Performance engineering in the PeCoH project

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Overview

1. Introduction
2. Performance engineering
3. Performance awareness
4. Certification
5. Tuning of packaged software
6. PeCoH web pages
7. Conclusion
Partners

- computer science at Universität Hamburg
  - Scientific Computing
  - Scientific Visualization and Parallel Processing
  - Software Engineering

- supporting HPC centres
  - DKRZ – Deutsches Klimarechenzentrum
  - RRZ – Regionales Rechenzentrum der Universität Hamburg
  - TUHH RZ – Rechenzentrum der TU Hamburg
Work packages and topics

- WP1 Management
- WP2 Performance Engineering
- WP3 Performance awareness
- WP4 HPC Certification Program
- WP5 Tuning sw configurations
- WP6 Dissemination
Performance engineering

Goals

■ improve productivity
■ bring software engineering closer to HPC

Topics

■ determination of concepts
■ benefit of data analytics
■ benefit of in-situ visualization
■ compiler-assisted development
■ code co-development
Software engineering techniques in HPC

Goal: motivate HPC users to

- use an integrated development environment (IDE) *(eclipse)*
- use the IDE for debugging
- employ automated testing (unit testing)

Interesting tool found

- *Visual Studio Code* (open source)
  - plugins for: bash, Fortran, . . .
  - full screen debugging based on *gdb*
Motivation

- HPC hardware and its operation are costly
- resources are requested in abstract terms
  - compute time, storage/archive capacity
- limited feedback on resource utilization
  → users and even experts are often not aware of cost

Goals

- Raise performance awareness by providing cost feedback
  → reduce overall cost and increase scientific output
  → help to make decisions on optimization effort
Approach and tasks

- model cost of resources (storage, compute, …)
- integrate cost models into workload manager
- deploy feedback tools on production systems
Cost models

Simple model
- divide total machine cost by node hours

Refined model
- procurement costs: compute, storage, infrastructure
- operational costs: energy, service, staff

Example data
- compute: 0.33 € to 0.47 € (per node hour)
- disk: 12.80 € (per month and TB)

Write-up
https://wr.informatik.uni-hamburg.de/_media/research/projects/pecoh/d3_1-and-d3_3-modelling-hpc-usage-costs.pdf
Cost modelling: a simple example

Question: What is the value of optimization?

Assumptions

- unoptimized run needs 10,000 node hours
- the optimizing scientist costs 60 k€ per year

Example alternatives

1. run code as is
2. spend an hour to make code run 2% faster
3. spend a day to make code run 5% faster
Cost modelling: a simple example

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1. run code as is
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Answer: alternative 2 leads to lowest cost

- saving: 200 node hours ≈ 66€
- investment: one working hour ≈ 36€
- total cost: 1. ≈ 3300€, 2. ≈ 3270€, 3. ≈ 3423€
Feedback on costs of HPC usage

We studied practical options to give feedback

- compute Time → SLURM epilogue
- online storage → daily/monthly reporting
- archive space → instrumentation of archiving commands

Scripts that use cost models were implemented

- script 1: job cost estimation
  - read a cost model configuration
  - analyse SLURM jobs accordingly
- script 2: statistical analysis of finished jobs
  - computes averages, std-deviations and quantiles
Feedback from DKRZ user group meetings

- most user representatives don’t find it necessary to provide cost information for every batch job
- some users would like to be able to convert between compute and storage resources according to their cost
HPC Certification / “HPC-Führerschein”

Motivation

- **HPC-Führerschein**
  (corresponds to a *Golf Proficiency Certificate* in Singapore)
  - provide HPC beginners with basic skills required for using HPC clusters
  - check success by self testing

- **HPC certification program**
  - provide HPC teaching material at all levels
  - establish HPC certificates (like other IT certificates)
  - *HPC-Certification Forum* started
    → [http://hpc-certification.org](http://hpc-certification.org)
Approach and tasks

- listing and classification of competences
- development of a certification program
- creation of workshop material
- provision of an online tutorial
- enabling an online examination
Listing and classification of HPC competences

Main topics

- general HPC knowledge
- performance engineering
- software engineering
- use of the HPC environment

Roles

- tester (running programs)
- builder (compiling programs)
- developer (writing programs)

Levels

- basic, intermediate, expert

Result

https://www.hhcc.uni-hamburg.de/files/hpccp-concept-paper-180601.pdf
The main topics are subdivided into a *skill tree*:

[HPC Skill Tree Diagram]

https://www.hhcc.uni-hamburg.de/en/hpc-certification-program/hpc-skill-tree.html
Our framework allows creation and selection of *views* on the skill tree, e.g.

- basic tester
- (intermediate) developer
- groups of users (chemists, climate researches, ...)
- analogy: targets and dependences in *Makefiles*
Content production workflow

Markdown

- easy to use lightweight markup language, widely used for documentation purposes (e.g. on GitHub)
- plain text editor is sufficient
- supports formulae, syntax-highlighting, tables, hyperlinks, inclusion of images
- content of a single skill is based on a list of Markdown files

Extensible Stylesheet Language Transformations (XSLT)

- XSLT-programs generate Makefiles for Pandoc from skill tree (XML) and contents (Markdown)

Pandoc

- conversions between many markup formats
- used to convert .md-skill content files to .html, .pdf, .tex
Tuning of packaged software

Goals

- provide settings for tuning parameters
  - runtime settings
    - e.g. $TMPDIR, process placement, thread number
  - compile time settings
    - e.g. compiler flags, libraries

Approach and tasks

- determination of tuning possibility (from manuals)
- setup of realistic use cases (cooperation with users)
- benchmarking (with use cases)
- documentation (success stories)
Tuning statistical computations with R

Compile time settings

- use OpenBLAS or MKL (slightly better than OpenBLAS)
- -O3 delivered best performance
- no benefit from *profile guided optimization*
- use at least simple parallelization via `foreach()`
Tuning results for R

Use case A: “R Benchmark 2.5” [Simon Urbanek]
- mix of matrix operations (cross product, eigenvalues) and other parts (recursions, loops)
- single process speedup: $\approx 4$ using MKL
- parallel speedup with OpenMP: $\approx 15\%$

Use case B: parallelization of regression analysis
- speedup $\approx 30$ on 4 nodes $\times$ 16 cores (64 cores)

Use case C: analysis of satellite night images
- parallelization with foreach()
- speedup: 126 on 32 nodes $\times$ 4 cores (128 cores)
  - no domain decomposition $\rightarrow$ every process has all data
Climate Data Interface (CDI) optimization

Problem: reading of compressed files with CDI is slow
Analysis: slowdown due to libaec and GribAPI
  ■ GribAPI is hard to change

Solution: parallelization of decoding
Result:
  ■ significant speedup on compressed data
  ■ slight slowdown on uncompressed data
    ■ caches become less effective, overheads are significant
  ■ decoding is concurrent to further processing steps
Measurements

Test case: copy data from one file to another
Memory size: 113GB (double), file size: 28GB (short), compressed: 13GB

<table>
<thead>
<tr>
<th></th>
<th>compressed time</th>
<th>compressed throughput</th>
<th>uncompressed time</th>
<th>uncompressed throughput</th>
</tr>
</thead>
<tbody>
<tr>
<td>sequential input</td>
<td>334s</td>
<td>340 MB/s</td>
<td>66s</td>
<td>1710 MB/s</td>
</tr>
<tr>
<td>→ disk access</td>
<td>5s</td>
<td>2600 MB/s</td>
<td>25s</td>
<td>1120 MB/s</td>
</tr>
<tr>
<td>→ decoding</td>
<td>329s</td>
<td>343 MB/s</td>
<td>41s</td>
<td>2756 MB/s</td>
</tr>
<tr>
<td>parallel input</td>
<td>66s</td>
<td>1710 MB/s</td>
<td>89s</td>
<td>1269 MB/s</td>
</tr>
<tr>
<td>→ disk access</td>
<td>27s</td>
<td>481 MB/s</td>
<td>57s</td>
<td>491 MB/s</td>
</tr>
<tr>
<td>→ overheads</td>
<td>41s</td>
<td>2756 MB/s</td>
<td>33s</td>
<td>3424 MB/s</td>
</tr>
<tr>
<td>parallel decoding</td>
<td>462s</td>
<td>244 MB/s</td>
<td>141s</td>
<td>801 MB/s</td>
</tr>
</tbody>
</table>

Cache effects heavily influence many values
Overheads are mostly extra memcpy() calls
PeCoH web pages

HHCC – Hamburg HPC Competence Center

- [https://www.hhcc.uni-hamburg.de](https://www.hhcc.uni-hamburg.de)

Scientific computing group

- [https://wr.informatik.uni-hamburg.de/research/projects/pecoh/start](https://wr.informatik.uni-hamburg.de/research/projects/pecoh/start)
Conclusion

- PeCoH brings Hamburg HPC centers closer together
- broad range of topics
- most results are in certification and training
  - topics were structured
  - framework for producing training material was developed
  - writing material is in progress