

European-US Summer School on HPC Challenges in Computational Sciences



organized by DEISA and TeraGrid sites

Oct 4 -7, 2010

Hotel Santa Tecla Palace, Acireale, Catania, Italy



Programme

Sun Oct 3, 2010:

19:00 – 21:00 Registration

20:30 Dinner

Mon Oct 4, 2010:

8:00 – 8:45 Registration

9:00 – 12:00 HPC Challenges and Technology

HPC Challenges

Barry Schneider, NSF, US

DEISA overview

Hermann Lederer, RZG, Germany

TeraGrid / XD overview

John Towns, NCSA, US

PRACE overview

Giovanni Erbacci, CINECA, Italy

10:20 – 10:40 Coffee Break

12:00 – 13:30 Lunch Break

13:30 – 15:30 Challenges by Scientific Disciplines I

Parallel track 1: Materials & Life Sciences

Nano technology

Thomas Schulthess, ETHZ, Zurich, & CSCS, Switzerland

Parallel track 2: QCD

Quantum Chromo Dynamics

Richard Brower, Boston University, US

15:30 - 15:50 Coffee Break

15:50 - 16:50 Challenges by Scientific Disciplines II

Parallel track 1: Materials & Life Sciences

Molecular Dynamics simulation packages I

Gromacs: David van der Spoel, Univ. Upsala, Sweden

Parallel track 2: Plasma Physics

Fusion energy research

Frank Jenko, MPI for Plasma Physics, Garching, Germany

Evening Networking Dinner

Tue Oct 5, 2010:

9:00 – 12:00 Programming

Overview on Mixed MPI/OpenMP Programming,

UPC, CAF, StarSs Model

Giovanni Erbacci, CINECA, Bologna, Italy

David Henty, EPCC, University of Edinburgh, UK

Josep M. Perez, Barcelona Supercomputer Center, Spain

- 10:20 – 10:40** Coffee Break
- 12:00 – 13:30** Lunch Break
- 13:30 – 15:20** **Challenges by Scientific Disciplines III**
- Parallel track 1: Astro Sciences**
 Astro sciences, Cosmology
Mike Norman, UCSD, San Diego, US
- Parallel track 2: Materials & Life Sciences**
 Molecular Dynamics simulation packages II
Amber: Thomas Cheatham, Univ. Utah, US
CP2K: Marcella Iannuzzi, Univ. Zurich, Switzerland
- 15:20 – 15:40** Coffee Break
- 15:40 – 16:35** **Challenges by Scientific Disciplines IV**
- Parallel track 1: Climate Research**
 Climate Research
Patrick Joeckel, DLR, Germany
- Parallel track 2: Materials & Life Sciences**
 Molecular Dynamics simulation packages III
QuantumEspresso: Paolo Gianozzi, Univ. Udine, Italy
- 16:35 – 17:30** **Algorithmic Approaches & Libraries I**
 Advanced algorithms for long-range interactions
Axel Arnold, University of Stuttgart, Germany
- Evening** Networking Dinner

Wed Oct 6, 2010:

- 9:00 – 12:00** **Performance Analysis & Profiling**
 Points package, Scalasca, etc.
Philip Blood, PSC, Pittsburgh, US
Bernd Mohr, FZJ, Juelich, Germany
- 10:20 – 10:40** Coffee Break
- 12:00 – 13:30** Lunch Break
- 13:30 – 17:00** **Algorithmic Approaches & Libraries II**
 Particle-in-Cell methods in plasma physics
Roman Hatzky, IPP, Garching, Germany
 Software environment for efficient flow simulations
Joachim Bungartz, TUM, Munich, Germany
 Numerical Libraries
Tony Drummond, LBNL, Berkeley, US
- 15:40 – 16:00** Coffee Break
- Evening** Summerschool Event Dinner

Thu Oct 7, 2010:

- 9:00 – 12:00** **Data Intensive Computing and Visualisation**
 Data intensive computing
John R Johnson, PNL, US
 Visualisation
Sean Ahern, ORNL, Knoxville, US
Uwe Woessner, HLRS, Stuttgart, Germany
- 10:20 – 10:40** Coffee Break
- 12:00 – 13:30** Lunch Break
- 13:30 – 16:00** **General Discussions, Collaborations**