1st PC² User Meeting

Prof. Dr. Christian Plessl

Director and chairman of the board
Paderborn Center for Parallel Computing

Paderborn University

10 December 2018
German HPC Center Landscape

- **Tier 0**
  - European network of high-performance computing centers (PRACE)
  - Access for users from Europe

- **Tier 1**
  - Federal HPC centers
  - Gauss Center for Supercomputing
  - Access for users from whole Germany

- **Tier 2**
  - State HPC centers
  - Gauss Alliance
  - Access for users from state (prioritized) and whole Germany
  - Co-financed by state and federal government

- **Tier 3**
  - Local computing centers
  - Financed by German Research Foundation
Paderborn Center for Parallel Computing (PC²)

- Central scientific institute of Paderborn University
  - rooted in theoretical computer science
  - founded in 1991, Leibniz award for B. Monien and F. Meyer auf der Heide
- Mission: Research institute and service provider
  - Development of methods for effectively using parallel computer systems
  - Operation of HPC systems for users of Northrhine-Westfalia and beyond
  - Support of users with consulting and services
- Study of innovative computing technologies
  - 1992: largest Transputer system in Europe with 1024 processors
  - 1999: first large HPC system with SCI network technology
  - 2003: one of the strongest playing Chess computers with FPGAs
  - 2004: HPC cluster with direct water cooling for CPUs
  - 2013: heterogeneous HPC cluster with GPUs and Xeon Phi
• PC² was always open for users from outside of Paderborn, e.g.:

• HPC System GCel (1992)
  – massive parallel computer system with 1024 processors
  – funded by NRW (¾) and ZiAM GmbH (¼)
  – parallel computing for industrial users (Europort initiative)

• HPC System OCuLUS (2013)
  – funded by 'major research instrumentation' program of Germany Research Foundation (DFG) proposal by Paderborn University with involvements of Universities of Bielefeld, Hamm-Lippstadt, OWL and University of Applied Sciences Bielefeld
  – established a cooperation between universities on the HPC infrastructure level
HPC is of central importance for Paderborn University but infrastructure does not account for future requirements:
- missing capacity and flexibility for power supply and cooling
- improving energy efficiency of cooling systems not possible or cost efficient
- lack of office space, computer lab space, seminar rooms for expected growth for PC², user support, and research collaborations

Strategic decision of Paderborn University with support of state of NRW:
- Proposal for establishing PC² as state-level Tier-2 HPC center (research infrastructure program of Council for Science and Humanities)
- Increase of HPC capacities and construction of new HPC-optimized compute center
- Provisioning of additional personnel

Start of Noctua Project in 2016

Athene Noctua
Lat. ‘Little Owl’
Research Infrastructure Proposal Noctua

• Proposal of University and NRW in Research Infrastructure Program (Forschungsbau) by Council for Science and Humanities (Wissenschaftsrat)
  – 10 M€ HPC systems
  – 15.4 M€ new computing center building

• Successfully evaluated in 2017, first 'Forschungsbau' of Paderborn University

• Implementation from 2018–2022
Noctua HPC Cluster (Phase 1)

- Cray CS 500 cluster system
- 256 CPU nodes
  - 2 Xeon Skylake Gold 6148, 40 cores, 2.4GHz
  - 192 GiB RAM / node
  - 540 TFLOPs LINPACK
- 16 FPGA nodes
  - 2 x Intel Stratix 10 GX2800 FPGAs (Bittware 520N)
  - additional network between FPGAs
  - at time of installation largest and most modern academic FPGA installation in HPC system
- 100 Gbps Intel Omni-Path network
- 700 TB Lustre ClusterStor L300N storage system
- Inauguration 9/2018
New HPC Computing Center

• Goals: Excellence in energy efficiency and flexibility
  – Energy efficient cooling of computers using free cooling (no chillers)
  – Modular concept for concurrent operation of several generations of HPC systems

• Key figures (preliminary)
  – White space for servers: 300m²
  – Additional technical areas: 1100m²
  – Operation of HPC systems with up to 1.1 MW electrical power (options for future upgrades)
  – Offices for 25 employees
  – Seminar rooms for user training
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<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>13:30</td>
<td>Welcome address</td>
<td>Prof. Dr. Christian Plessl, Director and head of the PC² management board, Paderborn University</td>
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<tr>
<td>13:40</td>
<td>Technical Overview of the Noctua HPC System</td>
<td>Dr. Jens Simon, Manager PC² Operations, Paderborn University</td>
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<td>14:00</td>
<td>How HPC helps exploring electromagnetic near fields</td>
<td>Prof. Dr. Jens Förstner, Paderborn University</td>
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<td>14:30</td>
<td>Poster Session – Discussions Among Participants</td>
<td>All participants</td>
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<td>15:30</td>
<td>How to Apply for Computing Time on PC² HPC Systems</td>
<td>Prof. Dr. Thomas D. Kühne, Head of the PC² Computing Time Committee, Paderborn University</td>
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<td>15:45</td>
<td>Atomistic Molecular Simulations for Engineering Applications</td>
<td>Prof. Dr. Jadran Vrabec, TU Berlin</td>
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<td>16:15</td>
<td>Prebiotic Chemistry in the &quot;Virtual Lab&quot;</td>
<td>Prof. Dr. Dominik Marx, Ruhr-Universität Bochum</td>
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<td>17:00</td>
<td>End of the event</td>
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Agenda