Performance engineering in the PeCoH project

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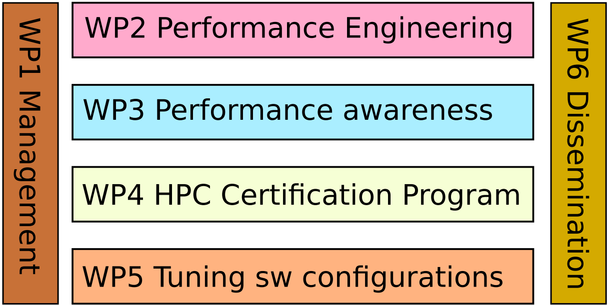
Overview

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



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*

Performance awareness

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

- devide 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

Question: What is the value of optimization?

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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

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 $\rightarrow$ SLURM epilogue
- online storage $\rightarrow$ daily/monthly reporting
- archive space $\rightarrow$ 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

$\rightarrow$ `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

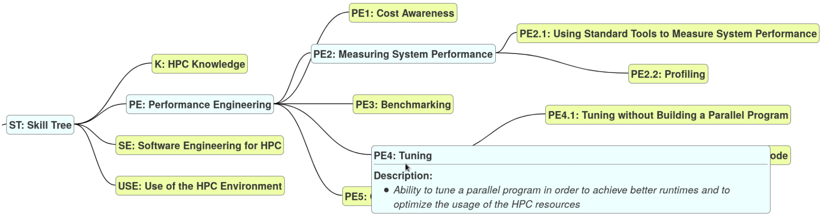
- basic, intermediate, expert

Result

- `https://www.hhcc.uni-hamburg.de/files/hpccp-concept-paper-180601.pdf`

Skill tree

The main topics are subdivided into a *skill tree:*



→ `https://www.hhcc.uni-hamburg.de/en/hpc-certification-program/hpc-skill-tree.html`

Views

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

- convertions 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: ≈ 4 using MKL
- parallel speedup with OpenMP: $\approx 15\,\%$

Use case B: parallelization of regression analysis

- speedup ≈ 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 Inferface (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

	compressed		uncompressed	
	time	throughput	time	throughput
sequential input	334s	340$^{MB}/_{s}$	66s	1710$^{MB}/_{s}$
→disk access	5s	2600$^{MB}/_{s}$	25s	1120$^{MB}/_{s}$
→decoding	329s	343$^{MB}/_{s}$	41s	2756$^{MB}/_{s}$
parallel input	66s	1710$^{MB}/_{s}$	89s	1269$^{MB}/_{s}$
→disk access	27s	481$^{MB}/_{s}$	57s	491$^{MB}/_{s}$
→overheads	41s	2756$^{MB}/_{s}$	33s	3424$^{MB}/_{s}$
parallel decoding	462s	244$^{MB}/_{s}$	141s	801$^{MB}/_{s}$

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`

Scientific computing group

- `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