGSZENTRUM

The LinkSCEEM-2 Project

What it does...and what it can do for you

13 July 2011 | Alan O'Cais
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Useful websites
Training: http://linksceem.eu/ATutor
Allocations: https://ssl.linklings.net/applications/linksceem/

Who is involved in LinkSCEEM?

The goals of LinkSCEEM-2 are fourfold:

- To facilitate the collaboration, coordination and improvement the HPC infrastructure of the Eastern Mediterranean
- To promote HPC as a scientific research tool and cultivate an HPC scientific community in the Eastern Mediterranean
- To assist in the generation of research of the highest calibre so that this effort can be sustainable
- To provide the technical and educational support necessary to achieve these goals

How is this achieved?

Networking/Coordination	Services	Research
• Networking • Access to resources • Training • Dissemination & Outreach	• User support • Connectivity • Integration of resources	• Cross disciplinary research • Climate research • Cultural Heritage research • Synchrotron Radiation research

Management & Coordination

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Management & Coordination

Networking/Coordination

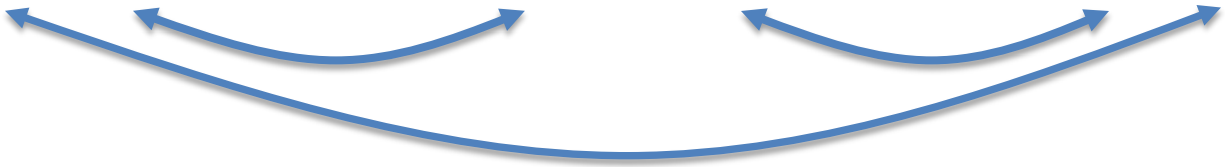
- Networking
- Access to resources
- Training
- Dissemination & Outreach

Services

- User support
- Connectivity
- Integration of resources

Research

- Cross disciplinary research
- Climate research
- Cultural Heritage research
- Synchrotron Radiation research



Management & Coordination

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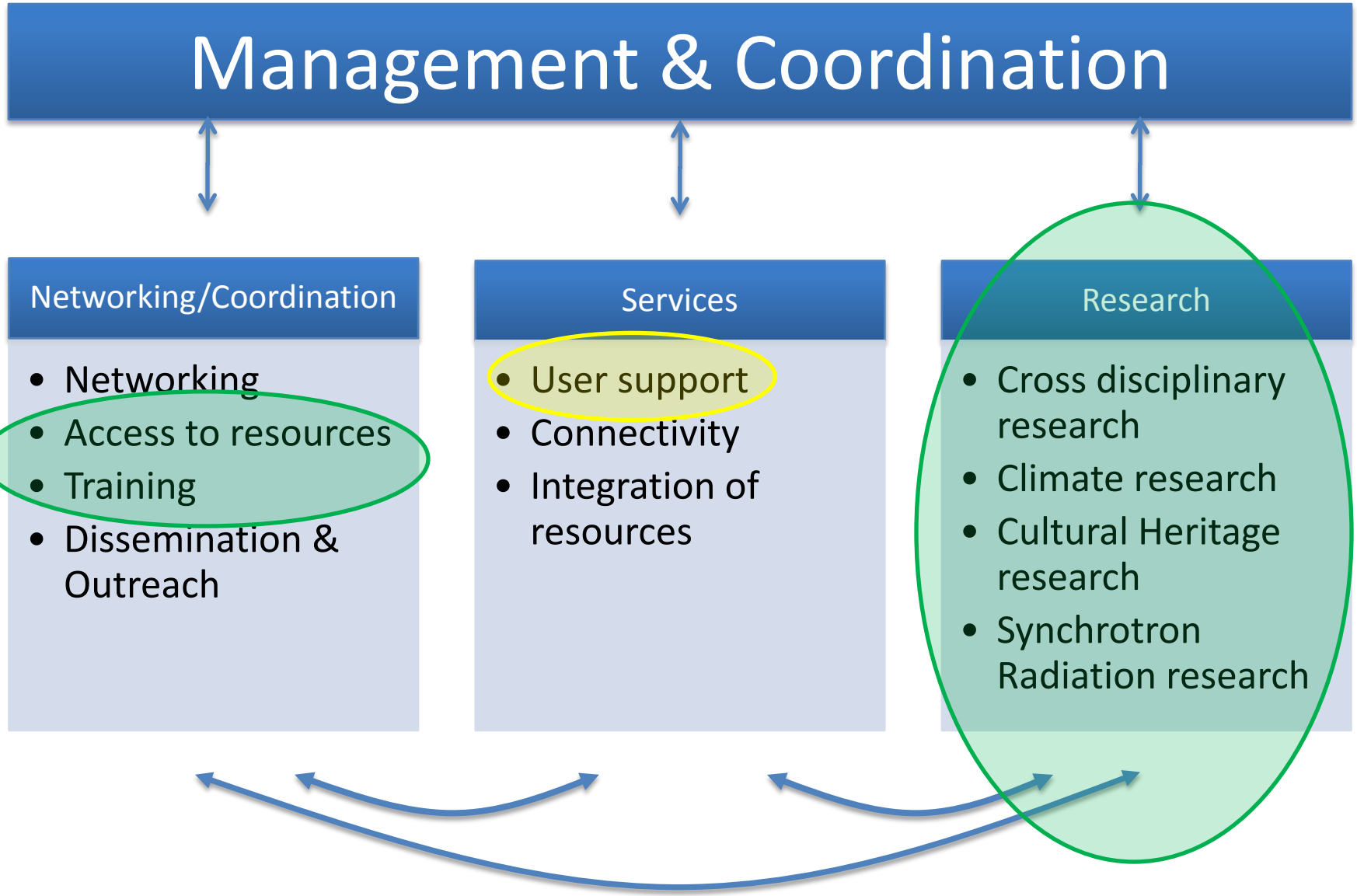


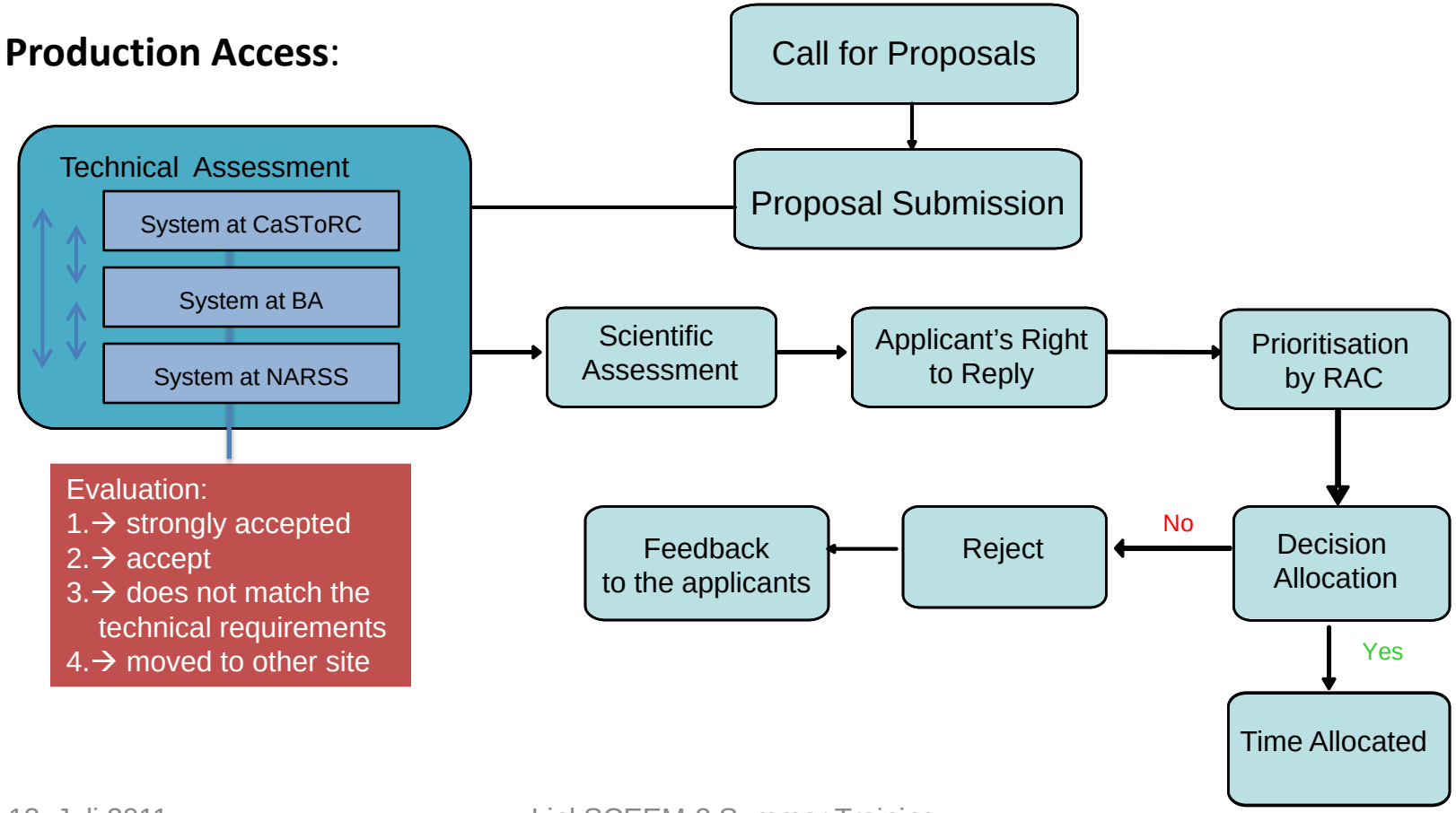
What Resources are available?

Cyl	BA	NARSS
Prototype: •Total peak performance ~1 TFlop/s •Total memory .192 TBytes •QDR Infiniband network for MPI •Lustre filesystems •16 GPUs **Cy-Tera:** •40+ Tflop •Fermi GPU •12 Core Nehalem	•130 8-core nodes •**Total peak performance 11.8 TFlops** •Total memory 1.05 TBytes (132 * 8GB) •DDR Infiniband @ 10 GBbps network •Lustre filesystems •Storage: 36 TByte	**Blue Gene/L:** •1024 dual processor compute nodes •Total peak performance per rack – 5.73 TFlops •Total memory .5 TBytes (1024 * .5GB) •3D toroidal network for peer-to-peer communication

Management of Access to Resources

- Create a peer review process for coordinating access to HPC, visualization and storage resources
- Form a Resource Allocation Committee to implement and oversee the process

Production Access:



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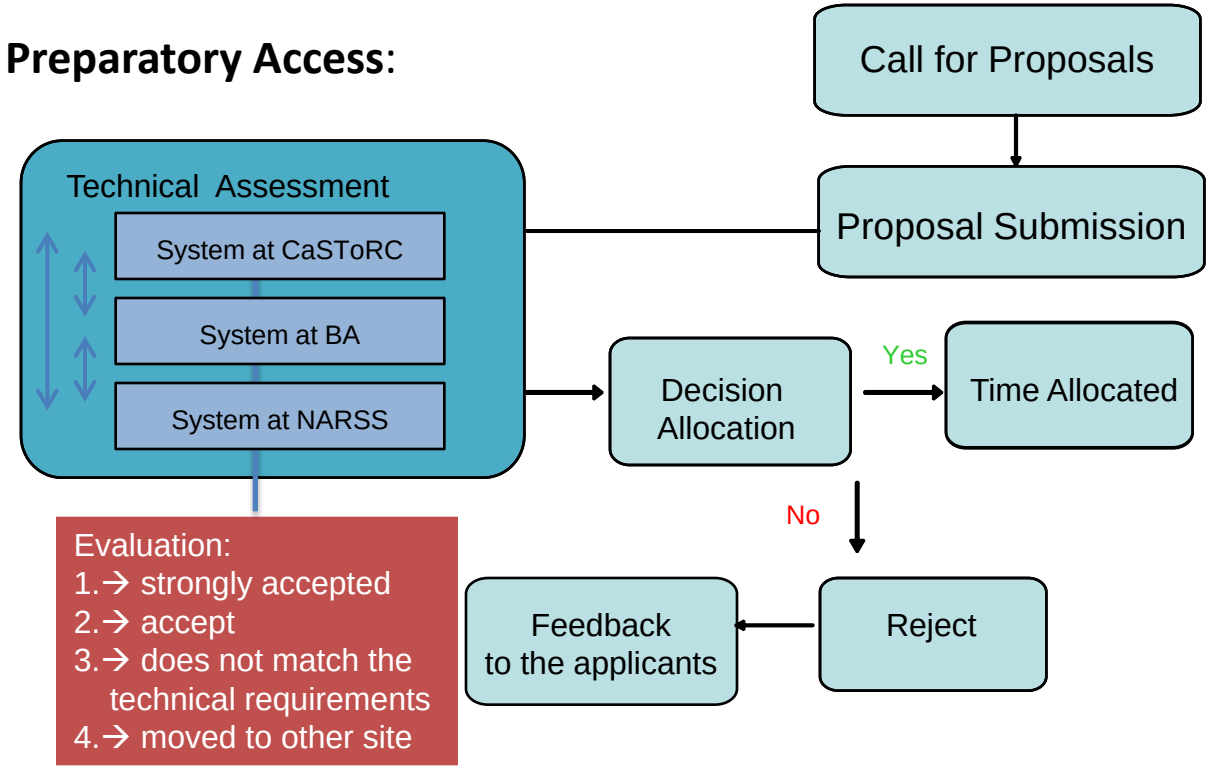

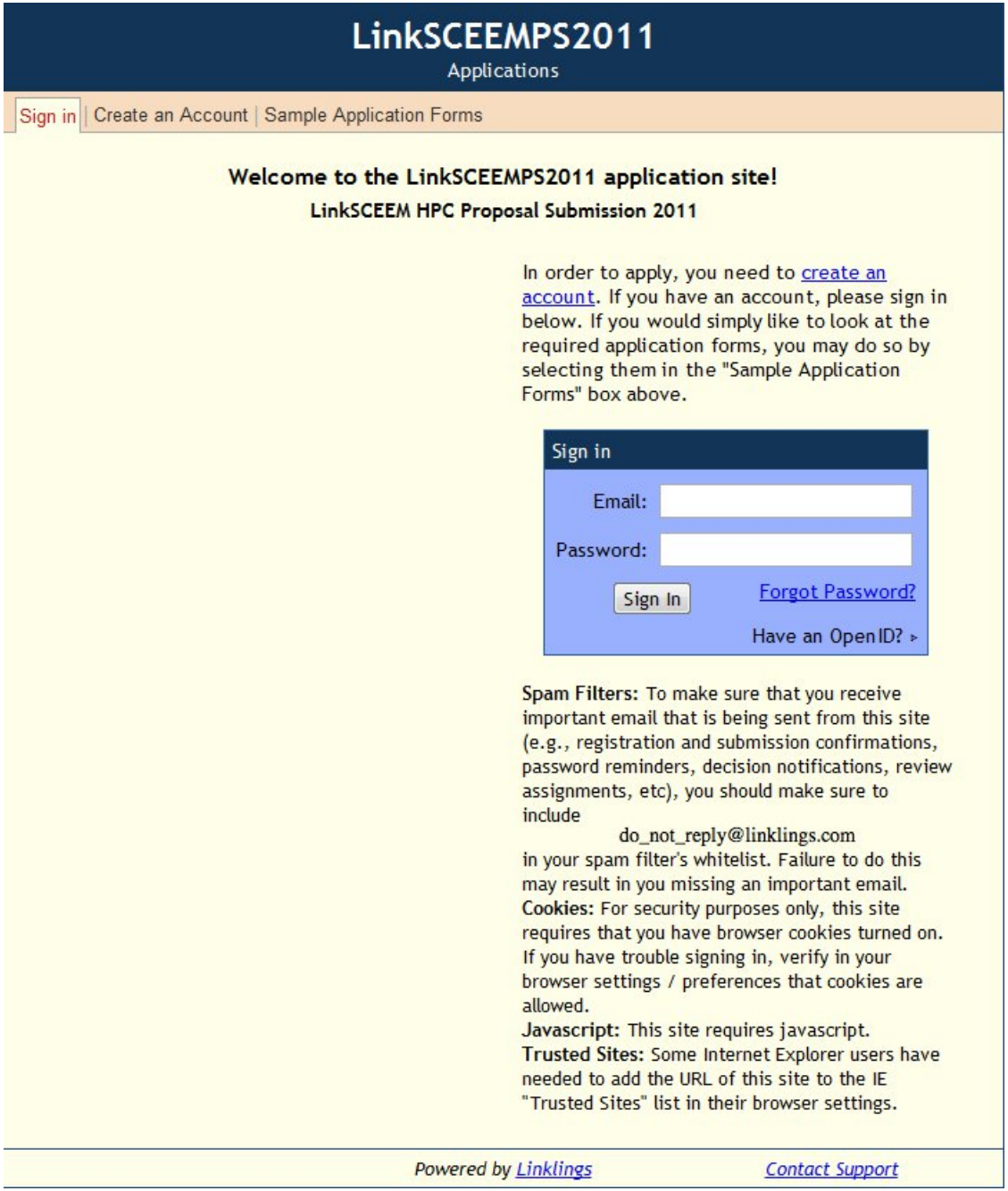

Applying for Resources

- Online system
- Year round preparatory access call – access to systems as soon as technical evaluation is complete
- Production access calls twice a year – access after decision of RAC (2 months)

Preparatory Access

Type of proposal & resources request

- Type A - Code scalability testing:
  Scalability testing to obtain scalability plots which can be used as supporting information when applying to future Cy-Tera or LinkSCEEM project calls.
  Please fill out questions 1.1-2.2 of the project information section of the application form.
- Type B - Code development:
  Code development and optimization by applicant (without Cy-Tera or LinkSCEEM support).
  Please fill out parts 1.1-2.3 of the project information section of the application form.
- Type C - Code development with support:
  Code development and optimization by applicant with support from Cy-Tera or LinkSCEEM experts.
  Please fill out parts 1.1-3.3 of the project information section of the application form.

Select the applicable category

- ○ Type A - Code scalability testing
- ○ Type B - Code development
- ○ Type C - Code development with support

Which resource centers are you requesting access to?

- ☐ Bibliotheca Alexandrina
- ☐ Cyl/CaSToRC
- ☐ NARSS

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Preparatory Access

- Scientific information

1.1: Summary of the project

1.1: Summary of the project (Maximum 200 words)	0 words

1.2: Scientific case for the project

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1.3: Computational Resources Requested

Please detail here the amount of computational resources you require, for example:

- Total CPU time required (in core hours)
- Total storage required (in Gbyte, *this is only available for the duration of the preparatory access project*)
- Maximum amount of memory per core (Mbyte)
- Any other resource dependencies known

1.3: Computational Resources Requested (Maximum 200 words)	0 words

Software information

2.1: Application software details

If known, please provide the following information on the simulation software required by your project:

- Name and version
- Any software dependencies (such as special compilers, libraries, software applications, etc.)
- Webpages or other references
- Licenses required; If the code is open source please state "open source".

2.1: Application software details (Maximum 200 words) 0 words

2.2: Algorithms and Parallelisation of Application Software

If known, please breifly describe the main algorithms used (e.g., conjugate gradient) and whether they have been parallelized.
If they are parallelized how is the parallelisation implemented (MPI, CUDA, etc.)?

2.2: Algorithms and Parallelisation of Application Software (Maximum 300 words) 0 words

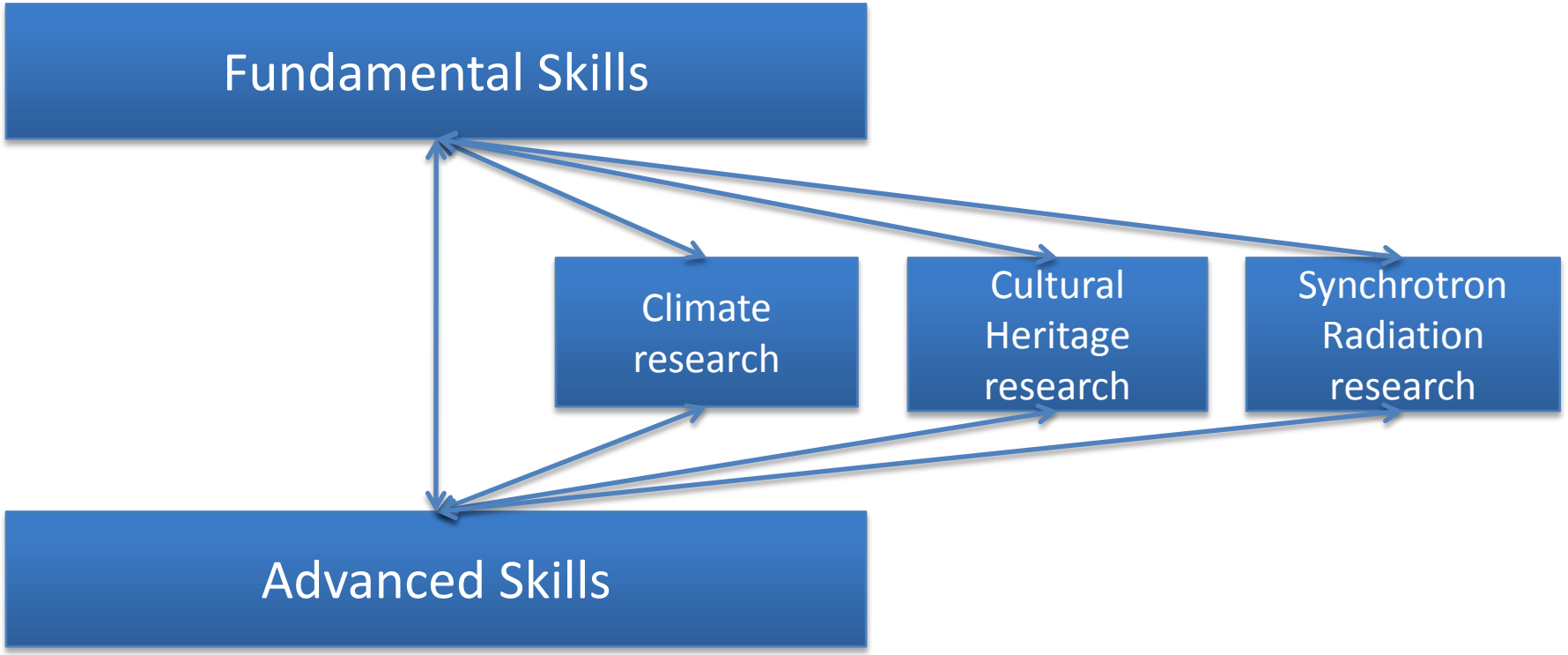
2.3: Enabling/optimization work required

Describe the application enabling/optimization work that needs to be performed to achieve the target performance.
This may include factors such as, for example:

- Implement parallelisation such as MPI, OpenMP, hybrid, CUDA, OpenCL etc.
- Improve I/O
- Reduce global communication

2.3: Enabling/optimization work required (Maximum 300 words) 0 words

HPC Training



- Tasks
  - Develop a tiered HPC training program to support new and existing users
  - Leverage material and skill developed at NCSA and JSC
  - Develop online training portal

- Impact
  - Prepare the regional scientific communities for using the LinkSCEEM e-infrastructure
  - Enable implementation of high-calibre research activities

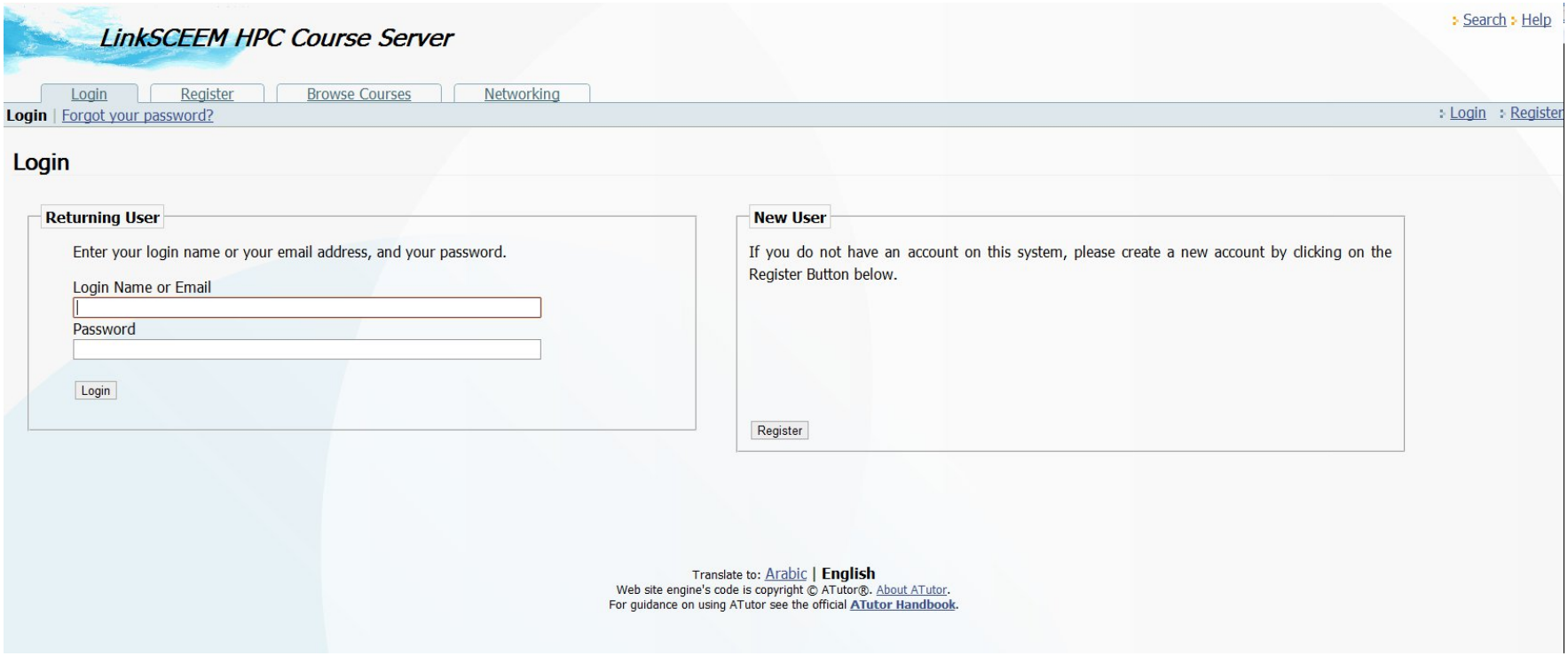
Training Program

- Four 1-day user meetings
- One 3-day basic user meeting
- One 3-day advanced cross-sectional workshop
- Three 3-day thematic workshops (one in each thematic area)
  - Climate Research
  - Digital Cultural Heritage
  - Synchrotron Radiation

BASIC	ADVANCED
▪ Basic system interaction • Introduction to MPI • Introduction to OpenMP • Introduction to GPU programming • Introduction to data management • Introduction to Performance Analysis • Optimisation and libraries • Debugging • Introduction to Visualisation • Application specific introductions	• Intermediate MPI • Hybrid programming • Intermediate GPU programming • Parallel I/O • Performance analysis • Porting workshop

Online Training Portal

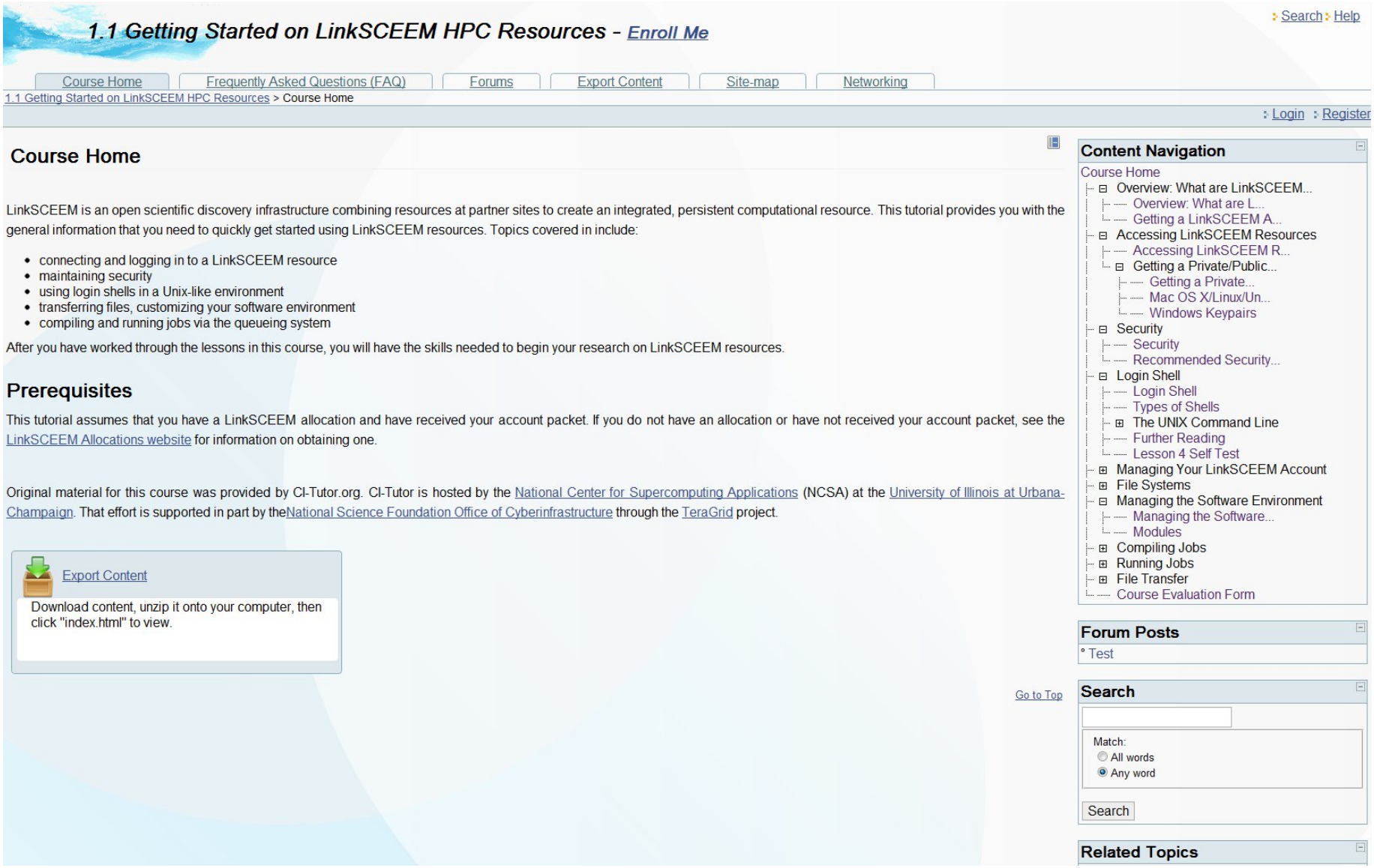
- Training content from Great Lakes Consortium
- Tailored for LinkSCEEM-2
- Offline browsing
- FAQ, forum, Q&A capabilities



Content

- Huge amount of content
- Many topics covered
- Exercises with solutions
- Material for all levels
- Expanding material based on hardware available within the project, new languages and emerging tools

Getting started



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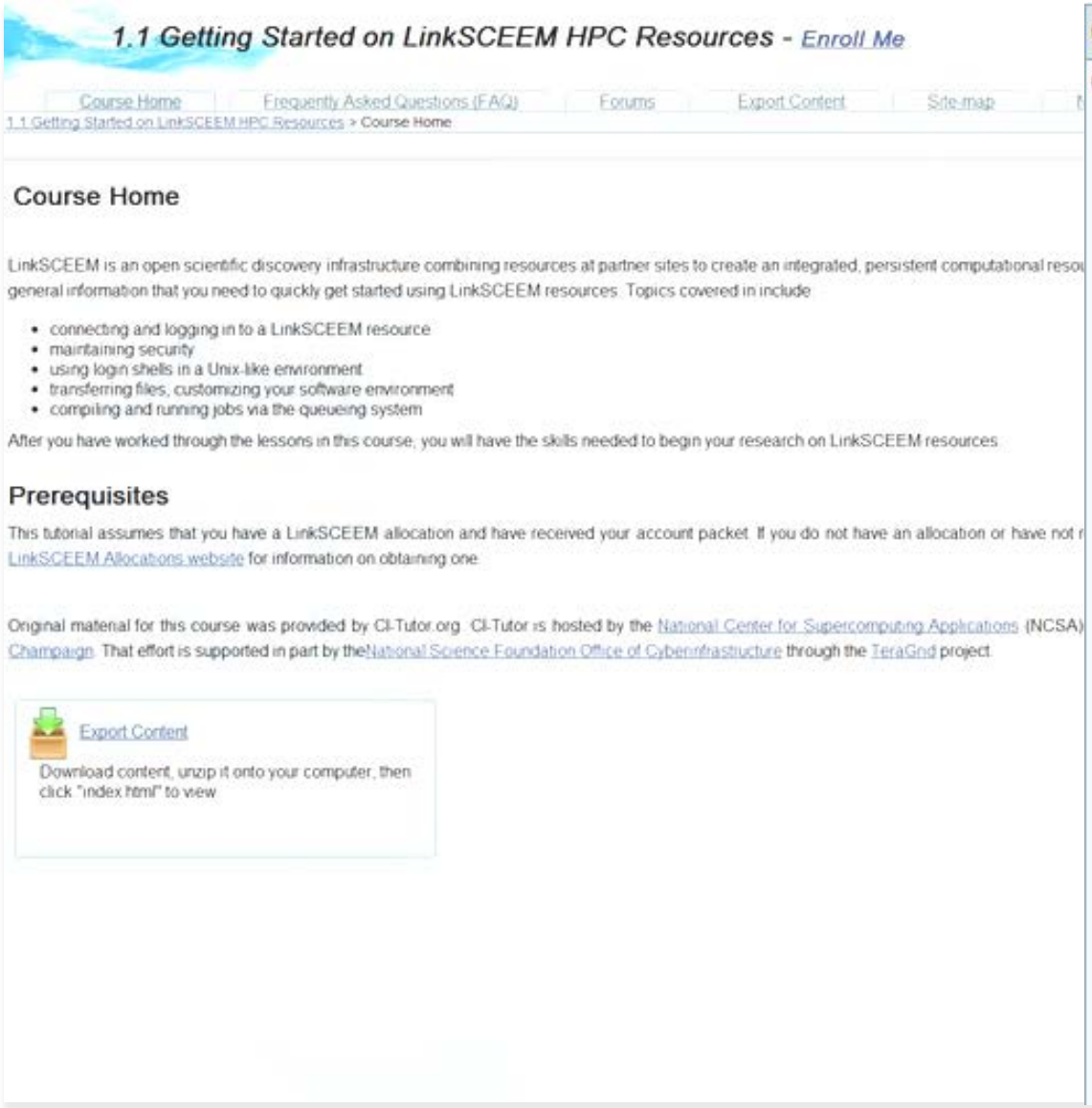
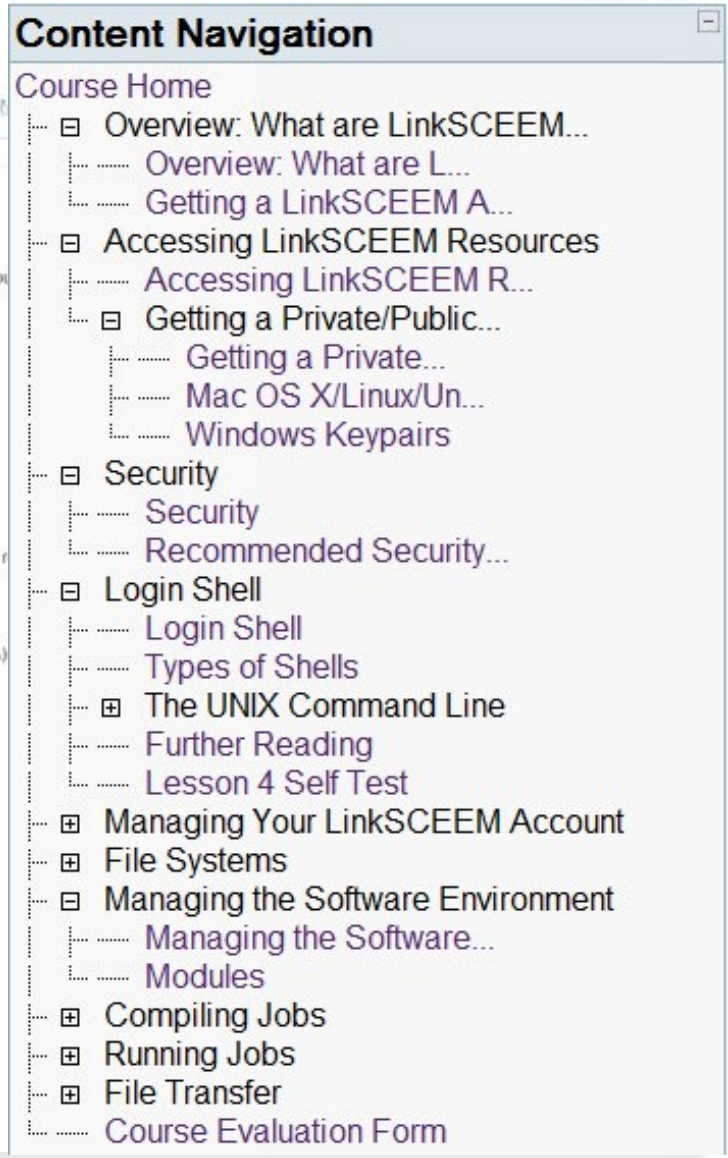
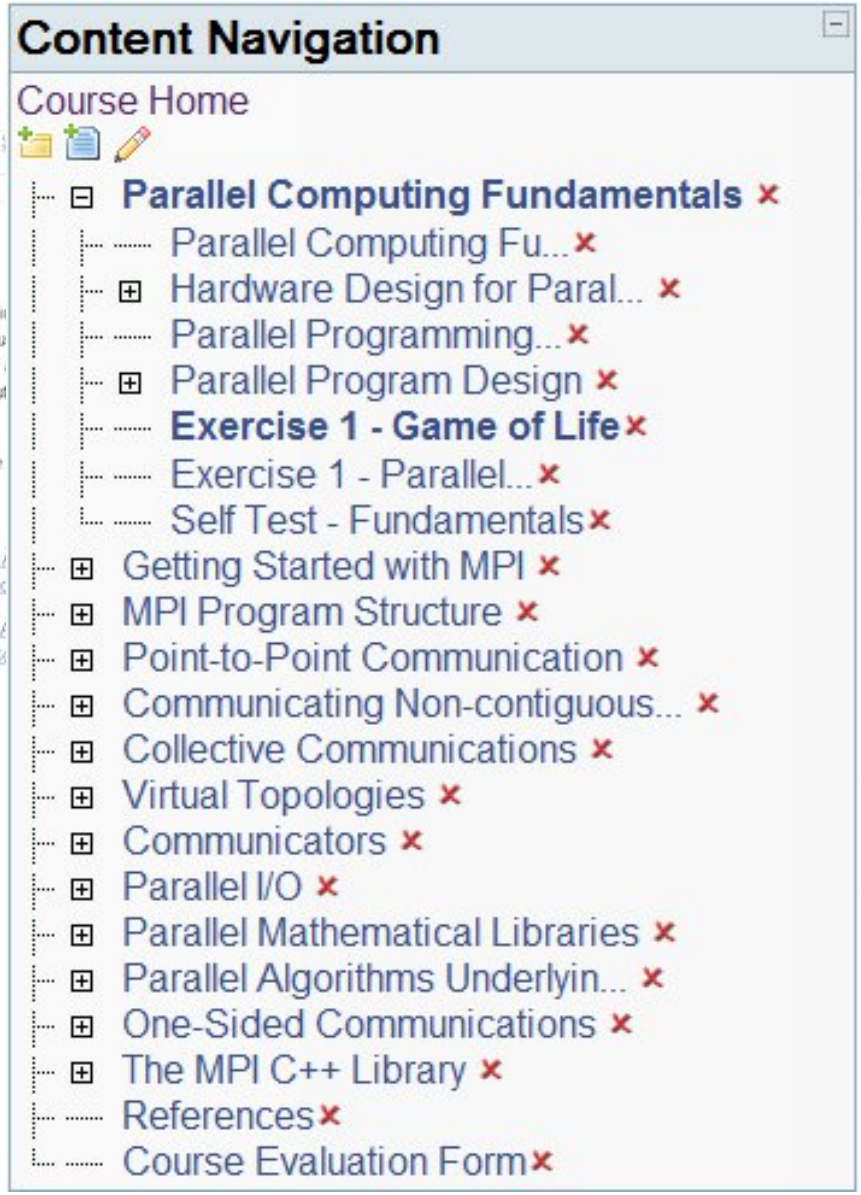
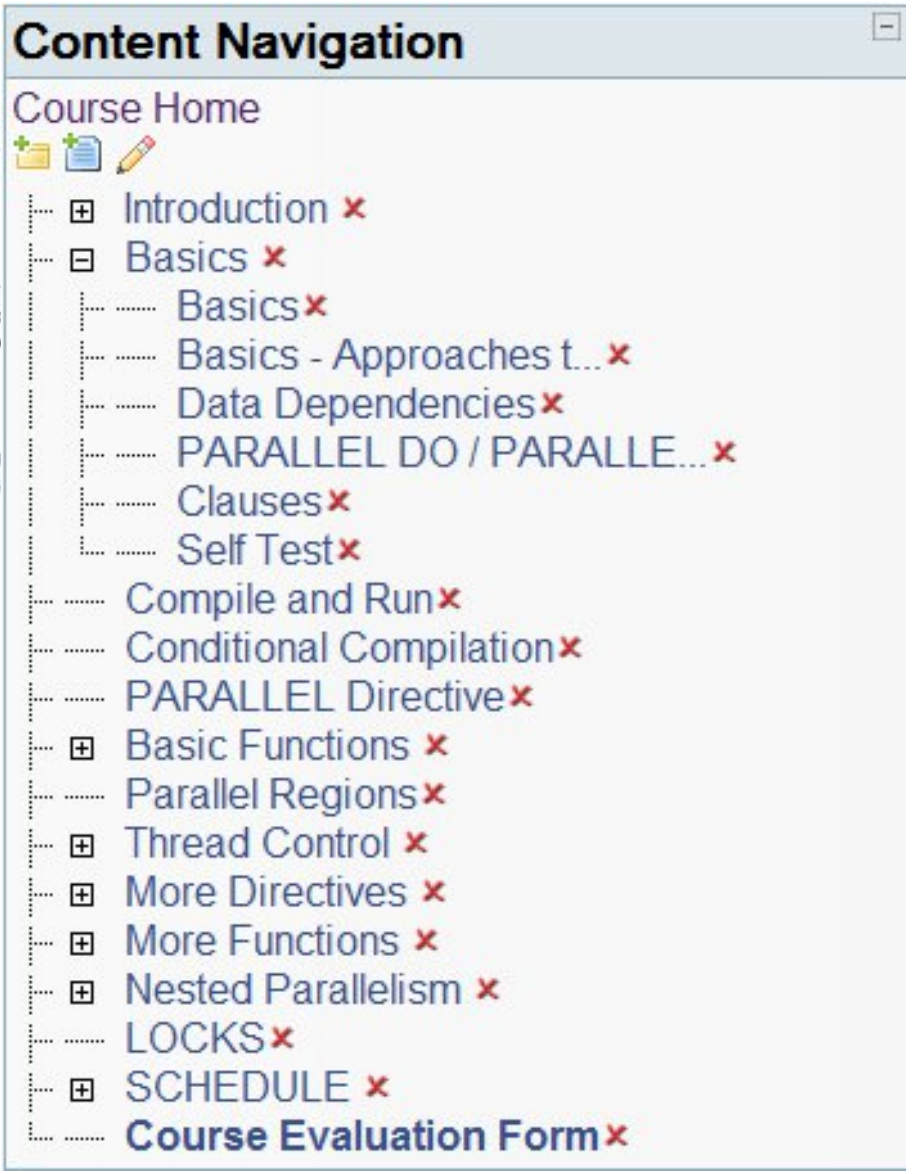




Introduction to MPI



Introduction to OpenMP



Research Activities

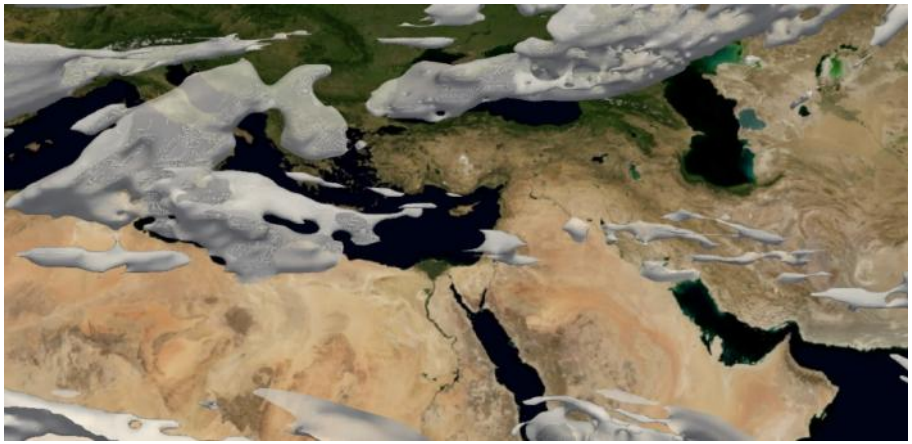
Cross-disciplinary research
CyI, NARSS, BA, JSC, NCSA, SESAME, IUCC
Climate research
CyI, MPG, NARSS
Cultural Heritage research
CyI, BA, NCSA
Synchrotron radiation research
CyI, SESAME, ESRF

Cross-disciplinary Research

- **Tasks**
  - **Optimization of parallel applications from Eastern Mediterranean computational scientists on large-scale HPC systems**
  - **Adaptation and development of tools for data repository management (for Cultural Heritage, Climate and Synchrotron data) and the visualization of complex data**

- **Impact**
  - **Provide know-how for scientific applications for use by the LinkSCEEM e-infrastructure users**
  - **Prepare data repository service for use with Cultural Heritage, Climate and Synchrotron data**
  - **Accumulate regional expertise on implementation of optimized parallel applications, data repository management and visualization.**

Climate Research



- Tasks
  - Porting, optimizing and sharing the existing global ECHAM5/MESSy Atmospheric Chemistry (EMAC) climate model to the CaSToRC and BA hardware and software computing environments
  - Study climate change and air quality scenarios in the Eastern Mediterranean

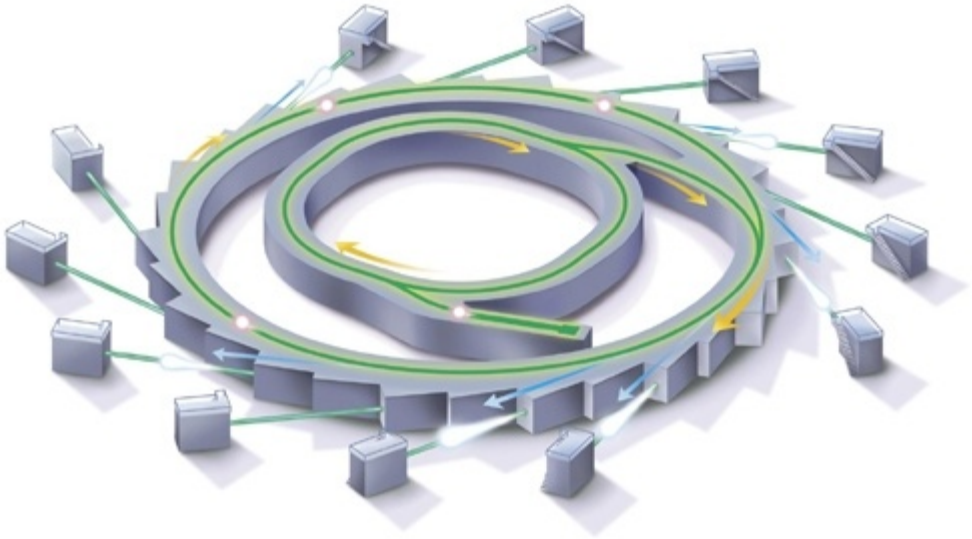
- Impact
  - Develop a custom, version of the EMAC model optimized to regional computational resources available through the LinkSCEEM e-infrastructure to regional users
  - Implement climate scenarios for the Eastern Mediterranean

Cultural Heritage Research

- **Tasks**
  - **Prototyping a novel, small object imaging centre at CaSToRC**
  - **Implementing a Digital Library of sufficient storage capacity to accommodate the high-resolution image-objects of cultural heritage artifacts.**
  - **Producing tools for tele-immersive collaborative environments and data**

- **Impact**
  - **Establish a small object imaging centre that can be used for developing high-resolution image objects for regional artefacts**
  - **Implement a pilot project to evaluate utility of the small object imaging centre**
  - **Develop and make available a Digital Library, open to regional users, to host high resolution image-objects of regional artefacts**
  - **Develop tools and expertise for creating tele-immersive collaborative environments**

Synchrotron Radiation Research



- Tasks
  - Port existing and develop new GPU programs to improve the efficiency and quality of experiments carried out on micro- and nano-focussing synchrotron beamlines
  - Provide support to package, distribute and install GPU programs in an HPC environment

- Impact
  - Implement a collection of tools optimized for the CaSToRC HPC infrastructure which includes GPU hardware made available to the regional user community through the LinkSCEEM e-infrastructure.
  - Develop regional expertise in synchrotron data analysis and simulation