Your Workshop Guide

Imprint:

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Welcome

Dear participants,

It is our distinct pleasure to welcome you at the Gustav-Stresemann-Institut e.V. to the **4th JLESC Workshop**, organized by the Jülich Supercomputing Centre. With about 100 participants coming from the six partner institutes of the **Joint Laboratory for Extreme Scale Computing** and their collaborating universities, this event gives an impressive illustration of the enormous effort undertaken within this coalition to address the challenges of today's and future high-performance computing.

The Joint Laboratory brings together researchers from the Institut National de Recherche en Informatique et en Automatique (Inria, France), the National Center for Supercomputing Applications and the University of Illinois at Urbana-Champaign (NCSA and UIUC, USA), Argonne National Laboratory (ANL, USA), Barcelona Supercomputing Center (BSC, Spain), and, since the beginning of this year, RIKEN Advanced Institute for Computational Science (RIKEN AICS, Japan) and the Jülich Supercomputing Centre (JSC, Germany). The key objective of JLESC is to foster international collaborations on state-of-the-art research related to computational and data focused simulation and analytics at extreme scales. Within JLESC, scientists from many different disciplines as well as from industry address the most critical issues in advancing from petascale to extreme scale computing. The collaborative work is organized in projects between two or more partners. This includes mutual research visits, joint publications and software releases.

Every six months, all JLESC partners meet during a workshop like this one to discuss the most recent results and to exchange ideas for further collaborations. This is what we are going to do here at GSI and this is what we will do at Lyon next June/July. For now, we wish you a stimulating and interesting workshop and a pleasant time at Bonn-Bad Godesberg.

Your local organizing committee,

Nadine Daivandy
Julia Kämpfer
Sarah Hansen
Sabine Höfler-Thierfeldt
Britta Hoßfeld
Robert Speck

Wednesday, December 2, 2015

Time	Main Lecture Room (S29/31)
08:00-12:00	Individual meetings at seminar rooms
12:00-13:00	*Registration & Snack*
13:00-14:30	**Welcome & News - Chair: Franck Cappello (ANL)** **Robert Speck (JSC):** Welcome (15 min) **Paul Hovland (ANL):** News (10 min) **William Kramer (UIUC):** News (10 min) **Yves Robert (Inria):** News (10 min) **Jesus Labarta (BSC):** News (10 min) **Thomas Lippert (JSC):** News (10 min) **Mitsuhisa Sato (RIKEN):** News (10 min) **Scott Poole (UIUC):** Collaboration in International Virtual Organizations (15 min)
14:30-15:00	*Break*
15:00-16:45	**Molecular Dynamics I - Chair: James Wilson (UIUC)** **Helmut Grubmüller (external):** Atomistic Simulations and Exascale Computing (keynote, 45 min) **Godehard Sutmann (JSC):** Parallel Molecular Dynamics for Materials Science (30 min) **Jaewoon Jung (RIKEN):** Development of GENESIS for large scale MD simulations (30 min)
16:45-17:00	*Intermission*
17:00-18:30	**Molecular Dynamics II - Chair: Godehard Sutmann (JSC)** **Jorge Estrada (BSC):** Interactive Drug Design with Monte Carlo Simulations (30 min) **S. Sankaranarayanan (ANL):** Big data challenges in molecular dynamics: From force field development to trajectory post-processing (30 min) **James Wilson (UIUC):** Molecular Dynamics simulations of nanoscale sensors (30 min)
19:00-22:00	***Dinner & Young Scientists Meeting***

Agenda

Thursday, December 3, 2015

Time	Main Lecture Room (S29/31)	Alternative Lecture Room (S25/26)
08:30-10:00	**Programming Models I - Chair: L. Kale (UIUC)** **A. Amer (ANL):** MPI+Threads: Thread-Safety Optimization Perspectives (30 min) **V. Beltran (BSC):** Implementing OmpSs on top of Argobots threads (30 min) **K. Pouget (Inria):** Programming-Model Centric Debugging for OpenMP/OMPss (15 min) **M. Sato (RIKEN):** Status of XcalableMP project and XMP 2.0 (15 min)	**Big Data & I/O I - Chair: G. Antoniu (Inria)** **N. Vandenbergen (JSC):** Update on Blue Gene Active Storage (30 min) **J. Polo (BSC):** Experiences with BGAS at BSC (15 min) **R. Sisneros (UIUC):** Blue Waters Data Analysis and Visualization (15 min) **B. Raffin (Inria):** DataMove (15 min) **B. Subramaniam (ANL):** Comparison of Virtualization and Containerization Techniques for High-Performance Computing (15 min)
10:00-10:30	*Break*	
10:30-12:00	**Programming Models II - Chair: M. Sato (RIKEN)** **M. Dreher (ANL):** Bredala: Pushing semantic into In-Situ applications to drive data redistribution (30 min) **L. Kale (UIUC):** Charm++ research overview (30 min) **M. Casas (BSC):** Hybrid OmpSs + Charm++ (15 min) **G. Ozen (BSC):** Heterogeneous Scheduling and Dynamic Parallelism Support in Accelerator Directives (15 min)	**Resilience I - Chair: Y. Robert (Inria)** **O. Subasi (BSC):** Spatial Support Vector Regression to Mitigate Silent Errors in the Exascale Era (30 min) **A. Hori (RIKEN):** Towards Realistic Fault Resilience (15 min) **V. Beltran (BSC):** Task-based resilience in OmpSs (15 min) **R. Speck (JSC):** Fault-tolerant Parallel- in-Time Integration with PFASST (15 min) **M. Schanen (ANL):** Asynchronous Two-Level Checkpointing Scheme for Large-Scale Adjoints (15 min)
12:00-13:30	*Lunch & individual meetings*	
13:30-15:00	**Double Feature: Automatic Differentiation - Chair: Robert Speck (JSC)** **Paul Hovland (ANL):** Automatic Differentiation: State of the Art and Collaboration Opportunities (keynote: 45 min) **Christoph Bischof (external):** Enhancing the Software Ecosystem for Automatic Differentiation (keynote: 45 min)	
15:00-15:30	*Break*	

15:30-17:00	**Numerics I - Chair: Y. Nakamura (RIKEN)** **T. Imamura (RIKEN):** Multi-platform Eigenvalue solver (30 min) **H. Suno (RIKEN):** Calculation of eigenvalues and eigenvectors for large sparse non-Herimitian matrices in lattice QCD (15 min) **K. Fröhlich (JSC):** Parallel Generation of Hierarchical Cartesian Meshes for CFD on HPC Systems (15 min) **B. Steinbusch (JSC):** PEPC - a Scalable, Multi-Physics O(N) Tree Code (15 min) **A. Bienz (UIUC):** Topology-Aware Asynchronous methods and the Sparse Matrix-Vector Multiply (15 min)	**FPGAs - Chair: F. Cappello (ANL)** **F. Cappello (ANL):** Introduction (15 min) **C. Alvarez (BSC):** OmpSs and FPGAs (30 min) **O. Unsal (BSC):** Accelerating Database Analytics Through FPGAs (15 min) **N. Maruyama (RIKEN):** Benchmarking FPGAs with OpenCL (15 min) **M. Sato (RIKEN):** Title missing (15 min)
18:00-23:00	***Social Event & Workshop Dinner***	

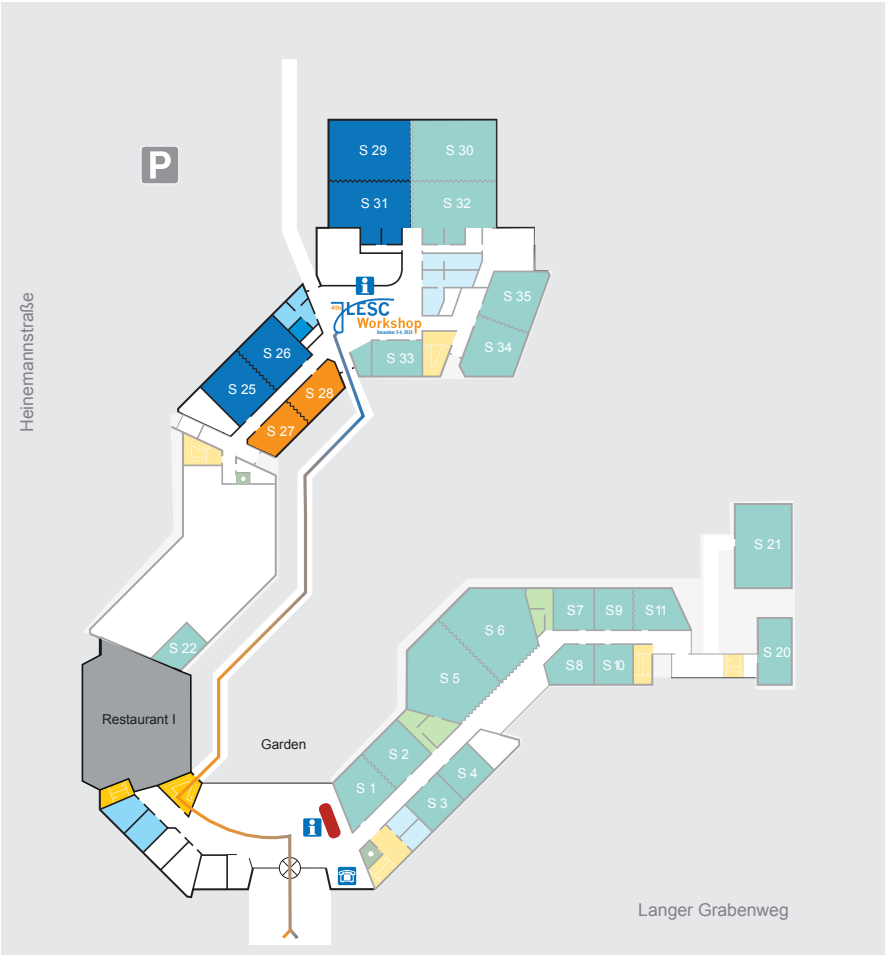
Friday, December 4, 2015

Time	Main Lecture Room (S29/31)	Alternative Lecture Room (S25/26)
08:30-10:00	**Big Data & I/O II - Chair: R. Sisneros (UIUC)** **M. Dorier (ANL):** Performance-Constrained In Situ Visualization of Atmospheric Simulations (30 min) **L. Pineda Morales (Inria):** Scaling Smart Appliances for Spatial Data S ynthesis (30 min) **A. Barcelo (BSC):** Exploiting locality through iterators on dataClay + PyCOMPSs (15 min) **M. Riedel (JSC):** Scientific Big Data Analytics (15 min)	**Numerics II - Chair: P. Hovland (ANL)** **D. Haensel (JSC):** How to do nothing in less time (30 min) **A. Schleife (UIUC):** Numerical Integrators for Fast and Scalable Quantum Molecular Dynamics (15 min) **Y. Nakamura (RIKEN):** Block and communication avoiding Krylov subspace methods (15 min) **P. Hovland (ANL):** open mic (30 min)
10:00-10:30		*Break*
10:30-12:00	**Big Data & I/O III - Chair: G. Antoniu (Inria)** **J. Wozniak (ANL):** Integrating big data tools for X-ray science (30 min)	**Resilience II - Chair: M. Casas (BSC)** **L. Bautista Gomez (ANL):** Opportunities for online data analytics in HPC (15 min)

Agenda

	O. Yildiz (Inria): Investigating the root causes of I/O interference in HPC storage systems (30 min) **G. Antoniu (Inria):** open mic (30 min)	**Y. Robert (Inria):** Optimal resilience patterns to cope with fail-stop and silent errors (15 min.) **J. Calhoun (UIUC):** Evaluating Lossy Compression for HPC (15 min) **S. Narayanan (ANL):** Separated at birth: checkpointing in resilience and algorithmic differentiation (15 min) **F. Cappello (ANL):** open mic (30 min)
12:00-13:30	*Lunch & individual meetings*	
13:30-15:00	**Performance Tools I - Chair: G. Llort (BSC)** **B. Wylie (JSC):** Developer tools for porting & tuning parallel applications (30 min) **B. Mohr (JSC):** Challenges and Opportunities of Visual Performance Data Analytics (15 min) **C. Heinrich (Inria):** Advances in simulation of parallel applications with SimGrid (15 min) **S. Shudler (JSC):** Exascaling Your Library: Will Your Implementation Meet Your Expectations? (15 min) **A. Peña (BSC):** Data placement on heterogeneous memory systems in HPC (15 min)	**Programming Models III - Chair: J. Labarta (BSC)** **S. Seo (ANL):** Performance Analysis and Optimizations of Argobots (30 min) **F. J. Conejero (BSC):** A brief overview of PyCOMPSs vs Spark comparison (15 min) **A. Denis (Inria):** Asynchronism in MPI (15 min) **J. Labarta (BSC):** open mic (30 min)
15:00-15:30	*Break*	
15:30-16:45	**Performance Tools II - Chair: B. Mohr (JSC)** **G. Llort (BSC):** Techniques for maximizing information and minimizing trace size (30 min) **S. Lührs (JSC):** JUBE - A Flexible, Application- and Platform-Independent Environment for Benchmarking (15 min) **B. Mohr (JSC):** open mic (30 min)	**Applications & Mini-Apps - Chair: M. Sato (RIKEN)** **N. Maruyama (RIKEN):** Title missing (30 min) **W. Kramer (UIUC):** Title missing (15 min) **N. Maruyama (RIKEN):** open mic (30 min)
16:45-17:00	*Farewell*	

Please check out the website (www.fz-juelich.de/ias/jsc/jlesc-4) for the most recent schedule.



Ground level

Floor Plan

- Registration Desk
- Sessions (S 31/29, S 25/26)
- Group Meetings (S 27, S 28)
- Restaurant/Lunch
- Information
- Stairs
- Elevator
- Restrooms
- Accessible restrooms

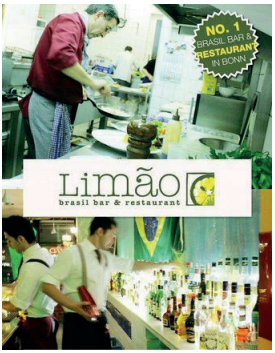
December 2, 2015: Dinner

If you have registered for the dinner on Wednesday and you are not a postdoc or student, you will meet in the lobby of the GSI at 7.15pm. You can enjoy a genuine evening and dinner at the GSI club rooms with excellent food and surely tasteful discussions on the future of HPC.

December 2, 2015: Young Scientist Meeting

If you have registered for the dinner on Wednesday and you are a postdoc or student, your bus will leave at 6.55pm in front of the GSI main entrance. Please be on time, so that the others do not have to wait.

Together with other students and postdocs, you can enjoy a stimulating and, of course, highly productive evening at:



Restaurant Limao
Moltkestraße 64
D-53173 Bonn

At 10.00pm, the bus will bring you back to GSI.

December 3, 2015: Social Event and Dinner

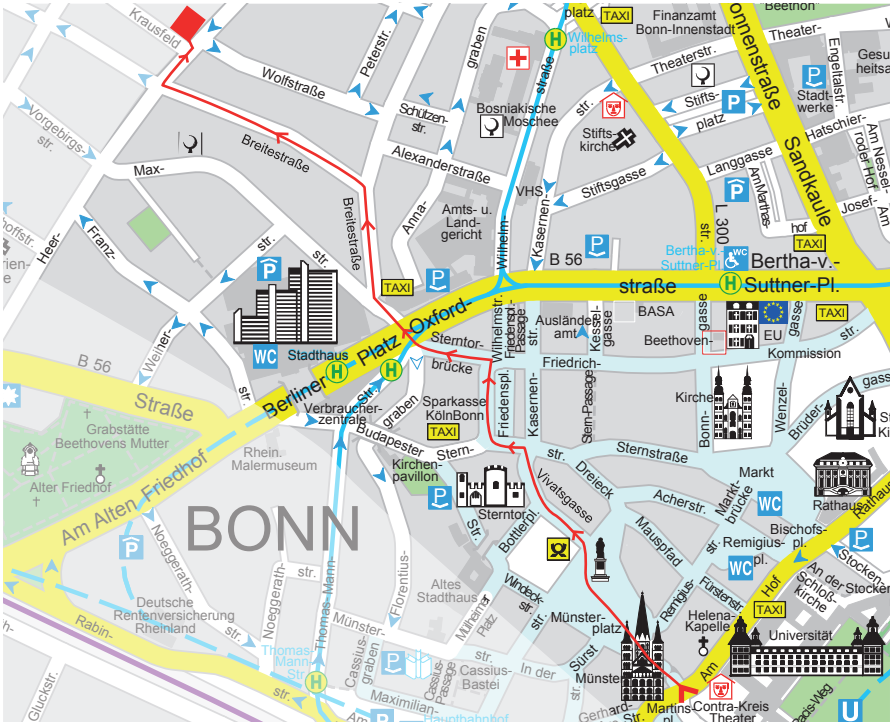
For those of you who have registered for the social event on Thursday, the bus will leave at 6.00pm in front of the GSI main entrance. Please be on time, so that the others do not have to wait. We will drive to the beautiful christmas market at the Münsterplatz in Bonn. There, you can enjoy regional specialities like “Glühwein” and buy first or final gifts. At 7.30pm, we will meet at

Bierhaus Machold
Heerstraße 52
D-53111 Bonn

for a classic conference dinner with local brewery specialities.

Details

A direct walk from Münsterplatz to the Bierhaus will take about 20 minutes, mostly across two Christmas markets. Follow the directions provided here or use the QR code above. Of course, you can arrive there earlier or later if you like. You can also meet us in front of the postal office, Münsterplatz, at 7.00pm for a joint walk to the Bierhaus. In any case, the dinner starts at 7.30pm.



December 4, 2015 and beyond: Dinners

If you have registered for a dinner on Friday, we will meet at 7.00pm at the lobby of the GSI. As for the lunches we will have dinner at the GSI canteen.

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If you have any questions or if you need anything, let us know!

Robert Speck

Julia Kämpfer

Look for an **orange dot** on our badges to find our staff members
Britta Hoßfeld, Myriam Czekala, Isabel Heisters, Andreas Müller, Julia Valder and My Linh Würzburger.

You can also write to

jlesc-workshop-2015@fz-juelich.de

to contact us. We will be happy to assist you.