

# The LinkSCEEM-2 Project What it does...and what it can do for you

13 July 2011 | Alan O'Cais a.ocais@fz-juelich.de

> Useful websites Training: http://linksceem.eu/ATutor Allocations: https://sel.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

- 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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#### Networking/Coordination

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

#### **Services**

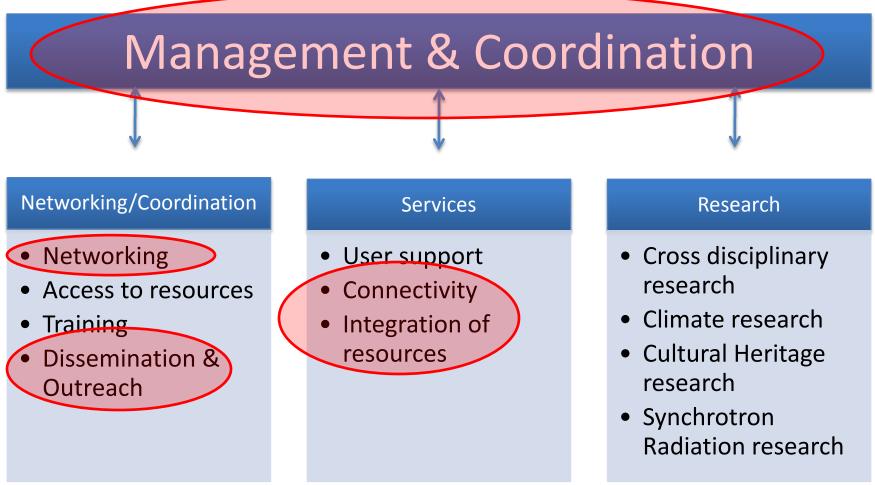
- User support
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#### Research

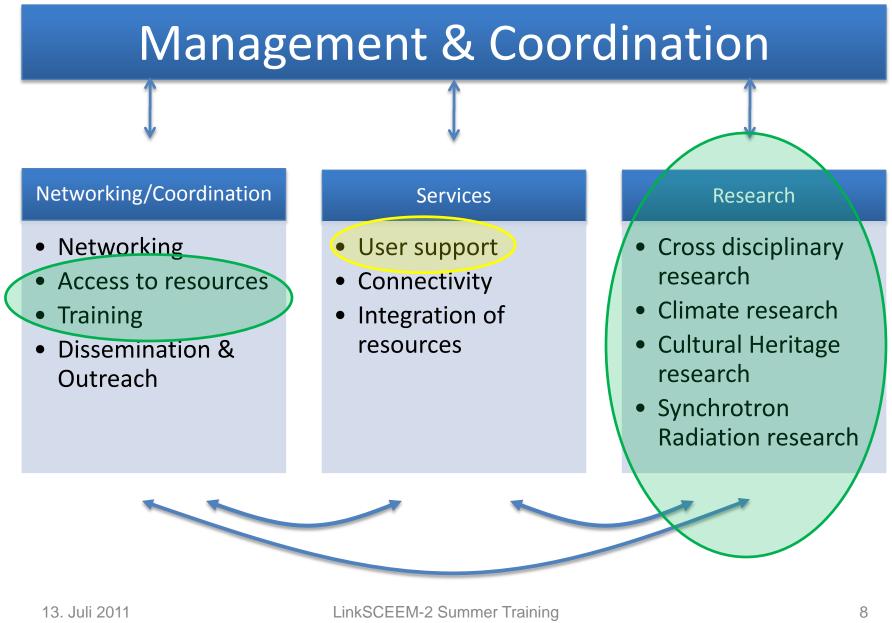
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- Synchrotron **Radiation research**













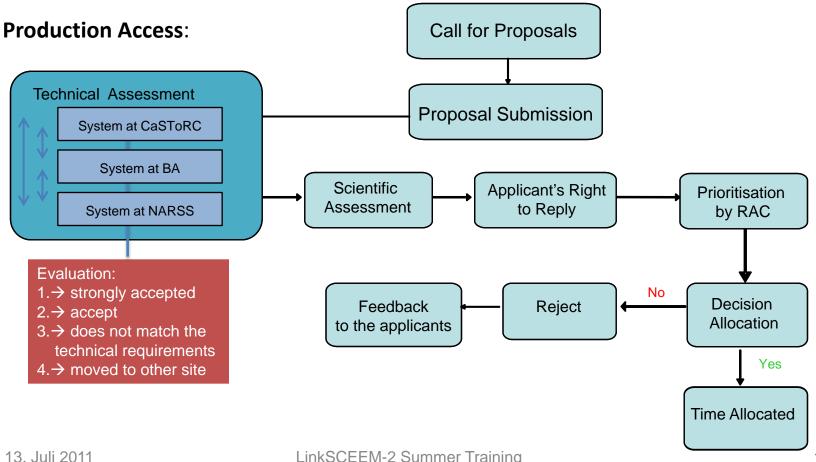
### What Resources are available?

СуІ	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	<ul> <li>•130 8-core nodes</li> <li>•Total peak performance 11.8</li> <li><b>TFlops</b></li> <li>•Total memory 1.05</li> <li>TBytes (132 * 8GB)</li> <li>•DDR Infiniband @ 10</li> <li>GBbps network</li> <li>•Lustre filesystems</li> <li>•Storage: 36 TByte</li> </ul>	<ul> <li>Blue Gene/L:</li> <li>1024 dual processor compute nodes</li> <li>Total peak performance per rack – 5.73 TFlops</li> <li>Total memory .5 TBytes (1024 * .5GB)</li> <li>3D toroidal network for peer-to-peer communication</li> </ul>

### Management of Access to Resources



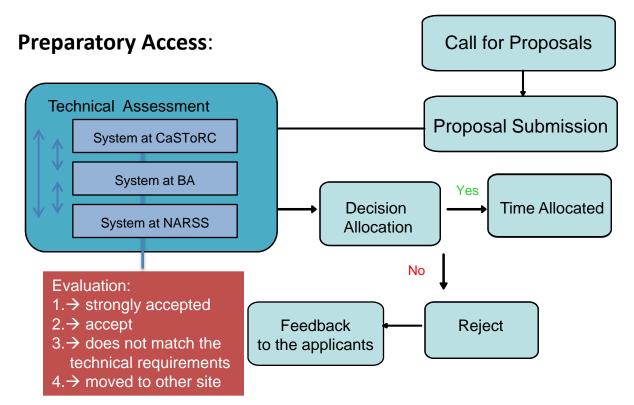
- Create a peer review process for coordinating access to HPC, visualization and storage resources
- Form a Resource Allocation Committee to implement and oversee the process



### **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



#### LinkSCEEMPS2011

Applications

#### Sign in Create an Account Sample Application Forms

#### Welcome to the LinkSCEEMPS2011 application site! LinkSCEEM HPC Proposal Submission 2011

In order to apply, you need to <u>create an</u> <u>account</u>. If you have an account, please sign in below. If you would simply like to look at the required application forms, you may do so by selecting them in the "Sample Application Forms" box above.

Sign in	
Email:	
Password:	
Sign In	Forgot Password?
	Have an OpenID? ⊳

Spam Filters: To make sure that you receive important email that is being sent from this site (e.g., registration and submission confirmations, password reminders, decision notifications, review assignments, etc), you should make sure to include

do\_not\_reply@linklings.com in your spam filter's whitelist. Failure to do this may result in you missing an important email. Cookies: For security purposes only, this site requires that you have browser cookies turned on. If you have trouble signing in, verify in your browser settings / preferences that cookies are allowed.

Javascript: This site requires javascript. Trusted Sites: Some Internet Explorer users have needed to add the URL of this site to the IE "Trusted Sites" list in their browser settings.



### 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)

Powered by Linklings

#### Contact Support

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### **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 🔲 CyI/CaSToRC 🔲 NARSS

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# Preparatory Access - Scientific information

1.1: Summary of the project (Maximum 200 words)	0 words
1.2: Scientific case for the project	
1.2: Scientific case for the project (Maximum 500 words)	0 words
1.3: Computational Resources Requested	
<ul> <li>Please detail here the amount of computational resources you require, for e</li> <li>Total CPU time required (in core hours)</li> <li>Total storage required (in Gbyte, this is only available for the duration access project)</li> <li>Maximum amount of memory per core (Mbyte)</li> <li>Any other resource dependencies known</li> </ul>	
1.3: Computational Resources Requested (Maximum 200 words)	0 words



#### 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:

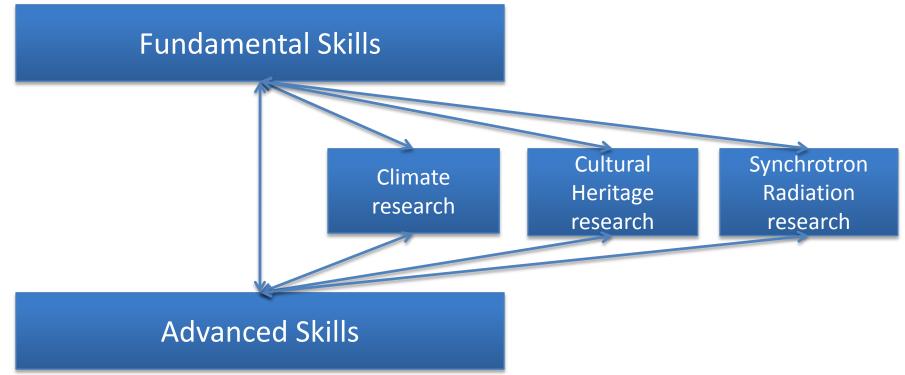
- Implement parallelisation such as MPI, OpenMP, hybrid, CUDA, OpenCL etc.
- Improve I/0
- Reduce global communication

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 einfrastructure
  - Enable implementation of high-calibre research activities

13. Juli 2011

LinkSCEEM-2 Summer Training

### **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)
  - o Climate Research
  - $\odot$  Digital Cultural Heritage
  - $\odot$  Synchrotron Radiation

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



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LinkSCEEM-2 Summer Training

### **Online Training Portal**

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

LinkSCEEM HPC Course Server		Search > Help
Login Register Browse Courses Networking		
Login Forgot your password?		: Login : Register
Login		
Returning User	New User	
Enter your login name or your email address, and your password. Login Name or Email	If you do not have an account on this system, please create a new account by clicking on the Register Button below.	
Password		
Login		
	Register	
Web site eng For guidance o	Translate to: <u>Arabic</u>   <b>English</b> gine's code is copyright © ATutor®. <u>About ATutor</u> . on using ATutor see the official <u>ATutor Handbook</u> .	



#### Course



1.1 Getting Started on LinkSCEEM HPC Resources Category: Parallel Computing

1.2 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



### 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**



1.1 Getting Started on Lin Course Home Frequently Asked Quest 1.1 Getting Started on LinkSCEEM HPC Resources > Course Hor		<mark>&gt; Search &gt; Help</mark>
1.1 Getting Stated on LinkSCLEW HPC Resources > Course hor	IIC	: Login : Register
Course Home	18	Content Navigation
<ul> <li>general information that you need to quickly get started usin</li> <li>connecting and logging in to a LinkSCEEM resource</li> <li>maintaining security</li> <li>using login shells in a Unix-like environment</li> <li>transferring files, customizing your software environme</li> <li>compiling and running jobs via the queueing system</li> <li>After you have worked through the lessons in this course, yo</li> </ul> Prerequisites This tutorial assumes that you have a LinkSCEEM allocati LinkSCEEM Allocations website for information on obtainin Original material for this course was provided by CI-Tutor.	ent ou will have the skills needed to begin your research on LinkSCEEM resources. on and have received your account packet. If you do not have an allocation or have not received your account packet, see the	Course Home      Ourview: What are LinkSCEEM      Overview: What are L      Getting a LinkSCEEM A      Getting a LinkSCEEM Resources      Overview: What are L      Getting a Private/Public      Getting a Private      Getting Private      Gettinte      Getting Private      Getting Private
click "index.html" to view.		Forum Posts
		° Test
	Go to Top	Search 🗉
		Match: All words Any word Search Related Topics
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### **Getting started**



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### **Introduction to MPI**



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D d Introduction to MDI		Content Navigation			
2.1 Introduction to MPI     Course Home Erequently Asked Questions (FAY My Start Page > 2.1 Introduction to MPI > Course Home     Course Home     The Message Passing Interface, or MPI, is a standard library of sub     coordination of a program running as multiple processes in a distribut	routines (Fortran) or function calls (C) that can be used to i	Course Home			
MPI library makes it very powerful and enables source code portab range of architectures, offers a great deal of functionality, including a user-defined data types and topologies, and support for heterogener	ality since MPI programs should compile and run as-is on number of different types of communication and special rout ous parallel architectures.	<ul> <li></li></ul>			
This tutorial is an introduction to MPI. No prior experience with Minecessary.		Exercise 1 - Parallel× Self Test - Fundamentals×			
Original material for this course was provided by CI-Tutor org. CI-T Champaron. That effort is supported in part by the <u>National Science F</u> The content for this particular course was provided by the followin <u>Supercomputer Center</u> (OSC), <u>Boston University</u> (BU), the <u>University</u>	oundation Office of Cybernfrastructure through the TeraGio ing institutions - the National Center for Supercomputing A	<ul> <li>            Getting Started with MPI ×            MPI Program Structure ×           MPI Program Structure ×           Point-to-Point Communication ×</li></ul>			
##		<ul> <li></li></ul>			
		<ul> <li>         ■ Parallel Mathematical Libraries ×         ■ Parallel Algorithms Underlyin ×         ■ One-Sided Communications ×         ■ The MPI C++ Library ×         ■ References×         ■ Course Evaluation Form×         ■     </li> </ul>			
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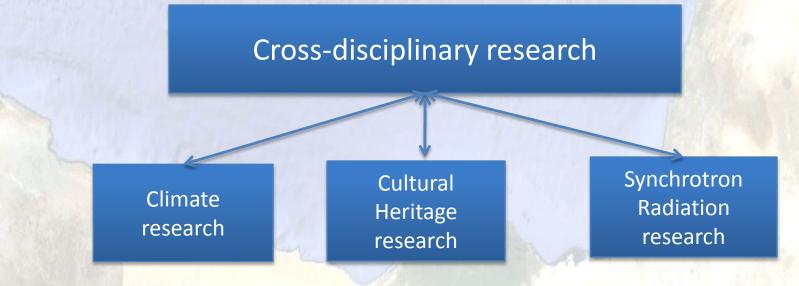
### Introduction to OpenMP



2.2 Introduction to OpenMP	Content Navigation
Course Home Frequently Asked Questions (EAQ) Forums Export Content My Start Page > 2.2 Introduction to OpenMP > Course Home	Course Home
Course Home  See A processing is a standardized API for parallelizing Fortran, C, and C++ programs on shared-memory architectures include to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent necessary to explain various points about OpenMP. Examples are provided to the extent ne	resent Basics × Basics - Approaches t× Data Dependencies × PARALLEL DO / PARALLE×
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### **Research Activities**

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





### **Cross-disciplinary Research**

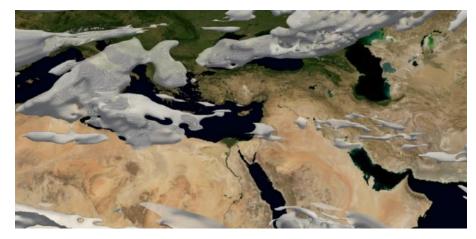
#### • Tasks

- 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 einfrastructure 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

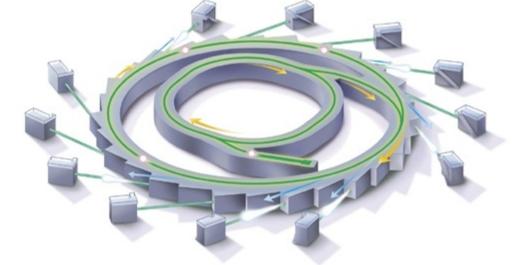


## **Cultural Heritage Research**

- 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 highresolution 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