

Albedo - The new HPC-System at AWI in 2022

Stephan Frickenhaus, Bernadette Fritzsch, Sebastian Hinck, Natalja Rakowsky, Malte Thoma

Computing Center, HPC & Data Processing and Storage & Server Alfred Wegener Institute for Polar and Marine Research, Bremerhaven

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HPC at AWI and beyond



HPC - High Performance Computing

- Tier-3 local resources at AWI: Ollie (2016-22), Albedo (2022-...) For code development, testing, and small projects.

 Click "HPC" in AWIID, approval by section head, and go!
- Tier-2 Network of 8 centres: National High Performance Computing (NHR) with specialised focus. DKRZ: Free within AWI share & application based HLRN: Small tests and projects are free, application for larger projects, support by BremHLR (Lars Nerger)
- Tier-0/1 Germany: Gauss Center for Supercomputing JSC Jülich, HLRS Stuttgart, LRZ Munich Europe: Partnership for Advanced Computing in Europe (PRACE)

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Albedo hardware - compute



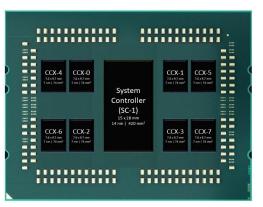
- vendor: NEC
- 240 compute nodes with
 - 2x AMD Rome Epyc 7702 2GHz (3.3GHz Boost), 64 Core, cTDP reduced from 200W to 165W
 - 256 GB RAM, 500GB SSD
- 4 "fat" nodes as above, 4TB RAM, 7.5TB SSD
- 1 GPU node with 1TB RAM, 4x NVIDIA A100/80
 More GPU nodes will follow later, after first experience
- 3 login nodes, one with GPUs 2x NVIDIA A40
- integrate test node with NEC SX-Aurora TSUBASA vector engine
- fast interconnect: HDR Infinband

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Albedo hardware - compute



AMD Epyc 7702 Multi-Chip Module: 8 Core-Dies and I/O Die



Each 8 Core Die is connected to 16GiB RAM ccNUMA - cache coherent Non Uniform Memory Access

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Albedo hardware - file systems

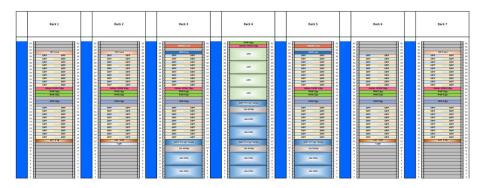


- 5 PB NEC GxFS (IBM Spectrum Scale)
 - /scratch, /home, /global
 - 220 TB as NVMe SSDs as fast cache and/or burst buffer
 - extension (capacity, bandwidth) possible
 - improved policy: small soft quota, large hard quota, grace period, project quotas e.g., for forcing data
- Dell EMC Isilon /isibhv connected to all nodes with 10GbE
 - main purpose: ease working with observation data
 - convenience: shared directories with other AWI servers
- local SSDs inside compute nodes
 - significant speed up of jobs that frequently read or write small amounts of data
 - reduce load on /scratch
 - as cache for GxFS?

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Albedo racklayout (offer)

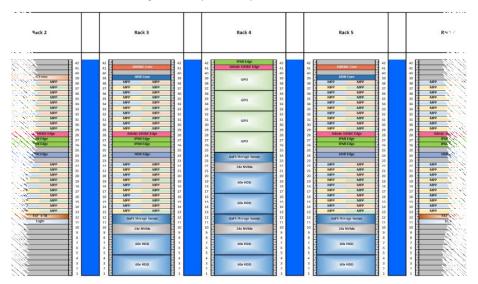




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Albedo racklayout (offer)





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Albedo racklayout: sidecooler





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Albedo racklayout: compute nodes





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Albedo racklayout: file system





Albedo Jan. 2022 10 / 15

Albedo software



- Alma Linux (Redhat clone; CentOS with rolling release no longer an option)
- Slurm batch system
- Programming Environment
 - Intel Compiler, MPI, MKL, Profiling: Intel oneAPI (now w/o license!)
 - Gnu Compiler Collection
 - AMD Optimizing C/C++ Compiler AOCC (includes Fortran)
 - Mellanox HPC-X MPI (OpenMPI)
 - NVIDIA compiler + MPI (GPUs)
 - NEC compiler + MPI (NEC SX-Aurora vector)
 - ARM DDT parallel debugger
- Application software → whatever you need!

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Albedo timeline



- 11/2021 procurement ended
- 12/2021 contract signed
- pprox 05/2022 start with a few compute nodes, Gigabit network (due to a severe delivery delay of Mellanox)
 - copy data from Ollie
 - install software, port applications
 - small projects
- \approx 07/2022 switch to fast Infiniband + most compute nodes
 - 30 days stability phase
 - production!
 - 2023 Evaluate, decide on extensions (GPUs, /scratch,...?)

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How to buy a supercomputer



- continuously:
 - inform and seek permissions from AWI boards and directorate
 - exchange with users, with other computer centers
 - get informations from vendors on new technologies (until procurement starts)
- write proposal to Helmholtz for a medium sized investment
- Prepare all documents (together with procurement)
 - call for competition
 - Leistungsverzeichnis with requirements, evaluation criteria
 - benchmarks (FESOM2, HPCC, IO500)
 - general paperwork . . .

How to buy a supercomputer



Call for Competition

Vendors apply with a concept for the installation of a supercomputer and the support. We evaluate the concepts and references. Three vendors will be admitted.

Negotiation Procedure

For Albedo: 40% price (investment + 7 years of support) 60% computing power

with fixed aspects like

- 170kW max. power consumption under "every day load"
- Fat and GPU nodes
- minimum size and speed of /scratch
- connection to /isibhy

Three rounds to fine tune the offers — award the contract

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Albedo Benchmark



FESOM2 fArc (640.000 2D nodes, 1800 steps) runtime of time stepping must be 3min or better, for example:

ollie.awi.de: 18 nodes (2x Intel Broadwell 18 core)

lise.hlrn.de: 7 nodes (2x Intel Cascade Lake 48 core)

albedo.awi.de: 6 nodes (2x AMD Rome 64 core)

Criterion

$$\Lambda = \frac{N}{n} \cdot \frac{3600s}{\tau} = \frac{240}{8} \cdot \frac{3600s}{135s} = 800$$

n number of nodes for benchmark (8 because of superlinear scaling) N number of compute nodes, τ benchmark runtime

Comparison: $\Lambda=1$ corresponds to 1 ollie node, thus $\Lambda_{\rm ollie}=316$