DEFAULT

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The software we rely on

- Version management via git
- Share scripts and configuration files across the team

- Batch scheduling system
- Optimized resource usage for multiple team members

- Automated installation across all nodes with Ansible
- Package management and OS configuration

- Software management via environment Modules
- Managing and organizing multiple versions of software

- CentOS as RedHat compatible operating system
- Industry standard

- Remote team coordination via Microsoft Teams
- File sharing and video conferences

The strategy we trust

Webinars

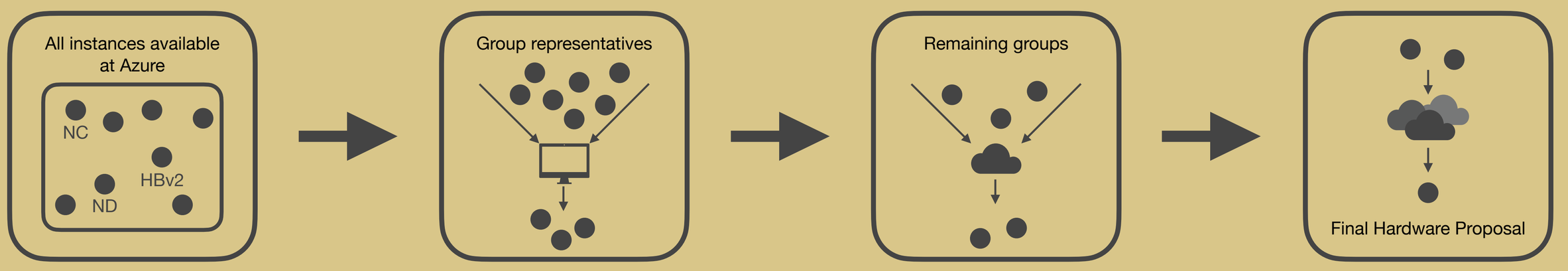
- Attended all SCC20 webinars + GROMACS-Talk by Alan Gray + MVAPICH User Group Meeting
- Short summary during weekly meeting
- Reproducing numbers, applying recommendations

Dedicated lecture by adviser

- Learning the basics of HPC systems to compare, describe and evaluate them
- Hands-on exercises with HPC resources of our university
- Setting up test cluster using VMs at FAU

Application Preparation

- Splitting team into subgroups of two
- Familiarizing themselves with one of the applications
- Preparing scripts and briefing the rest of the team during weekly meetings



- Identify & group similar hardware
- Select representative for each group

- Evaluate groups for every application and benchmark to identify suitable hardware

- Limited scalability runs to save budget
- Find hardware for which application scales

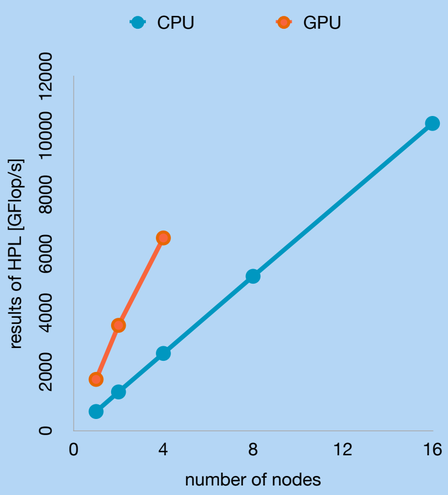
- Full scalability runs
- Select instance with best perf/$

Budget distribution

HPL & HPCG

We tried to find the optimal configuration by running HPL & HPCG with many different settings on the compute clusters of our university

- Parameter studies to optimize performance (NB, N, P, Q)
- Runs with multiple nodes exhibited good scaling
- Comparison of GPUs and CPUs: more than twice the CPUs are needed to achieve the same performance as GPUs
- Latest NVIDIA binaries for both benchmarks for GPU-focused optimization

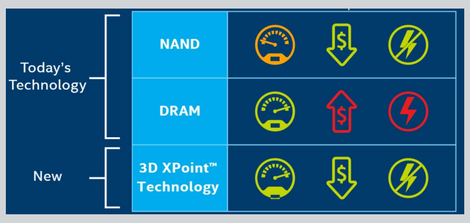


IO500

We are convinced that choosing a well performing composition of hardware and filesystem will have a more significant impact on the score than tuning the run parameters.

Our research made us settle on Intel Optane in combination with the DAOS file system

- Intel Optane provides fast and inexpensive non volatile memory
- Optane + DAOS occupy the first two places in the IO500 10 node challenge and first place in the IO500 list
- DAOS was developed specifically for Intel Optane: ideal interaction between hard- and software
- Overall better performance than other NAND storage units

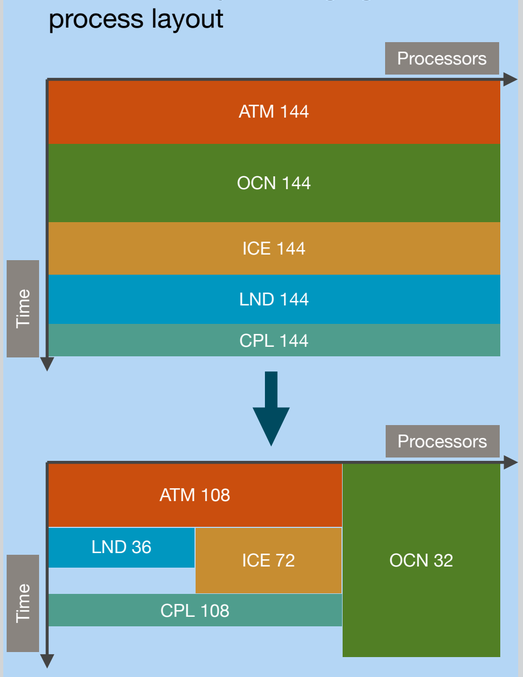


Comparison of speed, cost and volatility of different storage technologies

CESM

The performance of CESM lies in the complex computational characteristics

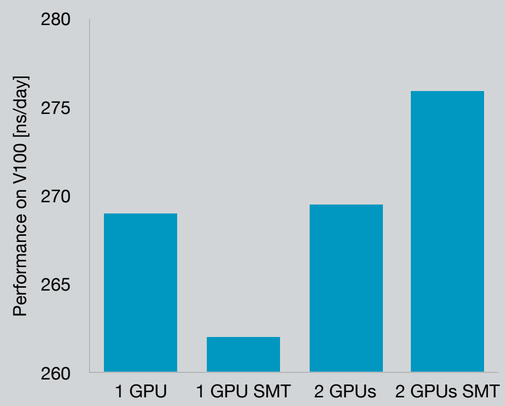
- Sequentially executing components with increasing process count does not equally result in better performance
- Adapt to hardware traits by utilizing tuning parameters such as NTHRD and NTASKS
- Major improvements can be achieved by rearranging process layout



GROMACS

Gromacs is a high performance molecular dynamics engine which utilizes CPUs and is supported by GPUs in many cases

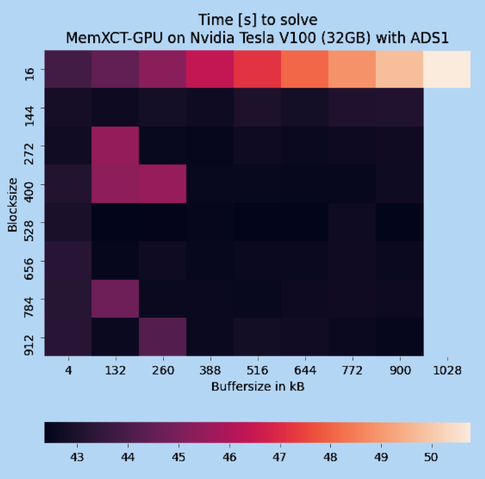
- Decent scaling only up to 4 GPUs
- Preparing for single-node 4 GPU runs as well as multi-node cpu runs, depending on the workload
- As the structure of the input may vary we write scripts for the system preparation wherever it is possible
- We try to tune the building and input parameter to reach better results with our sample data



MemXCT

MemXCT reconstructs computer tomography images using massive parallelization. We aim to reconstruct the results of the original paper and optimize performance

- Conduct parameter studies in order to find the ideal values for the tuning parameters
- Compile and run MemXCT with different MPI implementations (Intel MPI, OpenMPI, MVAPICH2) and compilers (Intel Parallelstudio, GNU)
- Perform test runs on V100 before gaining access to the Azure cloud



The awesome team

Diversity

- Ricardo and Marius are the first of their families to attend university, which is not typical in Germany
- Timur has a migration background
- Most of us are voluntary active which is not benefitted in Germany so it is unusual

Skillset

- Due to the structure of the CS mayor at our university we all have a strong fundamental base knowledge on parallel programming and distributed computing
- Topped by individual specialization where we can choose from a great variety reaching from operating systems, hardware oriented programming and computer graphics to deep learning
- As a result of our personal engagement in teaching, start-ups and voluntary work we gained a big spectrum of soft skills which are beneficial to work together as one team as they are complementary

University

- FAU reached the first place in Germany and second place amongst European universities in Reuters Top 100 The World's Most Innovative Universities 2019
- This ranking is based on patent filings and paper citations