# EU-US HPC Summer School August 7-12, 2011 South Lake Tahoe, California

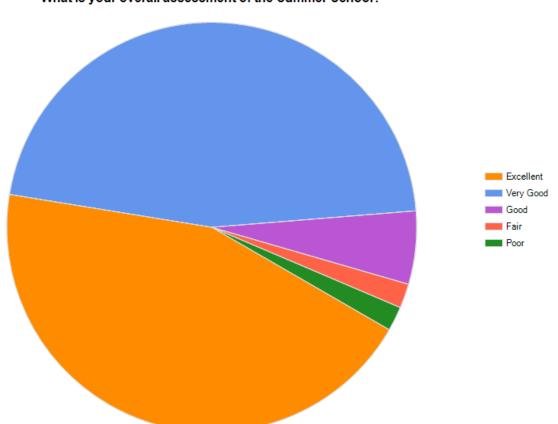
♪ The Eagles, Hotel California (intro) ♪

Venue: Embassy Suites, South Lake Tahoe, California Located on the California/Nevada border

## Student selection process & Diverse community

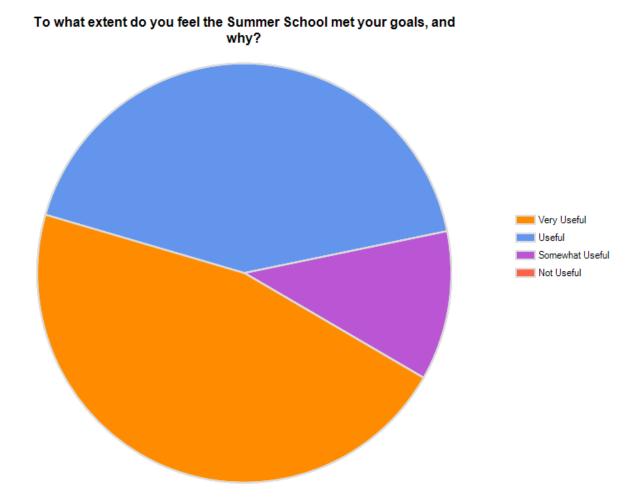
- March 15, 2011 deadline
- ~200 applications
- 60 students chosen by distributed selection committee
- 25 EU/PRACE
- 35 US/XSEDE
- 17 countries represented
- 30% female

### 95% post-event favorable feedback.



What is your overall assessment of the Summer School?

### Student goals met—time well spent...



### The academic program...

∫ Devo, Whip it (intro) ∫

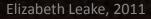
## Monday, August 8

- HPC Challenges and Technology Session
  - PRACE Overview Lennart Johnsson,
     University of Houston, and Royal
     Institute of Technology, Stockholm
  - XD Overview John Towns, NCSA
- Introduction of Participants
- Exascale Software Project
  - David Keyes, Columbia University and KAUST
- Lunch (Birds-of-a-feather lunch groupings, by discipline)
- Programming
  - Overview on Mixed MPI/OpenMP
     Programming, UPC, CAF, David Henty,
     EPCC, University of Edinburgh, UK
  - StarSs Model Alejandro Duran,
     Barcelona Supercomputing Center
- Electronic Poster Session



## BoFs were popular

- Birds-of-a-feather lunch group topics:
  - Monday—Disciplines
  - Tuesday—Activities
  - Wednesday—Tech themes
  - Thursday—sit with someone new!



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## Tuesday, August 9

- Challenges by Scientific Disciplines I
  - Parallel track 1: Materials Science
    - Thomas Schulthess, ETHZ, Zurich, & CSCS, Switzerland
  - Parallel track 2: Plasma Physics
    - Frank Jenko, Max Planck Institute for Plasma Physics, Garching
- Challenges by Scientific Disciplines II
  - Parallel track 1: Life Sciences
    - Amber: Thomas Cheatham, Univ. Utah, US
  - Parallel track 2: CFD / Engineering
    - Ulrich Rist, University of Stuttgart
- Challenges by Scientific Disciplines II
  - Parallel Track 1: Cosmology
    - Britton Smith, Michigan State University
  - Parallel Track 2: Metagenomics Earthmicrobiome Project
    - Folker Meyer, University of Chicago
- Lunch and Team Building
- Performance Analysis & Profiling PAPI, IPM, PerfSuite, TAU, Vampir, Scalasca
  - Philip Blood, PSC, Pittsburgh, US
  - Bernd Mohr, FZJ, Juelich, Germany





## Wednesday, August 10



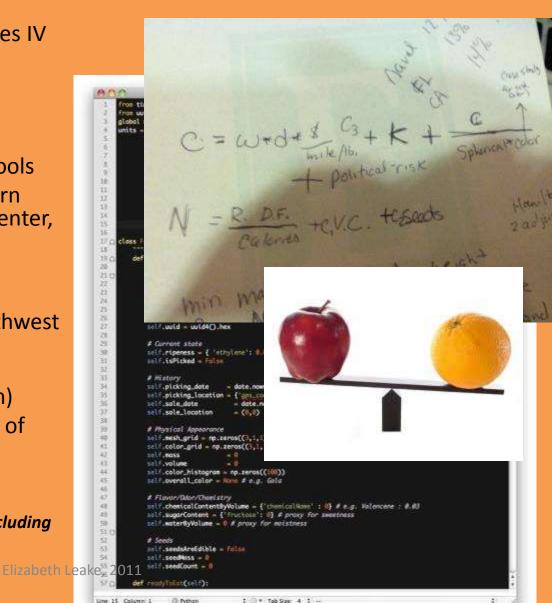
- Challenges by Scientific Disciplines III
  - Parallel track 1: Life Sciences
    - GROMACS Erik Lindahl, University of Stockholm
  - Parallel Track 2: Engineering A Software Environment for Efficient Flow Simulations
    - Hans-Joachim Bungartz, Technical University of Munich
- Numerical Algorithms & Parallel I/O
  - Parallel track 1: Scalable fast algorithms for Coulomb interactions
    - Olaf Lenz, University of Stuttgart
  - Parallel Track 2: Parallel I/O
    - Lonnie Crosby, National Institute of Computational Sciences (NICS)
- Community Building Time
- Lunch and Team Building
- GPU/CUDA programming with Wen-Mei Hwu, NCSA



## Thursday, August 11

- Challenges by Scientific Disciplines IV
  - Parallel Track 1: Numerical Libraries
    - Tony Drummond, LBNL, Berkeley, US
  - Parallel Track 2: Workflow Tools
    - Scott Callaghan, Southern California Earthquake Center, USC
- Data Intensive Computing
  - John R Johnson, Pacific Northwest Laboratory
- Scientific Visualization (hands-on)
  - Amy Szczepański, University of Tennessee/NICS

John Johnson's "apples and oranges" exercise stimulated discussion on FaceBook, including shared notes, and positive feedback..



### Who would you like to meet?...

∫ Manu Chao, Me Gustas Tu (intro) ∫

## **The Social Network**

#### lasting relationships are made outside of the classroom





- Wiki--Bios of all participants, presentations, photographs, announcements, etc;
- Dynamic exchange on FaceBook;
- FB community created July 25—time to get to know each other in advance;
- 64 members (most students, some faculty);
- FB used for announcements, social banter, homework results, and more;
- Rich repository of student photographs;
  - "Friending" among participants assured continued contact;
- Survey feedback: FB highly effective tool for ~95% of the participants;
- LinkedIn group offered for professional networking.

## Participants encouraged to mix it up

- Four course-filled days is not much time to meet 87 people;
- Tight social groupings were discouraged (in and outside of class);
- Head-shots and bios shared in advance;
- Organizers and faculty encouraged to mingle in and outside of class.



## Multiple Levels of Interpersonal Social Engagement

- Students provided with a sheet of star stickers in a color that represented their field of study;
- Each was encouraged to share stars and collect others and to learn something unique about each person;
- First prize awarded to Adam Sullivan who had collected the most stickers and could tell us something unique about each person.





### By Thursday everyone needed a break... Today I don't feel like doing anything

S Bruno Mars, the Lazy Song (intro) S

## **Extracurricular Activities**

On Thursday afternoon students chose from the following (ala carte) recreation options:

- Riverboat Cruise (20 students);
- Hiking (30 students);
- Helicopter ride (Three students);
- Casinos (Three students);
- Others had to leave Thursday evening.







### In their own words...

S Edward Maya and Vika Jigulina, Stereo Love (intro);
Red Hot Chili Peppers, Road Trippin (in the USA-intro) S

The EU/US HPC summer school was the most enjoyable learning experience. Not only did we have breathtaking views of Lake Tahoe each day, the school provided me with the opportunity to learn about HPC challenges and state-of-the-art technologies. The friends I made in multidisciplinary research fields will offer future potential collaborations.



#### Man (Melody) Luo

Eshelman School of Pharmacy University of North Carolina, Chapel Hill, US

#### Mohamad M. Nasr-Azadani

Ph.D. Candidate, Department of Mechanical Engineering, University of California at Santa Barbara, USA

My research involves numerical simulations of turbidity currents or, simply said, underwater avalanches. Thanks to the talks presented by knowledgeable and experts in HPC about parallel I/O and visualization, I think I will be performing better research during my final academic year. I loved the diversity of people coming from different countries and various backgrounds. Thanks to organizers for choosing Lake Tahoe. I loved the hikes we all did together!

I am so grateful that I spent this wonderful week in South Lake Tahoe, and hope to meet everyone again in the future!

### Shuang (Susan) Gao

PhD student at the University of Tennessee, Knoxville, USA.

Research in high performance computing (GPGPU, GPU, parallel HPC and computer architecture).

Presentations about performance tools, workflow, and software for Exascale were interesting and helpful. **The location (South Lake Tahoe)** was beautiful. I was able to interact with international fellow students and experts on HPC. I was able to increase my skills on code acceleration, new tools for massively parallel codes and efficient parallel processing of large amounts of data.

### **Paulo Abreu**

PRACE partner Post-Doc at Institute for Plasmas and Nuclear Fusion, Technical University of Lisbon, Portugal

Home of the Original



The EU/US Summer School provided a comprehensive overview of the different aspects of HPC. All lectures were well prepared and presented. Especially interesting to me where the presentations on tools, parallel programming, GPU programming, and the opportunity to get to know HPC experts and colleagues from around the world. The location and organization of the event were excellent, providing the perfect atmosphere. Thanks to everyone who made it possible!

Estela Suarez, Forschungszentrum Jülich, Germany

#### Mohsen Eshraghi PhD Student Mechanical Engineering Department Mississippi State University, USA



I enjoyed meeting people from different disciplines and different countries and made invaluable friendships. It was good knowing about the HPC challenges in other disciplines. I learned a lot especially from useful talks presented afternoons about some new HPC tools for programming, profiling and visualization that for sure will influence my research work. *Many thanks to everybody who provided this wonderful opportunity for me!* 





#### Maria Minakova

PhD student: Chemistry Department at the University of North Carolina, Chapel Hill and Chemistry Department at the University of Maryland, College Park



Thanks to NSF for this wonderful opportunity! I've met inspiring and very knowledgeable people, learned the difference between OpenMP and MPI, got both amazed and frightened by CUDA, and discovered many new fields of interest where my analytical skills can be applied!

The 2<sup>nd</sup> EU-US HPC Summer School exposed me to several tools and techniques, specially in parallel programming with MPI and GPUs, that can be very useful to my research. Very prominent professors, researchers, and organizers made this summer school a successful event.

Cuauhtemoc Munoz University of Texas at El Paso Ph.D. student in Computer Science



Thank You! The 2011 HPC Summer School at Lake Tahoe, California was an amazing and enriching experience for me. The talks by the experts, discussions with fellow attendees and the light fun moments made it a cherished one too! <sup>©</sup>

Prachi Pradeep PhD student in Computational Sciences Marquette University, Milwaukee, USA



#### **Benjamin Payne** PhD Candidate Missouri University of Science and Technology

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e

I attended the 2010 EU/US HPC Summer School in Catania Sicily, and was invited to return as a student mentor, and technical assistant. I also helped organize some of the extracurricular activities.

It was great to meet the staff, attendees, and presenters. I especially enjoyed talking with Scott Callaghan about GridFTP client setup and documentation. It was good to learn that I am already using version control and automated workflow best practices, and that metadata standards are needed, but have not yet been developed.

The experience will benefit me in the future, as I plan to apply for a Computational Physics Postdoctoral position with a national laboratory.

# Ripple Effect:

- Student Ben Payne teaches fellow Missouri students what he learned at HPC Summer School:
  - http://mominer.mst. edu/2011/09/08/stgraduate-studentgives-lecture-oncomputertechnology/



By Barry Closser on 9/08/11 • Share 🖬 Facebook 📧 Twitter 🖬 del.icio.us

Computing has come a long way from its early days. We now have computers all around us; they are in our homes, cars, and even our pockets. Most people do not see some of the more powerful and clever uses for computers today. Many research teams use computers to view and analyze their data from research done. The physics department is just one department that deals with mass amounts of data as a result of their experiments. One person has made it a point to try and stream line the process of analyzing and organizing this data. Ben Payne, a physics graduate student, is currently studying the characterization of wave propagation. He has worked with his advisor for five years now, in that time he has had four publications based on their combined efforts.

Payne gave a talk last Wednesday on how computers could be used for repetitious tasks. The talk was a result of various summer schools Payne attended that focused on the role computers play in research. One in particular, was a summer school on high performance computing that was held in Lake Tahoe, California. There are also some upcoming conferences on supercomputing and its benefits that Payne plans to attend this fall. He wants to bring this information back to the S&T campus to help his fellow students process the data received from their projects.

The talk focused mainly on version control and automation. These are probably two of the most useful tools available to research teams on campus. Version control is the ability to keep an entire team up to date on computer code written specifically to analyze the specific parts of data received. Often times, this code needs to be changed on the fly to improve the accuracy of results or to fine-tune the calculations to the new specifications of the instrumentation used. Automation is pieces of code used to make looking for specific files or pieces of files among hundreds or even thousands of folders easier. The strings of code are often times command line executions of actions that need to be repeated. This allows the user the ability to just launch one program to find or change many separate files.

Payne has worked with the Linux User Group that is run by the IT department, along with the high performance computing group, to help spread these techniques to students in other departments. Payne said that "any student or faculty member who manages data or source code can benefit" from version control and automation. These are not ideas that are specific to any one department, but a wide range of techniques that can be applied across the board to data management and computer code.

If you would like Payne to speak to your group on the benefits of using these tools, feel free to contact him via e-mail at <u>ben.is.located@amail.com</u>. He is also available if you would like to speak one-on-one about these topics to gain further technical insight. He also has knowledge in various other uses for technology in aiding the research and data processing that he would be more than happy to share.

Attending the EU/US HPC Summer School in Lake Tahoe was a valuable learning experience. The skills I learned will help me streamline and improve my research in the future. The friends I made will make my research in HPC more enjoyable in the future. And, of course, the location in beautiful Tahoe added a wonderful spice to the mix.

### Organizers – thank you for all of your work in creating this excellent event!

Vera Dadok PhD Candidate University of California, Berkeley

#### Raman Shah

Physical Chemistry University of Chicago, USA

The EU/US HPC Summer School was a fantastic experience. Working at the interface of theory and experiment within an experimental research group, I seldom get chances to talk in depth with colleagues about computation. The summer school gave me a chance not only to learn about cutting-edge hardware and software used to solve scientific problems but also to absorb some of the unwritten lore in developing highperformance code and ultimately getting computational science done.

The chance to make new friends throughout Europe and the USA and to work in a beautiful and stimulating setting was also a pleasure. Now back home, I am refreshed and more productive than ever!



I wish to thank the EU/US HPC summer school program organizers for their outstanding effort! They chose a beautiful location and selected a diverse group of attendees and faculty. I appreciate the creative ways they encouraged us to mingle. By meeting so many new people, the exchange of ideas will surely form future collaborations. Thanks to the speakers for taking time to prepare up-to-date content that broadened my knowledge. I had such a meaningful and fun week. I hope the summer school will continue in the future so that many more young researchers

will benefit as I have

#### Xuefei Rebecca Yuan

Petascale Postdoctoral Fellow Lawrence Berkeley National Laboratory SYLVAIN LAIZET RESEARCH ASSOCIATE in Computational Fluid Dynamics IMPERIAL COLLEGE LONDON

> During this amazing summer school, in an amazing location, I had the chance to meet colleagues in the field of HPC. I also had the opportunity to increase my knowledge thanks to impressive lectures/talks by experts. It was a great experience!



As if breathing in fresh mountain air, taking invigorating lake dips and meeting peers and potential collaborators were not enough reasons to appreciate this summer school; my research course has also been influenced, particularly from the following experiences:



Learning where-to-start/how-to-do performance engineering by using the tools and procedures outlined by Philip Blood

Dirtying my hands with CUDA after an extremely informative heterogeneous computing session facilitated by Wen-mei Hwu

Figuring out which tools to use with regards work flow structure as explained by Scott Callaghan

Many thanks to all involved.





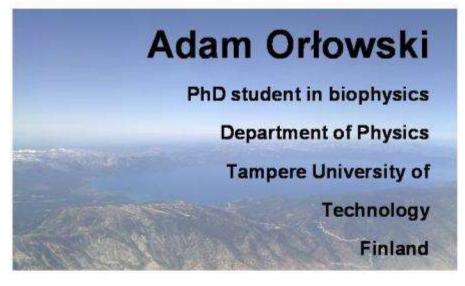
The school provided a unique environment and an excellent opportunity to come in contact with members of the international HPC community. I developed new friendships and partnerships with both the presenters and attendees that will foster the exchange of ideas and collaboration.



Theo Christoudias Computational Scientist Cyprus Institute I not only learned about new topics and computing resources through lectures, but I also had a chance to try them out first hand. These hands-on workshops were a wonderful way for me to come away with a better knowledge of GPU acceleration, Coarray Fortran, and more!

> Anjali Tripathi PhD Student in Astronomy Harvard University USA

# **Thank You!**



The EU/US HPC Summer School broadened my knowledge and will definitely improve my research.

I had a chance to meet wonderful people and spend time with them in a beautiful place. The organization was perfect.

Each lecture and hands-on session was well prepared. It was an interesting and unique meeting.



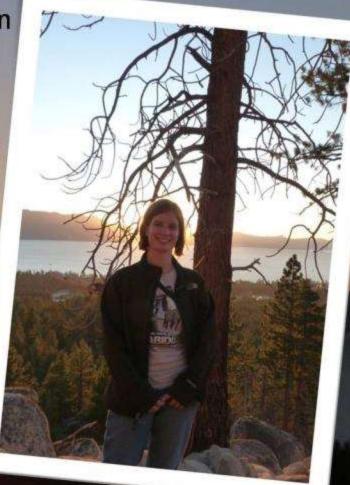


Many thanks to the EU/US HPC Summer School organizers for a great location and choice of attendees/presenters! People were very open and friendly. Hmm, a joint proposal to EU/FP7 funds in the near future sounds good! The tools presented in the profiling talks like *TAU*, *Vampir* and *Scalasca* will definitely be discussed in my research group. We'd also like to go forward with GPU programming. A short course on GPU programming helped a lot.

## Miloš Ivanović, PhD

Assistant Professor Faculty of Science Department of Mathematics & Informatics University of Kragujevac Serbia This summer school allowed me to be inspired by experts and colleagues in the HPC field and to learn about different programs that I can utilize in the future. It has helped me create valuable relationships that will continue to help me as I pursue a career in this field. Thank you for this wonderful opportunity!





## Theresa Foster

Doctor of Pharmacy Student University of New England, Portland, Maine

# Thank You....

...for showing HPC put to work.... and outside my field

# ...and superb team spirit out of class...

I firmly believe.

...great team

...helps me become....

...that this intensive training

...well, somewhat more valuable player

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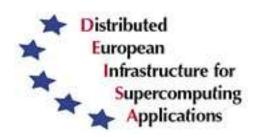
Michal Stepniewski Helsinki University, Faculty of Pharmacy/Centre for Drug Research





### Peng Bai

Department of Chemical Engineering and Materials Science University of Minnesota, USA



After five days in idyllic Lake Tahoe, not only did I learn from talks by experts in the field and see a variety of tools that might be useful in my future work, I met people from other disciplines and countries and had really interesting discussions with them!





#### Second EU/US Summer School on HPC Challenges:

Interesting lectures and hands-on sessions, especially the programming, profiling, and visualization exercises;

Nice talks with students and staff over coffee or during lunch and dinner;

Inspiring and motivational atmosphere;

Superb accommodations and Organization;

Great group activities!

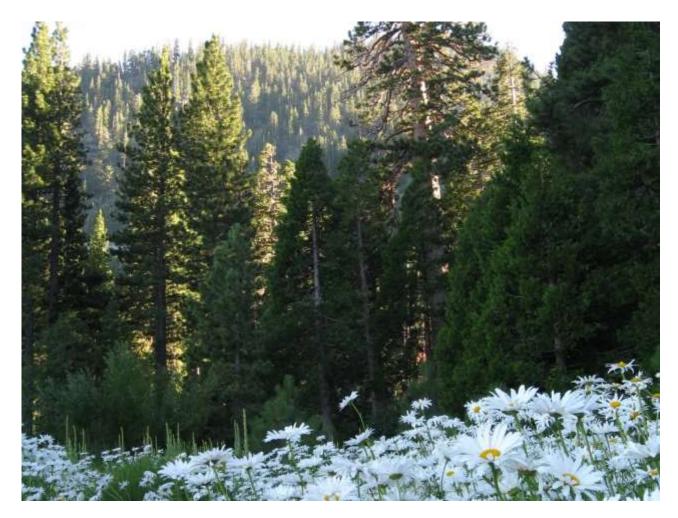






Thank you to all the organizers and participants for the great time!

Andrea Beck, Institute of Aerodynamics and Gasdynamics, University of Stuttgart



The supercomputing resources that are available to the world are **limited** and **expensive**.

Often, the solution to the problem is not to build a larger or faster machine but to use currently available resources in a **smarter** way: we will need to use **collaborative** and **creative** strategies.



#### **Ben Madej**

University of California San Diego, San Diego Supercomputer Center AMBER and molecular dynamics

#### • (\* 18. w) 2 zone study for optimal color Processes of Educating Series,

## HPC challenges require thinking outside the box

a case study about "oranges", intense discussions with colleagues, Lake Tahoe as the very inspiring background...

I would like to thank the organizers, the speakers and my fellow students for opening the box

Konstantin Koschke PhD Student at the Max Planck Institute for Polymer Research, Mainz, Germany Using HPC to improve icecream





The EU/US Summer School was a great opportunity for me to interact with others who use HPC resources so that I could begin to learn how to incorporate them into my research. The GPU/CUDA class was particularly useful to my work. Thank you for the opportunity to participate.

~ Ryan Field, PhD student, Bioelectronic Systems Laboratory, Columbia University.

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Elizabeth Leake, 2011

QUEEN OF THE LAKE BALLE