Symposium on High Performance Computing (HPC)
on the occasion of the inauguration of Marvin

October 20
2023
1 pm - 5.30 pm

Free participation. Mandatory: Register here

Speaker

Estela Suarez (Computer Science department, University of Bonn & Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH)

Jürgen Dölz (Institute for Numerical Simulation, University of Bonn)

Thomas Luu (Institute for Advanced Simulation 4, Forschungszentrum Jülich GmbH & HISKP, University of Bonn)

Peter Krawitz (Institute for Genomic Statistics and Bioinformatics (IGSB), University Hospital Bonn)

Julian Klaus (Department of Geography, University of Bonn)

Petra Mutzel (Institute for Computer Science, University of Bonn)

Jan Steiner (HRZ HPC Team, University of Bonn)

Location

Research and Technology Center for Detector Physics; Presentationroom FTD

Contact

Daniel Minge (TRA Modelling Manager)
traleuni-bonn.de
# Symposium on High Performance Computing (HPC)

20.10.2023  
1.0 pm - 5.30 pm  
Research and Technology Center for Detector Physics  
Presentation room FTD

## Session I

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<td>“Modular Supercomputing: heterogeneous hardware for diverse applications”</td>
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<td>1.30 pm</td>
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<td>“HPC and Physics: Strange Bedfellows or the Perfect Couple?”</td>
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<td>Prof. Dr. Petra Mutzel</td>
<td>“Quantum Annealing versus Digital Computing” &amp; “News from the HPC/A-Lab”</td>
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<td>Jan Steiner</td>
<td>“What Everyone Should Know about Marvin”</td>
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<td>5.25 pm</td>
<td><strong>Conclusion</strong> and end of the event</td>
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Contact

Daniel Minge (TRA Modelling Manager)  
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Abstracts

Session I

1.05 pm  “Modular Supercomputing: heterogeneous hardware for diverse applications”

Prof. Dr. Estela Suarez
Computer Science department, University of Bonn, and Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH

The Modular Supercomputing Architecture combines various hardware components like CPUs, GPUs, accelerators, and emerging technologies into specialized compute modules. These modules are linked through a fast network and share a common software stack, creating a versatile system where users can adjust hardware resources by selecting the appropriate nodes per module. This setup enables efficient execution of complex multi-physics and multi-scale simulations across modules and allows users to tailor their hardware resources by selecting the appropriate nodes per module. MSA optimizes system workload distribution by assigning tasks to the most suitable hardware, following each application part's inherent parallelism.

1.30 pm  “On Computational Uncertainty Quantification”

Prof. Dr. Jürgen Dölz
Institute for Numerical Simulation, University of Bonn

We discuss computational aspects in the uncertainty quantification of partial differential equations. The later is commonly referred to as studying how errors and uncertainties in the input data of partial differential equations affect the solution or, vice versa, how the behaviour of the input data can be statistically estimated from measurements. In this context, we discuss efficient computational methods and their implementation.

1.55 pm  “HPC and Physics: Strange Bedfellows or the Perfect Couple?”

Prof. Dr. Thomas Luu
Institute for Advanced Simulation 4, Forschungszentrum Jülich GmbH & HISKP, University of Bonn

I discuss the general role of HPC in physics, emphasizing how HPC has become an essential tool in performing non-perturbative, strongly-correlated physical systems. I highlight certain successful examples and discuss various physical problems that can (hopefully) be addressed with future HPC resources. Finally, I point out how physics in turn benefits HPC, thus providing a means for "closing the loop" and cementing the marriage of HPC and Physics.
The amount of genetic sequencing data in research and healthcare is growing faster than processing power and storage space. This means that intelligent algorithms for sequence assignment, assembly, and variant detection are crucial. Once these first steps of clinical bioinformatics are done, the data must also be interpreted in the context of the patient’s phenotype. Again, an increasing amount of medical images need to be analyzed. To solve these challenges, we need GPU clusters and experts who can handle them.

3.00 pm  “Why does Clinical Bioinformatics need Marvin?”

Prof. Dr. Peter Krawitz
Institute for Genomic Statistics and Bioinformatics (IGSB), University Hospital Bonn

Today we are experiencing a global water crisis with more than two billion people lacking access to safe drinking water. The observed non-stationarity of hydrological systems, together with increasing anthropogenic pressure on catchments, are challenging our current capabilities to understand changes in the global water cycle, impacting our capability to predict floods and droughts around the world, and eventually impacting adaption and resilience of society to global change. In this presentation, I will focus on computational approaches to understand and predict processes in the water cycle from small to large scales.

3.25 pm  “Predicting water cycle processes under global change”

Prof. Dr. Julian Klaus
Department of Geography, University of Bonn
Quantum annealing is getting increasing attention in combinatorial optimization. The quantum processing unit of the D-Wave 2000Q is constructed to approximately solve Ising models on so-called Chimera graphs. Ising models are equivalent to quadratic unconstrained binary optimization (QUBO) problems and to maximum cut problems on the associated graphs.

A conventional digital computer front end is used to transform a given combinatorial optimization problem to one or more instances of the Ising problem that are fed to the annealing hardware for approximate solutions. These solutions are finally transformed to a solution of the original problem. The transformation steps are problem dependent, and in general quite involved. As an example, we will point out the problems in solving combinatorial optimization problems such as the Traveling Salesman Problem by quantum annealers.

In the pursuit of a fair comparison, we neglect the digital front end phases and concentrate only on the solution of the Ising instances given to the annealing unit. It has been a matter of discussion in the literature how well the D-Wave hardware performs at its native task. In our experiments we examine how reliably the D-Wave computer can deliver true optimum solutions of the Ising problem. We also compare the annealer’s performance in terms of solution time and solution quality with the performance of a heuristic by Alex Selby designed for digital computers and present some surprising results. (This is joint work with Michael Jünger, Elisabeth Lobe, Gerhard Reinelt, Franz Rendl, Giovanni Rinaldi, and Tobias Stollenwerk).

At the end I will briefly present some news from our HPC/A-Lab.