The Abdus Salam International Centre for Theoretical Physics

# Advanced School in High Performance and GRID Computing

Cosponsor(s): Co-sponsored by : Central European Initiative (CEI), Democritos INFM, eLab, E4 Computer Engineering S.p.A., EuroTech S.p.A., IBM Italia S.p.A., Spring Firm S.r.l.
Organizer(s): Directors: S. Cozzini, A. Kohlmeyer
Trieste - Italy, 03 - 14 November 2008

## Final programme

**DAY 1:**
**Introduction to Linux and HPC** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
**Chairperson: Stefano Cozzini**

**3 November 2008**

**08:30 - 09:30** **Registration**

**09:30 - 09:40** **Stefano Cozzini / Axel Kohlmeyer** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy / University of Penn., Philadelphia, U.S.A*
**Introduction to the School**

**09:40 - 10:30** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Introduction to HPC and Cluster computing**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 11:45** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A*
**Introduction to Linux**

**11:45 - 12:30** **Riccardo di Meo** / *ICTP EU-IndiaGrid project, Trieste, Italy*
**Tools for Linux Workstations**
-Compression and packaging utilities: tar/gzip -ssh basic -packages management: yum/rpm etc.. -wget -gnuplot and/or other tool for plotting

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** (Room: Adriatico Guest House Informatics Lab.)
**Piero Calucci/ Moreno Baricevic/ Riccardo di Meo** / *Sissa/eLab and ICTP/EundiaGrid, Trieste, Italy*
**Crash Course on Linux: Intermediate Lab (part 1)**
A small crash course on bash scripting etc.etc. Materials are available starting from here: http://www.democritos.it/hpc-wiki/index.php/Main/MasteringLinux

**14:00 - 16:00** (Room: Adriatico Guest House - Eklund Informatics Lab (Lower Level 1))
**Iztok Gregori & Stefano Cozzini** / *Sissa/eLab, Trieste, Italy*
**Crash Course on Linux: Beginner's Lab (part 1)**
A small crash course on bash scripting etc.etc. Materials are available starting from here: http://www.democritos.it/hpc-wiki/index.php/Main/MasteringLinux

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** (Room: Adriatico Guest House Informatics Lab.)
**Piero Calucci/ Moreno Baricevic/ Riccardo di Meo** / *Sissa/eLab and ICTP/EundiaGrid, Trieste, Italy*
**Crash Course on Linux: Intermediate Lab (part 2)**
A small crash course on bash scripting etc.etc. Materials are available starting from here: http://www.democritos.it/hpc-wiki/index.php/Main/MasteringLinux

**16:30 - 18:30** (Room: Adriatico Guest House - Eklund Informatics Lab (Lower Level 1))
**Iztok Gregori & Stefano Cozzini** / *Sissa/eLab, Trieste, Italy*
**Crash Course on Linux: Beginners Lab (part 2)**
A small crash course on bash scripting etc.etc. Materials are available starting from here: http://www.democritos.it/hpc-wiki/index.php/Main/MasteringLinux

**18:30 - 19:15** **Homework: blog about the day**

**DAY 2: Scientific Computing** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
**Chairperson: Axel Kohlmeyer**

**4 November 2008**

**09:00 - 09:45** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Floating Points Numbers: How to work with them correctly and efficiently**

**09:45 - 10:30** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A.*
**From Source Code to Executable: Preprocessing/Compiling/Linking/Makefiles (part I)**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 11:45** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A.*
**From Source Code to Executable: Preprocessing/Compiling/Linking/ Makefiles (part II)**

**11:45 - 12:10** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A.*
**From Source Code to Executable: Preprocessing/Compiling/Linking/ Makefiles (part III)**

**12:10 - 12:30** **Antonio Messina** / *ICTP, Trieste, Italy*
**Working with svn**
A short introduction how to use svn (http://subversion.tigris.org/)

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Laboratory: Install compilers and programming tools on your workstation**
Exercise Instruction available here: http://www.democritos.it/hpc-wiki/index.php/Main/InstallingTheGNUPGIAndIntelCompilerPackages

**16:00 - 16:30** **Coffee Break**

**16:30 - 18:30** **Laboratory Part 2: Test Compilers on IEEE floating point arithmetic**
Exercise Instructions available here: http://www.democritos.it/hpc-wiki/index.php/Main/TestTheCompilersAndPlayWithFPNumbers

**18:30 - 19:15** **Homework: blog about the day**

**DAY 3: Modern architecture for HPC and how to use them efficiently** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))

**5 November 2008**

**09:00 - 09:45** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Modern architectures for HPC computation**
Review of modern architecture: details about memory hierarchy etc..etc.

**09:45 - 10:30** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Using Compilers and Profilers to Optimize your Code for Performance**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 11:45** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A.*
**Mathematical Libraries part I**
review the main libraries for linear algebra and fftw

**11:45 - 12:30** **Luca Heltai** / *S.I.S.S.A. - International School for Advanced Studies, Trieste, Italy*
**Mathematical Libraries Part II**
Petcs and other toolkits..

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 14:20** **Peter McGrath** / *TWAS, Trieste, Italy*
**The EuroAfrica-ICT project**

**14:20 - 16:00** **Laboratory part 1: Optimize simple codes provided by Lab; Measure memory hierarchy speed**
Exercise Instructions available here: http://www.democritos.it/hpc-wiki/index.php/Main/OptimizeSimpleCodesProvidedByLab http://www.democritos.it/hpc-wiki/index.php/Main/MeasureMemoryHierarchySpeed

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **Laboratory Part 2: Play with mathematical libraries**
Exercise Instructions are here: http://www.democritos.it/hpc-wiki/index.php/Main/ComparePerformancesOfDifferentOptimizedLibrariesOnMatrixMultiplication

**18:30 - 18:45** **Homework: blog about the day**

**DAY 4: Parallel Computation** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))

**6 November 2008**

**09:00 - 09:45** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Parallel Computing with Linux: the cluster approach..**

**09:45 - 10:30** **Giuliano Taffoni** / *INAF, Trieste, Italy*
**Introduction to Grid computing**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 12:00** **Luca Heltai** / *SISSA, Trieste, Italy*
**Introduction to MPI**

**12:00 - 12:30** **Ershaad A. Basheer** / *JNCASR, Bangalore, India*
**General instructions on compiling MPI codes on clusters**

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Laboratory part 1: install MPI libraries and run parallel codes on your workstation**
Exercise Instructions are here: http://www.democritos.it/hpc-wiki/index.php/Main/TestSimpleMPIProgramsOnASingleProcessor

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **Laboratory Part 2: Set up Mini Clusters to Test MPI**
Exercise Instructions are here: http://www.democritos.it/hpc-wiki/index.php/Main/SetUpMiniClustersToTestMPIOnTrueParallelMachines

**18:30 - 19:15** **Homework: blog about the day**

**DAY 5: Tools and methods for HPC** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))

**7 November 2008**

**09:00 - 09:30** **Stefano Cozzini** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**How to benchmark your application**

**09:30 - 10:15** **Shawn T. Brown** / *Carnegie Mellon University, Pittsburgh Supercomputing Center, U.S.A.*
**How to find the best resources for your Application**

**10:15 - 11:00** **Shawn T. Brown** / *Carnegie Mellon University, Pittsburgh Supercomputing Center, U.S.A.*
**Introduction to OpenMP ( first part)**

**11:00 - 11:30** --- Coffee Break ---

**11:30 - 12:30** **Axel Kohlmeyer** / *University of Pennsylvania, Philadelphia, U.S.A.*
**Error Messages and Debugging**

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Axel Kohlmeyer/Stefano Cozzini** / *University of Pennsylvania, Philadelphia, U.S.A. / CNR-INFM Democritos*
**Question&Answer open session**

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **Laboratory Session second session: OpenMP examples Use of OpenMP threaded libraries**
http://www.democritos.it/hpc-wiki/index.php/Main/OpenMPExamples http://www.democritos.it/hpc-wiki/index.php/Main/UseOfOpenMPThreadedLibraries

**18:30 - 19:15** **Homework: blog about the day**

**DAY6: MPI tutorial** (**Saturday**)

**8 November 2008**

**09:00 - 10:30** **Axel Kohlmeyer / Shawn T. Brown** / *University of Penn., Philadelphia, U.S.A. / CMU, PSC, Pittsburgh, U.S.A.*
**MPI tutorial: first part**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 12:30** **Axel Kohlmeyer / Shawn T. Brown** / *Un. of Pennsylvania, Philadelphia, U.S.A. / CMU, PSC, Pittsburgh, U.S.A.*
**MPI tutorial: part 2**

**12:00 - 17:00** --- Lunch and free time ---

**DAY 7: FREE TIME** (**Sunday**)

**Advanced Topic session:** (Room:Adriatico Guest House Kastler Lecture Hall)

**10 November 2008**

**09:00 - 09:10** **Stefano Cozzini/Axel Kohlmeyer** / *CNR-INFM Democritos, Trieste, Italy/University of Penn., Philadelphia, U.S.A.*
**Presentation of the second week activities**

**09:10 - 09:45** **Ershaad A. Basheer** / *JNCASR, Bangalore, India*
**Introduction to GPU programming in the nvidia CUDA environment**

**09:45 - 10:30** **Ershaad A. Basheer** / *JNCASR, Bangalore, India*
**Introduction to GPU programming in the nvidia CUDA environment (second part)**

**10:30 - 11:00** --- Coffee Break ---

## 11 November 2008

**09:00 - 09:45** **Piero Calucci** / *S.I.S.S.A. - International School for Advanced Studies, Trieste, Italy*
**Queue systems for HPC platform**

**09:45 - 10:05** **Carlos Jaime Barrios Hernadez** / *Laboratoire Informatique de Grenoble, France*
**High Bandwidth Data Transfer**

**10:05 - 10:30** **Carlos Jaime Barrios Hernadez** / *Laboratoire Informatique de Grenoble, France*
**Modeling and Evaluation of Performance of Scalable Architectures (Grid/Cluster Monitoring tools and procedures)**

**10:30 - 11:00** --- Coffee Break ---

## 12 November 2008

**09:00 - 09:45** **Piero Calucci** / *S.I.S.S.A. - International School for Advanced Studies, Trieste, Italy*
**An Introduction to the Lustre Parallel File System**

**09:45 - 10:30** **Jorge Zuluaga** / *CRESCA- Universidad de Antioquia, Medellin, Colombia*
**Rocks: what is and how to install it**

**10:30 - 11:00** --- Coffee Break ---

**Application Optimization and Parallel Programming** (Room:Adriatico Guest House Lundqvist Lecture Hall)
**Chairperson: Axel Kohlmeyer and Shawn T. Brown**

**Cluster Installation and management lab: how to setup HPC facilities**
**Chairperson: Piero Calucci and Moreno Baricevic**

**10 November 2008**

**11:00 - 12:00** (Room: Adriatico Guest House Kastler Lecture Hall)
**Moreno Baricevic** / *CNR/INFM Democritos, Trieste, Italy*
**Installation procedures for clusters**

**12:00 - 14:00** --- Lunch Break and transfer to SISSA lab ---

**14:00 - 18:00** (Room: SISSA MediaLab)
**LAB Session: Installation Procedure for a Cluster Master Node**
http://www.democritos.it/hpc-wiki/index.php/Main/InstallationProcedureForAClusterMasterHeadNode

## 11 November 2008

**11:00 - 12:00** (Room: Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
**Piero Calucci** / *SISSA, Trieste, Italy*
**How to set-up a Queue system on your cluster**

**14:00 - 18:00** **Installing and configuring PBS and monitoring services**

## 12 November 2008

**11:00 - 12:00** (Room: Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
**DEMO on I/O procedures by PANASAS**

**14:00 - 18:00** **Lab: I/O configuration and Infiniband installation**

## 13 November 2008

**14:00 - 18:00** **Final Lab: completing all the exercises proposed**

**GRID computing Lab** (Room:Adriatico Guest House Informatics Lab.)
**Chairperson: Stefano Cozzini and Antun Balaz**

**10 November 2008**

**11:00 - 12:30** **Antun Balaz / Stefano Cozzini** / *Institute of Physics, Belgrade, Rep. of Serbia /CNR/INFM Democritos and Sissa/eLab, Trieste, Italy*
**Grid tutorial part 1: introduction to gLite and Gridseed**

Introduction to gLite middleware (Antun Balaz) 40'

Introduction to GRIDSEED (Stefano Cozzini) 20'

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Riccardo Murri / Antun Balaz** / *Swiss Centre for Scientific Computing, Manno, Switzerland/Institute of Physics, Belgrade, Republic o*
**Grid tutorial 2: Security and basic Job Submission**

GRID authentication/authorization mechanism (Riccardo Murri) 35'

Basic Job Submission (Antun Balaz) 35'

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **Giuliano Taffoni** / *INAF/OATS, Trieste, Italy*
**Grid tutorial part 3: data management**

## 11 November 2008

**11:00 - 12:30** **Antun Balaz** / *Institute of Physics, Belgrade, Republic of Serbia*
**Grid Tutorial part 4: advanced job submission**

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Giuliano Taffoni** / *INAF/OATS, Trieste, Italy*
**Grid tutorial hands-on session on data management and advanced job submission**

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **Stefano Cozzini / Riccardo di Meo** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy/S.I.S.S.A. - International School for Advanced St*
**Grid Tutorial part 5: how to port application on the grid and parallel computing on the GRID**
We will present a general overview how to port application on the grid and then we will focus on: -MPI approach on the GRID -SMP calculation on the GRID -client/server mechanisms

## 12 November 2008

**11:00 - 12:30** **Grid Tutorial 7: problem assignments to participants**

**12:30 - 14:00** --- Lunch Break ---

**14:00 - 16:00** **Grid LAB: personal/group work on assigned problems**

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **GRID LAB: personal/group work on assigned problems**

## 13 November 2008

**14:00 - 16:00** **GRID Lab: personal/group work on assigned problems**

**16:00 - 16:30** --- Coffee Break ---

**16:30 - 18:30** **GRID LAB: personal/group work on assigned problems**

**Vendors&Sponsors Session**
**Chairperson: Stefano Cozzini**

**13 November 2008**

**09:00 - 09:30** **Panasas presentation**

**09:30 - 09:50** **E4 presentation**

**09:50 - 10:10** **Eurotech presentation**

**10:10 - 10:30** **IBM presentation**

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 12:20** (Room: Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))
**Stefano Cozzini/Axel Kohlmeyer** / *CNR-INFM Democritos, Trieste, Italy/University of Penn., Philadelphia, U.S.A.*
**Special Topic: How to organize a similar school in your country/institute**
We will discuss with interested people how to setup a similar event in other places with or without the help of ICTP. Logistic details (how/where to submit a proposal ) and technical ones as well will be discussed.

**12:20 - 14:00** --- Lunch Break ---

**14:00 - 15:30** **CEI Round Table**
Participants coming from CEI countries will discuss future regional initiatives in the area of HPC/GRID

**Closing Session** (Room:Adriatico Guest House - Kastler Lecture Hall Area (Lower Level 1))

**14 November 2008**

**09:00 - 09:45** **Stefano Cozzini/Axel Kohlmeyer** / *CNR-INFM Democritos, Trieste, Italy/University of Penn., Philadelphia, U.S.A.*
**Future Perspectives in GRID and HPC**

**09:45 - 10:30** **Presentations from Participants**
15 minutes each

The SEE-GRID project (Antun Balaz) 15'

Benchmarking WRF on different clusters (Irene Gallai) 15'

**10:30 - 11:00** --- Coffee Break ---

**11:00 - 12:00** **Presentations from Participants**

Public Cluster: An open cluster approach (Zaenal Akbar - Research Center for Physics, Indonesian Institute of Science) 20'

APPLICATION OF GRID COMPUTING IN MODELING TSUNAMI AND DENGUE (Teh Su Yean, Kew Lee Ming and Koh Hock Lye ) 20'

MPICH-G2 Communication Model on the Grid (Mehdi Sheikhalishahi) 20'

**12:00 - 12:30** **Stefano Cozzini / Axel Kohlmeyer** / *CNR/INFM Democritos and Sissa/eLab, Trieste, Italy / University of Penn., Philadelphia, U.S.A*
**Wrap-up and conclusions**