

**EU-US HPC Summer School  
Report  
December 24, 2010**



The first European US Summer School on HPC Challenges in Computational Sciences organized jointly by Europe's DEISA project and the US/NSF TeraGrid project was held at Santa Tecla Palace in Acireale, Sicily from Oct 3-7, 2010.

The attendees were asked about their goals for attending and the extent to which the summer school met those goals. Overwhelmingly, the attendees said that the summer school met their goals, and quite a few people indicated that the event fully and completely met their goals, and a couple people said the event exceeded their expectations. Two people indicated that there were topics that could have been covered in more depth to aid them including fault tolerance, and more on numerical algorithms. When asked for their overall assessment of how well the summer school met their goals, the attendees responded as follows:

- Excellent – 16 - 33.3%
- Very good – 25 - 52.1%
- Good – 6 - 12.5%
- Fair – 1 - 2.1%
- Poor – 0

Among the participants were sixty graduate students or post-docs, selected from more than 100 applications: 24 from US and 35 from EU universities and research institutions. Students came from a variety of disciplines, among them astronomy, atmospheric sciences, chemistry, computer science, engineering, mathematics and physics.

Approximately 20% of the attendees were female students. The list of attendees is included in Appendix B.

Twenty-five high level speakers addressed major fields of computational science, with nine speakers from the US and sixteen from Europe. Areas covered included Challenges by Scientific Disciplines, Programming, Performance Analysis & Profiling, Algorithmic Approaches & Libraries, and Data Intensive Computing and Visualization.

“The summer school HPC Challenges in Computational Sciences was an excellent opportunity for me to get an overview of the complete spectrum of High Performance Computing and Computational Science. Attending talks from the large number of distinguished speakers from almost every domain of computational science and High performance computing has enabled me to get a very clear idea of the current trends in the area”, one of the students stated afterwards.

This was planned from the outset and a joint DEISA-TeraGrid effort. “Our primary objective for the student experience was to advance computational sciences by enabling and stimulating future international collaboration, innovation, and discovery through the most effective use of HPC,” said Hermann Lederer from the DEISA coordination team at RZG, Garching. “We hope to continue with such events every year— alternating between EU and US destinations,” said TeraGrid Forum Chair John Towns, National Center for Supercomputing Applications. “The overwhelmingly positive feedback of the students, in which 85% rated the event as very good or excellent, can be taken as a mandate”, he added.

The agenda for the event is included as Appendix A. The presentation slides are available at: <http://www.deisa.eu/Summer-School/talks>

A survey was conducted among the attendees and presenters to capture feedback from the event to assess the impact of this event, and to help plan for future events. A total of 50 responses were provided from among the 60 participants, and 13 responses were collected from the 35 presenters.

The make-up of the attendees responding to the survey included:

- Postdoc – 6 - 12.2%
- Graduate – 36 - 73.5%
- HPC Center staff – 4 - 8.4%
- Other – 3 - 6.1%

The make-up of the presenters (and staff) responding to the survey included:

- Faculty – 3 - 37.5%
- Researcher – 2 - 25%
- HPC Center staff – 2 - 25%
- Other – 1 – 12.5%

The attendees were from among the following fields:

- Physics – 14
- Computer science – 10
- Chemistry – 7
- Engineering – 6
- Astronomy – 2
- Other – atmospheric science, biology, mathematics

The survey respondents were asked to indicate what they found to be *most* useful from the summer school experience. Many of the responses indicated that they felt very positive about the broad range of topics that were covered including scientific areas and technological areas related to HPC. The attendees felt they learned a great deal about HPC tools, resources, and the directions that others in the community were taking that would help to guide their own endeavors. Many of the attendees enjoyed learning about the challenges addressed in a diverse array of disciplines, which in turn helped them to understand they faced similar challenges and similar opportunities for advancing their own research. A number of attendees also mentioned that it was beneficial to learn about career opportunities.

The survey respondents were asked to indicate what they found to be *least* useful from the summer school experience. A number of attendees mentioned that they would like to have heard less about the detailed scientific results and the theory behind the science, with a preference for more information about the computational details and computational methodologies that were applied to advance the research. A number of attendees would have preferred more hands-on aspects during the summer school, although some attendees said that would only have reduced the time to learn about the breadth of topics that were covered, that were overall considered to be very good by the vast majority of people responding to the survey. Some respondents mentioned that they would like to have heard more about algorithms. There was a very strong negative response by many attendees to the situation with the Internet access, which required work by the staff at the site to rectify lack of access and charges to use the Internet. These problems were worked out with the hotel on-site. There were a few negative comments about offering parallel sessions, as these people wanted to attend the competing sessions, yet many people appreciated the parallel sessions as they weren't interested in both topics, and eliminating the parallel tracks would make the summer school much longer. A couple people suggested that the presentations could be shortened.

When asked to provide advice for future, many respondents said that all of the talks should address the HPC challenges, general computational problems and solutions, and the talks should address less on the specific research work and specific formulas. Some respondents would like to hear more about GPU programming, and more coverage of other fields of science including chemistry and biology. It was suggested that young researchers should talk about their research and seek advice from the group, including the more senior presenters, to guide them in their research. It was mentioned that slides from

all presenters should be made available as soon after the presentations as possible. The attendees suggested that the use of Google Docs would help to address this. A number of people again repeated the request for hands-on sessions. A few people suggested that the summer school could be between ½ a day and full day longer to cover more topics.

The survey respondents recommended conducting the summer school so as not to compete with classes, and to be closer to a major airport to eliminate the travel hassles of getting to the meeting site. The attendees liked the BOF sessions during lunch, and suggested that they start earlier in the week to allow people to meet and share information on topics of common interest. The attendees would like to have received a list of all participants and presenters, and their fields of research to help people make connections during the summer school.

When asked how the summer school would impact their own work, most of the respondents said the summer school would not change their research plans, but many of them planned to apply the tools they learned about to enhance their research. Many of the attendees plan to apply the code profiling, tuning, and optimization techniques on their own codes, plan to explore the use of numerical libraries, and utilize the visualization tools they learned about. Some of the attendees plan to explore some of the new frameworks they learned about (e.g. UPC, StarSs), and to share what they learned with their colleagues.

Overall, nearly all of the respondents felt that the event was well organized, that the location was wonderful (except for transportation issues to and from the airport), and that the accommodations were quite good (except for early Internet problems). Some people felt that being near a major airport and near a city to offer more off-hours opportunities would be useful. One person mentioned that the hotel did not provide ample options for vegetarians.

A major emphasis for the event was to facilitate interactions among the attendees and the presenters, and to allow ample time for people to share ideas, explore challenges and opportunities, and to establish new colleagues and collaborations. The vast majority of attendees felt that the summer school did allow plenty of time for people to interact and talk. A number of people mentioned that they have new colleagues to share ideas. A few indicated that new collaborations may result from the event. A few people indicated that there were not enough others in the same field of study to build new connections, but that the event overall was still very useful to their learning. A few people said more could be done to encourage presenters to spread out among the attendees, and not sit together during meals.

In summary, the attendees and presenters strongly recommended that further summer schools be conducted in the US and Europe.

## Appendix A - Summer School Agenda

*Mon Oct 4, 2010:*

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*

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*

15:50 – 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*

*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 (Lecture 1, Lecture 2, Lecture 3, Lecture 4), EPCC, University of Edinburgh, UK*  
*Josep M. Perez, Barcelona Supercomputer Center, Spain*

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*

15:40– 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*

*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*

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*

*Thu Oct 7, 2010:*

9:00 – 12:00 - Data Intensive Computing and Visualization

- Data intensive computing: *John R Johnson, PNL, US*
- Visualization  
*Sean Ahern, ORNL, Knoxville, US*  
*Uwe Woessner, HLRS, Stuttgart, Germany*

## Appendix B – Attendees, Staff and Presenters

### Attendees

First Name	Last Name	Institute	Country
Xavier	Abellan Ecija	Barcelona Supercomputing Center	Spain
Shannen	Adcock	University of Arkansas	USA
Fabio	Affinito	CINECA	Italy
Sean	Ahern	University of Tennessee	USA
Axel	Arnold	University of Stuttgart, ICP	Germany
Thomas	Auckenthaler	TU München	Germany
Mirco	Bazzani	Physics department, Parma University	Italy
Philip	Blood	Pittsburgh Supercomputing Center, Carnegie Mellon University	USA
Steven	Böing	Delft University of Technology	Netherlands
Jonathan			
Richard	Brower	Boston University	USA
Hans-Joachim	Bungartz	TUM, Department of Informatics	Germany
Benjamin	Byington	University of California, Santa Cruz	USA
Ramon	Calderer	University of Illinois at Urbana-Champaign	USA
Thomas	Cheatham	University of Utah	USA
Galen	Collier	Clemson University	USA
Benjamin	Cruz Perez	University of Puerto Rico at Mayaguez	USA, Puerto Rico
Tony	Drummond	Lawrence Berkeley National Laboratory	USA
Philipp	Edelmann	Max-Planck-Institute for Astrophysics	Germany
Giovanni	Erbacci	CINECA	Italy
Johannes	Feist	ITAMP, Harvard-Smithsonian Center for Astrophysics	USA
James	Ferguson	National Institute for Computational Sciences	USA
Daniel	Fletcher	University of Warwick (EPSRC)	UK
Wolfgang	Gentzsch	Max-Planck-Institute	Germany
Paolo	Giannozzi	University of Udine and IOM-Democritos	Italy
Andreas	Goetz	San Diego Supercomputer Center	USA
Luca	Graziani	Max-Planck-Institute for Astrophysics, Garching	Germany
Thomas	Guillet	CEA/DSM	France
Roman	Hatzky	IPP	Germany
Andreas	Hauser	Genzentrum, LMU	Germany

Tobias	Heidig	MPI Magdeburg	Germany
David	Henty	EPCC	UK
Matthew	Hogan	University of Massachusetts	USA
Lorenz	Hüdepohl	Max-Planck-Institut für Astrophysik	Germany
Marcella	Iannuzzi	University of Zurich	Switzerland
Sebastian	Illi	University of Stuttgart, IAG	Germany
Sam	Jacobs	University of Antwerp	Belgium
Frank	Jenko	IPP	Germany
Patrick	Jöckel	DLR Institute for Atmospheric Physics	Germany
John	Johnson	Pacific Northwest National Laboratory	USA
Alan	Kelly	University of Glasgow	UK
Hans- Joachim	Klingshirn	MPI für Plasmaphysik	Germany
Elizabeth	Leake	University of Chicago	USA
Hermann	Lederer	Garching Computer Centre, Max- Planck-Society	Germany
Angelo	Limone	Max-Planck-Institut für Plasmaphysik	Germany
Jeremy	Logan	University of Maine	USA
Katie	Maerzke	Vanderbilt University	USA
Chris	Malone	Stony Brook University	USA
Bernd	Mohr	Jülich Supercomputing Centre	Germany
Giuseppa	Muscianisi	University of Messina	Italy
Sreeja	Nag	Massachusetts Institute of Technology	USA
Stefan	Nagele	Vienna University of Technology	Austria
Terrence	Neumann	Marquette University	USA
Michael	Norman	SDSC, UCSD	USA
Szilárd	Páll	Center For Biomembrane Research, Stockholm	Sweden
Benjamin	Payne	Missouri Science and Technology	USA
Renate	Pazourek	Vienna University of Technology	Austria
Christian	Pelties	Department of Earth & Environmental Sciences, LMU Munich	Germany
Josep M.	Perez	Barcelona Supercomputing Center	Spain
Marcelo	Ponce	Rochester Institute of Technology	USA
Johannes	Reetz	Garching Computer Centre, Max- Planck-Society	Germany
Martin	Roderus	Technische Universität München	Germany
Dominic	Roehm	Institute for Computational Physics	Germany
Anastasia	Romanova	Max-Planck-Institute for Mathematics in the Science	Germany
Romelia	Salomon	San Diego Supercomputing Center	USA



	Ferrer		
Annika	Schiller	Jülich Supercomputing Centre	Germany
Barry	Schneider	National Science Foundation	USA
Mandes	Schönherr	Institute of Physical Chemistry	Switzerland
Thomas	Schulthess	ETHZ	Switzerland
Jacob	Searcy	University of Oregon	USA
Daniele	Selli	Technische Universität Dresden	Germany
Cengiz	Sen	University of Tennessee	USA
Andrey	Sharapov	University of Pittsburgh	USA
Pablo	Souza	University of Michigan	USA
Filippo	Spiga	IBM and University of Milano Bicocca	US and Italy
Julien	Thibault	University of Utah	USA
Daniel	Told	MPI für Plasmaphysik	Germany
John	Towns	NCSA/University of Illinois	USA
Volodymyr	Turchenko	University of Calabria	Italy
Ikram	Ullah	Royal Institute of Technology (KTH)	Sweden
David	van der Spoel	Department of Cell & Molecular Biology, Uppsala University	Sweden
Xingyu	Wang	New York University	USA
Susann	Wangnett	Garching Computer Centre, Max- Planck-Society	Germany
Stefan	Wenk	Munich University, Geophysics	Germany
Katelyn	White	University of California, Santa Cruz	USA
Daniel	Wilde	EPCC	Scotland
Uwe	Woessner	HLRS	Germany
Guoxing	Xia	Max-Planck-Institute for Physics	Germany
Anastasia	Yanchilina	Lamont Doherty Earth Observatory, Columbia University	USA
Haseeb	Zia	Technische Universität München	Germany

### Staff and Presenters

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Sean	Ahern	University of Tennessee	USA
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Elizabeth	Leake	University of Chicago	USA
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Bernd	Mohr	Jülich Supercomputing Centre	Germany
Michael	Norman	SDSC, UCSD	USA
Josep M.	Perez	Barcelona Supercomputing Center	Spain
Barry	Schneider	National Science Foundation	USA
Thomas	Schulthess	ETHZ	Switzerland
John	Towns	NCSA/University of Illinois	USA
David	van der Spoel	Department of Cell & Molecular Biology, Uppsala University	Sweden
Uwe	Woessner	HLRS	Germany