Performance Conscious HPC (PeCoH) – 2019

Kai Himstedt¹, Nathanael Hübbe¹, Sandra Schröder¹, Hendryk Bockelmann², Michael Kuhn¹, Julian Kunkel³, Thomas Ludwig^{1,2}, Stephan Olbrich¹, Matthias Riebisch¹, Markus Stammberger⁴, Hinnerk Stüben¹

Universität Hamburg ² *Deutsches Klimarechenzentrum (DKRZ)* ³ *University of Reading* ⁴ *Technische Universität Hamburg*

Contact: kai.himstedt@uni-hamburg.de

INTRODUCTION

This poster presents project outputs and ongoing activities. For the sake of completeness, it also gives a brief overview of the major project goals and partners involved in the project.

Data centers often face **similar challenges when supporting analysis and optimization** of relevant applications. From the user perspective, the **benefit of performance engineering is difficult to quantify** and so are the costs involved in this tuning/optimization.

The German state of Hamburg has **three data centers, each independently providing compute power and support** to their users. Two general purpose data centers are responsible for the needs of Universität Hamburg and Technische Universität Hamburg, respectively. The third data center is a Tier-2 center supporting climate research. Although near to each other, the collaboration of support staff between the data centers has been limited. As part of the project, this **collaboration will be strengthened**.

PERFORMANCE AWARENESS: PROVIDING COST FEEDBACK

10000

Percentile of jobs

Statistical analysis of costs per

job that were executing during

a single day on a supercompu-

ter, each line shows the result

of a different cost model

The usual approach to accounting on a scientific supercomputer is that the scientists apply for compute time with their projects, get their projects granted, and then use their compute time to reach their project goals. Grants usually include an amount of node hours and a quota for disk storage.

This approach has several problems, which essentially boil down to the fact that scientists only works against limits. The true costs associated with their actions are not visible to them. Our cost modelling efforts were aimed at providing more information about the true costs to HPC users, enabling them to make more informed decisions. On the other hand, our cost models can also be used to derive statistics of the use of an HPC system. The figure on the right shows the results of performing this analysis on a day's worth of jobs.

Most interestingly, the vast majority of jobs does not consume any significant amount of resources, the costs are driven by the few very large and long running jobs, which are usually prepared by much smaller jobs. As such, it seems very important to educate users to efficient HPC usage during the time span in which they are still running many small jobs, before they start their really big runs. This can have a positive effect on the scientists ability to make the best scientific use from an HPC system.



HPC Software Engineering

This activity broadens the use of software engineering techniques in the field of HPC in order to increase the performance of parallel programs.



Efficiently Create, Maintain and Reuse Code

Programming Concepts for HPC	Programming Best Practices for HPC	Software Configuration Management	Agile Software Development
Programming Languages	Integrated Development	Terminology (IEEE Standard)	Test-driven Development
languages typically used in HPC,	Environments	IEEE 729-1983, IEEE 828	and Agile testing
such as C, C++, FORTRAN, HPX	use development environments	Version Control	unit testing
Parallel Programming	like Eclipse	Git, SVN	challenges of testing scientific
Programming Shared Memory +	Debugging	Issue Tracking and Bug Tracking	applications
Message Passing Systems	common debugging concepts	apply issue tracking in order to	
Efficient Algorithms and Data	and workflows	manage tasks and bug reports	developing test strategies
Structures	GDB, DD1, IotalView	during development	Extreme Programming (XP)

GOALS

The objectives of PeCoH are to

- 1. raise awareness and knowledge for performance engineering and to
- 2. coordinate performance engineering within Hamburg's institutions.

To reach these goals, we have established the **Hamburg Regional HPC Competence Center** conduct various practical activities on established techniques but also explore some supportive and alternative approaches as research.

PARTNERS

German Climate Computing Center (DKRZ) DKRZ is a partner for Climate Research, providing tools and the associated services to investigate the processes in the climate system. The HLRE-3 supercomputer Mistral consists of more than 3,000 compute nodes, providing a peak compute performance of 3.6 PFLOPs. The system is backed by a 60 Petabyte Lustre file system. The used scripts and a docker image to test the SLURM extension are available online at https://github.com/pecoh/cost-modelling

DEVELOPMENT OF THE HPC CERTIFICATION PROGRAM

Users should have a set of validated skills before they start using an HPC system.

For the classification of HPC competences and the definition of certificates we implemented an HPC skill tree (based on XML).

Beside its name and description, a skill in the tree has additional attributes to describe e.g. its special significance to a scientific domain, in order to

- enable the creation of different views of the skill tree to consider the users' varied backgrounds
- give the user an overview of custom-tailored skills which he has to acquire to pass the exams

A certificate definition

- bundles an appropriate set of HPC skills
- is used to certify a users' HPC qualification by successfull exams

For the development of the certification program, we separated the certificate definition from the providing of content, similar to the concept of a high school graduation exam (Zentralabitur in German).

We helped to setup the HPC Certification Forum, an international board that will sustain this activity and curate the skills, certificate definitions, and exam questions.

The certification board has the role of a (virtual) central authority, which results in major advantages:

• Generally accepted certificates and corresponding exams can be established by the HPC Certifi-

assess the efficiency of algorithms and data structures oad Balancing domain decomposition strategies scheduling algorithms O Programming general concepts of HPC I/O systems	Programming Idioms idioms for a programming language, e.g. FORTRAN, Python, C, C++ Logging Log Levels (ERROR, WARN, INFO) Libraries for FORTRAN, C, C++ etc. Exception Handling exception handling concepts in FORTRAN, C, C++	Release Mana plan and mana software and t Deployment M build tools like continuous int and deployme	age releases of scientific to document the release Management te waf, make, or cmake tegration, delivery, ent		practices of XP: pair programming, continuous process, system metaphor, small releases etc. SCRUM concepts of SCRUM, e.g. Sprint, Backlog, Planning, Stand up meeting, project velocity etc.
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Software Quality Software Architecture		Documentation
Coding Standards	Requirements Elicitation	Requirements Documentation
common coding conventions to	and Analysis	IEEE standard for Software
	identify, specify and document	Requirements Specification
ensure portability and maintainability	functional and non-functional	Software Architecture
Code Quality	requirements of the software	Documentation
assess code quality using metrics,	Object-Oriented Design	document the different views of
e.g. lines of code, coupling,	understand and use concepts of	architecture using a framework, e.g.
code coverage	object-orientation	4+1 views or decision frameworks
Defectoring	write modular and reusable code by	Source Code Documentation
Keractoring	applying design principles, e.g.	document source code using
improve code quality using well	Separation of Concerns,	documentation generators like
established refactoring, e.g. move	Information Hiding, KISS etc.	doxygen or pydoc
or extract method, rename class	Software Architecture	Documentation for Reproducibility
Code Reviews	architecture design patterns for HPC	documenting the software stack,
knowing and applying the single steps of a code review define checklists for code reviews	component-based architecture	build instructions, input data, results
	importance and impact of software architecture during development and maintenance	using tools for literate programming like activepapers, knitr, or jupyter

Assess Practicability with Scientists

ACTIVITIES TO DATE

We particitpated for the presentation of the PeCoH project in the

• ISC 2017

June 18–22, 2017, Frankfurt, Germany

- PeCoH project poster
- Handout to the work in progress of our HPC Certification Program
- FEPA workshop July 20–21, 2017, Erlangen, Germany
- 7th Gauß Allianz HPC-Status-Conference December 4–5, 2017, Stuttgart, Germany

• ISC 2018

June 24–28, 2018, Frankfurt, Germany

PeCoH project poster



Regional Computing Center at Universität Hamburg (RRZ) RRZ provides many central IT services to Universität Hamburg. Amongst these, it operates an HPC cluster with 396 nodes and 400 Terabyte BeeGFS file system.

> Universität Hamburg DER FORSCHUNG | DER LEHRE | DER BILDUNG

Technische Universität Hamburg (TUHH-RZ) RZT provides central IT services to the Technische Universität Hamburg. It operates a 244 node cluster with a 250 Terabyte BeeGFS file system. cation Forum without the burden of being responsible for the learning material

• The learning material can be provided by different scientific institutions

The recently kick-started HPC Certification Forum (HPC-CF) welcomes international collaborators.

ONGOING ACTIVITIES

Tuning: We have successfully started our examination with performance improvements for examples using the language R, along with efficient libraries like OpenBLAS or MKL and parallelizing loops with the foreach() paradigm in OpenMP and MPI environments.

For collecting further success stories we will focus on the following tuning possibilities to transfer performance engineering know-how:

- Tuning without the need to (re-)build a parallel program, e.g. by tuning a parallel program from the outside via runtime options
- Tuning without modifying the source code, e.g. by using optimized libraries and setting appropriate compiler/linker options
- Tuning of individual software based on co-development with users

Workshop Material and Online Tutorial: In the PeCoH project we have a focus on the HPC Certification Program and the role as certification provider. As we have additionally the role as content provider for basic HPC skills in the project, we designed a workflow based on XSLT programs and the well-known Pandoc-Tool to convert the Markdown content files associated with each single skill to various target formats like HTML, PDF, and TeX.

- To efficiently equip new users with certified HPC skills, we will
 - finish the coordination with other stakeholders that may provide content
 - work on the completion of the complementary open source workshop material
 - develop a multiple choice questionnaire to validate the basic HPC skills

- 8th Gauß Allianz HPC-Status-Conference October 8–9, 2018, Erlangen, Germany
- SC 2018

November 11–16, 2018, Dallas, Texas

 Extended abstract titled "Towards a HPC Certification Program"

All contributions are available for download.¹

A concept paper for the HPC certification program is available for download.²

We are hosting a mailing list for the HPC certification program.³

In the sense of a spin-off of the PeCoH project we established the HPC Certification Forum.⁴

We submitted a BoF (Birds of a Feather) titled "HPC Certification Program" in the field of education and training for the ISC 2019 together with international partners.

REFERENCES

¹HHCC. *Hamburg HPC Competence Center – Downloads*. https://www.hhcc.unihamburg.de/en/support/downloads.html

²HHCC. *Hamburg HPC Competence Center – HPC Certification Program: Concept Paper - Draft Version 0.91 – June 1, 2018.* https://www.hhcc.uni-hamburg.de/en/files/hpccp-concept-paper-180601.pdf



SKILL TREE MODELING



XML Schema Definition for Showing the Essential Skill Tree Structure

HPC SKILL TREE

The developed HPC Skill Tree contains descriptions of the various skills that are relevant in the field of HPC (we are still in the process of refining it and open to suggestions). The skills will be linked to the relevant teaching material. Our current HPC Skill Tree is available online via our interactive skill tree viewer (https://www.hhcc.uni-hamburg.de/en/hpc-certification-program/ hpc-skill-tree.html). This viewer can easily be included into third party web-sites and can be configured to provide different views of the skill tree data.



Interactive HPC Skill Tree viewer with the description of the skill "PE4: Tuning"

³HHCC. *Hamburg HPC Competence Center – Mailing List of the HPC Certification Program*. certification.hhcc@lists.uni-hamburg.de

⁴HPCCF. *The HPC Certification Forum – Home Page*. https://www.hpc-certification.org

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Please visit also the HPC Certification Forum
https://hpc-certification.org.