The Hessian competence center for high performance computing (www.hpc-hessen.de)

Christian Bischof
Spokesperson of the Directorate of HPC-Hessen

University Computing Center (HRZ)
Institute for Scientific Computing
Technische Universität Darmstadt
Rationale for a HPC Competence Center

Software is essential

• for competitiveness in science
• for efficient use of computing resources, i.e.
  • The code performs well (% of peak performance)
  • The code is energy-efficient (e.g. Impact of compilers on energy efficiency of HPCG benchmark, A. Jäger et al.)

“In the context of engineering sciences, many TOP500 systems achieve only a fraction of their peak computation capability.”
Harlacher et.al. DOI 10.1007/978-3-642-23869-7 22
Hessian competence center for high performance computing (HKHLR):

- A distributed competence center with staff at each site, but a common place to turn to.
- Educational offers to teach competences needed for HPC
- Advice on efficient use of our systems and efficient programming
- Outreach activities
Funding

• HKHLR has been funded by the Hessen State Ministry for Higher Education, Research, and the Arts.
  • Review by German Science Foundation (DFG) in June 2013
  • First round funding 7/13-3/16
  • Second review by DFG in July 2015
  • Second round funding 7/16-12/20, ~ 600 T€/yr.
  • Evaluation scheduled for end of 2018.
  • Universities committed to 25% and 50% co-funding in 2019 and 2020.

• 7 FTE scientific staff (2 each in DA/F, 1 each in GI/MR/KS), and 1 FTE for managing directorate.
# Tickets and Introduction Sessions

<table>
<thead>
<tr>
<th>Standorte</th>
<th># Tickets</th>
<th>Summe 2014</th>
<th>Summe 2015</th>
<th>Summe 2016</th>
<th>Summe 2017</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Clustereinführung</td>
<td># Teilnehmer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HKHLR-insgesamt</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1129</td>
<td>1293</td>
<td>1015</td>
<td>677</td>
</tr>
<tr>
<td></td>
<td></td>
<td>35</td>
<td>148</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TU Darmstadt</td>
<td># Tickets</td>
<td>472</td>
<td>500</td>
<td>328</td>
<td>188</td>
</tr>
<tr>
<td></td>
<td>Clustereinführung</td>
<td># Teilnehmer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td>25</td>
<td>69</td>
<td>53</td>
</tr>
<tr>
<td>GU Frankfurt</td>
<td># Tickets</td>
<td>487</td>
<td>488</td>
<td>422</td>
<td>291</td>
</tr>
<tr>
<td></td>
<td>Clustereinführung</td>
<td># Teilnehmer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td>-</td>
<td>68</td>
<td>44</td>
</tr>
<tr>
<td>JLU Gießen</td>
<td># Tickets</td>
<td>50</td>
<td>73</td>
<td>16</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>Clustereinführung</td>
<td># Teilnehmer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td>-</td>
<td>11</td>
<td>-</td>
</tr>
<tr>
<td>Uni Kassel</td>
<td></td>
<td>o.A.</td>
<td>81</td>
<td>9</td>
<td>15</td>
</tr>
<tr>
<td>Uni Marburg</td>
<td># Tickets</td>
<td>120</td>
<td>126</td>
<td>92</td>
<td>65</td>
</tr>
<tr>
<td></td>
<td>Clustereinführung</td>
<td># Teilnehmer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-</td>
<td>10</td>
<td>8</td>
<td>10</td>
</tr>
</tbody>
</table>
Engagement with users

• Lessons learned: Introduction sessions *before* users engage with the machine avoid a lot of tickets!

• So we try to engage with users early on: Each month intro sessions in DA and F, on demand at other sites.

• Earn the users’ trust by providing a reliable place to turn to.
Empowering the HPC Users: The High-Performance Computing in Hesse (HiPerCH) Workshop Series

• For the users, it is very convenient if HKHLR staff writes their scripts, parallelizes and optimizes their code.
• This approach does not scale, there is not enough staff.
• This approach does not have a lasting impact, the changes by HKHLR staff are much less likely to be reflected in the main development branch of the codes.
• HiPerCH provides training on:
  • Linux and software development tools
  • Vectorization, CUDA, OpenCL, OpenMP, MPI
  • Debugging and profiling tools (Funding for Totalview)
HiPerCH 7

Previous event
This introductory course is especially recommended for new LOEWE-CSC and FUCHS cluster users.

Agenda

Monday - Wednesday, March 13-15
8:30 - 18:00

Module 1:
Parallelization with MPI and OpenMP
DR. R. RAUSCHENBECHER (HiPER) and STAFF

The focus of this three-day workshop is on the programming models MPI and OpenMP. Hands-on sessions (in C and Fortran) will allow users to immediately test and understand the basic constructs of the Message Passing Interface (MPI) and the shared memory directives of OpenMP. Content: Level 70% for beginners, 30% advanced.

- Hardware architectures and parallel programming models
- Parallel programming with Message Passing Interface (MPI-2) and OpenMP
- Tools for performance optimization and parallel debugging
- Short introduction to Portable, Extensible Toolkit for Scientific Computation (PETSc)

Prerequisites: Unix / C or Fortran

ATTENDANCE FEE: 50,00 €
INCL. EVENING EVENT (MONDAY)

Evening event
Monday, March 13
18:30

Guided tour

Monday, March 13
20:00

Dinner

Thursday, March 16
9:00 - 15:00

Module 2:
Introduction to the TotalView Debugger
HiPER STAFF

This course consists of lectures supplemented with practical exercises.

Prerequisites: For the tutorials all participants are kindly asked to use their own laptop (Eduroam WLAN access is available).

All modules can be booked separately.

December 06, 2016
HiPerCH 8

**Agenda**

**Tuesday, September 26**
- 09:00 - 18:00

**Module 1:**
- **Linux - Basic use and useful tools**
  - STAFF: JOHANNES GUTENBERG UNIVERSITY MAINZ
  - ATTENDANCE FEE: 15,00 €

**Wednesday, September 27**
- 09:00 - 18:00

**Module 2:**
- **Introduction to the TotalView Debugger**
  - STAFF: HIHLER STAFF
  - ATTENDANCE FEE: NO ATTENDANCE FEE

**Module 3:**
- **Python - Basics**
  - STAFF: HIHLER STAFF
  - ATTENDANCE FEE: 30,00 € INCL. EVENING EVENT (THURSDAY)

**Evening event**
- Thursday, September 28
- 19:30
- INCL. MODULE 3: DINNER

---

**HiPerCH 8**

**Building Hochschulezentrum**
- ROOM 06467 „Schulungsräume HRZ“
  - HANS-MEERWEIN-STRASSE, 35032 MARBURG

This course consists of lectures supplemented with practical exercises.

**Prerequisites:** For the tutorials all participants are kindly asked to use their own laptop (Eduroam WLAN access is available).

---

**HiPerCH 8**

**Building Hochschulezentrum**
- ROOM 06467 „Schulungsräume HRZ“
  - HANS-MEERWEIN-STRASSE, 35032 MARBURG

This course consists of lectures supplemented with practical exercises.

**Prerequisites:** For the tutorials all participants are kindly asked to use their own laptop (Eduroam WLAN access is available).

---

**HiPerCH 8**

**Building Hochschulezentrum**
- ROOM 06467 „Schulungsräume HRZ“
  - HANS-MEERWEIN-STRASSE, 35032 MARBURG

This course consists of lectures supplemented with practical exercises.

**Prerequisites:** For the tutorials all participants are kindly asked to use their own laptop (Eduroam WLAN access is available).

---

All modules can be booked separately.
### HiPerCH over the years

<table>
<thead>
<tr>
<th>HiPerCH</th>
<th>2, DA Sept 14</th>
<th>3, GI March 15</th>
<th>4, DA Sept 15</th>
<th>5, KA Feb 16</th>
<th>6, DA Sept 16</th>
<th>7, F March 17</th>
<th>8, MA Sept 17</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total</strong></td>
<td>49</td>
<td>25</td>
<td>49</td>
<td>36</td>
<td>56</td>
<td>61</td>
<td>38</td>
</tr>
<tr>
<td>HKHLR</td>
<td>6</td>
<td>4</td>
<td>9</td>
<td>5</td>
<td>9</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>TU Darmstadt</td>
<td>19</td>
<td>4</td>
<td>18</td>
<td>7</td>
<td>23</td>
<td>11</td>
<td>8</td>
</tr>
<tr>
<td>Goethe-Uni Frankfurt</td>
<td>7</td>
<td>3</td>
<td>7</td>
<td>7</td>
<td>7</td>
<td>31</td>
<td>3</td>
</tr>
<tr>
<td>JLU Gießen</td>
<td>3</td>
<td>7</td>
<td>4</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>6</td>
</tr>
<tr>
<td>Uni Kassel</td>
<td>2</td>
<td>1</td>
<td>14</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>Philipps Uni Marburg</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>4</td>
<td></td>
<td></td>
<td>8</td>
</tr>
<tr>
<td>FRA-UAS</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>JGU Mainz</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other extern</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Speakers and Aides</td>
<td>6</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>7</td>
<td>2</td>
<td>4</td>
</tr>
</tbody>
</table>
Yearly online survey (2016)

This is the third survey:

<table>
<thead>
<tr>
<th>Year</th>
<th>Participants</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014</td>
<td>210</td>
</tr>
<tr>
<td>2015</td>
<td>230</td>
</tr>
<tr>
<td>2016</td>
<td>240</td>
</tr>
</tbody>
</table>

Little change in topical emphasis over the years

Parallel performance of the used software:
- 64% is part of your research
- 19% is important for the success of your research
- 9% doesn't matter
- 5% is unknown to you
- 3% not answered
- 3% not answered
Online Survey 2016

Which topics for workshops are of interest to you?

- What is serial/parallel performance?
- How to measure code performance?
- MPI for beginners
- MPI advanced
- Debugger (TotalView)

Legend:
- high interest
- nice to have
- no interest
- not answered
Improving codes and scripts

- HKHLR staff provides tuning support for codes and scripts
  - To demonstrate the need and potential of performance tuning (earning trust)
  - To improve efficiency of use of our systems by focussing on the “power users” and their codes.

- Following “best-practices“ to maximize return on time investment. (e.g. Enhancing Brainware Productivity through a Performance Tuning Workflow, C. Iwainsky, R. Altenfeld, D. an Mey, C. Bischof, in Euro-Par 2011: Parallel Processing Workshops, M. Alexander et al., Eds, LNCS 7156, pp. 1987-207, Springer Verlag, 2012.)
Tuning Examples

• Physics code@Darmstadt: 8x speedup
  • Replace \texttt{pow(2,2)} by 4 and \texttt{pow(2,3)} by 8: 4x
  • Optimize \texttt{cpow(x,2)} by squaring: 2x

• Biophysics code@Frankfurt: 2x speedup
  • Educate user in proper SLURM usage

  SLURM script generator developed at Kassel

• Plasmapic code@Gießen: 2x speedup
  • Function inlining, memory layout changes and optimization of inner loops.

• OpenMP+MPI-parallelized code@Marburg: 2x speedup
  • Explicit setting of thread number
Lessons learned

- There are many ways how users’ codes cannot perform well.
- Users by and large are not performance-aware, and not familiar with HPC environments and tools.

HKHLR tries to provide structures to streamline support:
- Common knowledge base at all sites.
- Development of specialist knowledge.
- „Early intervention“ with our users.

On-site personnel presence is essential.
Monitoring Resource Usage

• **Goal:** To better understand what is going on the system, *to assist, not to complain.*

• Issues deducible from scheduler protocols include, e.g.:
  - Resources used vs. required (CPU, RAM)
  - Code crashes

• But measuring may significantly perturb the application

• „This looks strange“ ≠ „something is wrong“

• Related Projects funded by German Science Foundation:

  - ProPE
  - Profit-HPC
  - PeCoH
Outreach

• HPC is a growing field, with growing demands.

• But why is HPC important for science and industry?
• And why does one need a competence center focusing on software?

To answer these questions:
• Short video clips with researchers highlighting the importance of HPC for their work.
• HPC-Hessen at ISC
Research Portraits

- **Combustion**
  - Dr.-Ing. Florian Kummer
  - IFS Center, Fluid Dynamics

- **Fluid Dynamics**
  - Dipl.-Ing. Daniel Deising
  - Mathematical Modeling and Analysis

- **Fluid Interfaces**
  - Sandy Bruszas
  - Labradir, University of Jena, Fakultät für Maschinenbau

- **Insurance**
  - Hessisches Kompetenzzentrum für Hochleistungsrechnen

- **Investment**
  - Peter Schober
  - University of Jena, Fakultät für Wirtschaftswissenschaften

- **Black Holes**
  - Prof. Luciano Rezzolla
  - Chair of Theoretical Astrophysics, Institute for Theoretical Physics
ISC High Performance, 19.-21. Juni 2017
Messe Frankfurt

Competence Center for High Performance Computing in Hessen
HPC Hessen (www.hpc-hessen.de)
Reaching out beyond Hesse: Enabling Performance Engineering in Hesse and Rhineland-Palatine

- Expand and deepen HPC support in areas where existing scientific expertise coincides with critical user needs.
- Bundle the distributed expertise for HPC support in Hesse and Rhineland-Palatine
- Funded by German Science Foundation

- Darmstadt: Bischof, Sternel, Wolf
- Frankfurt: Lindenstruth
- Kaiserslautern: Gauger
- Mainz: Brinkmann
www.hpc-hessen.de

apply

educate

investigate

support

brainware for science