HPC Research Group

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Our Group

Main topics:

- generic technologies in HPC
- scientific computing

Important synergy

- scientific programs use generic technologies
- generic technologies are inspired and tested on scientific software

Generic technologies

All about software adaptability

- software efficiency depends on HW and input
- autotuning CUDA/OpenCL kernels, by *Kernel Tuning Toolkit*
- autotuning FFT settings by *cuFFTAdvisor*
- autotuning graphic pipelines by *Umpalumpa*

Typical output

- computer science papers
- software

Recent work

Standardization

- how to test and compare autotuning searchers/frameworks (collaboration with NTNU, eScience Centre)?
- unified specification for tunable code (collaboration with multiple institutions)
- autotuning benchmark (collaboration with NTNU, eScience Centre)
- mainly Filip's work, now abandoned

Umpalumpa

- specification of pipeline (what to do with data) decoupled with details, such as distribution on heterogeneous node and autotuning
- data-centric architecture, describe physical and logical properties of data
- in principle allows autotuning on level of the pipeline
- David's PhD

Recent work

Tuning space analysis

- how to be sure we have defined a good tuning space?
- detect opportunity for adding faster configurations
- detect always-poor configurations
- collaboration with UAB

Tuning budget estimation

- autotuning optimizes the runtime... and requires runtime
- how to decide how much resources invest into autotuning?
- Jaro's PhD

Scientific computing

Holistic approach

- change mathematics/introduce approximative solution: *CaverDock*, *4D-GRAPHS*
- parallelize/optimize the code: *CaverDock*, *Xmipp*
- introduce GPU acceleration: *Xmipp*, some small projects

Typical output

- non-computer science papers (e.g., structural biology), some computer science papers
- software

Recent work

CaverDock 2.0

- utilizing RRT algorithm as an alternative for the original CD algorithm
- allowing the receptor to change conformance
- Petra's PhD

Xmipp

- GPU acceleration of continuous heterogeneity
- improving accelerated FlexAlign
- David's PhD, multiple bachelor's and master's thesis

Achieved Results

Journal papers

- O. Vávra et al. pyCaverDock: Python implementation of the popular tool for analysis of ligand transport with advanced caching and batch calculation support. *Bioinformatics.* (IF 6.9, Q1)
- D. Střelák et al. Umpalumpa: a framework for efficient execution of complex image processing workloads on heterogeneous nodes. *Computing.* (IF 3.2, Q2)
- F. Petrovič, J. Filipovič. Kernel Tuning Toolkit. *SoftwareX.* (IF 3.4, Q2)
- D. Herreros et al. ZART: A Novel Multiresolution Reconstruction Algorithm with Motion-blur Correction for Single Particle Analysis. *Journal of Molecular Biology.* (IF 5.6, Q1).
- D. Herreros et al. Estimating conformational landscapes from Cryo-EM particles by 3D Zernike polynomials. *Nature Communications.* (IF 16.6, D1)

Conferences/workshops

- J. O. Tørring et al. Towards a Benchmarking Suite for Kernel Tuners. *IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW).*

Publication performance

	Q1	Q2	Q3	confs/books	sum
2017	0	0	0	1	1
2018	0	0	0	1	1
2019	2	2	0	1	5
2020	2	0	2	0	4
2021	3	1	2	1	7
2022	0	1	0	2	3
2023	3	2	0	1	6

Tabulka: Papers of our group where Fila is an co-author.

Autotuning

Searching and analysis of tuning spaces

- analysis of performance counters allows to understand limitations of tuning space
- potential for visual tool ("tuning space profiler")
- further development of profile-based searcher

Dynamic autotuning

- new playground: spMV (CUSP)
- practical implementation of tuning budget planing

Scientific Computing

CaverDock

- we are finishing the version 2.0
- unclear what to do next

Xmipp

- we expect to continue

Other projects

- rather limited by our capacity

Bigger Picture

What goes well

- quite good publication record
- strenghten international collaboration

Challenges

- projects
- people