DISCOVERER

Explore, Endeavor, Elevate

What is DISCOVERER
Sofia Petascale Supercomputer

► **Discoverer** is a Petascale supercomputer can execute:
  - 4,6 PetaFlops   Rmax
  - 6,0 PetaFlops   Rpeak

    [1 PetaFlops= 10^{15} Flops = 10^6 Flops x 10^9 Flops]

166th
(91st)

► **In** in oct 2021 **Discoverer** was ranked at 91st place among the worlds top 500 supercomputers (in oct 2023 it is 166th)

► Discoverer's infrastructure is **co-funded by EuroHPC JU (35%) and by PetaSC** and the Bulgarian government (65%).

► **PetaSC Bulgaria** is a legal consortium combining the knowledge and 15 years of expertise of the National Center for Supercomputing Applications, the Strategic Center for Artificial Intelligence and **Sofia Tech Park** (where it is hosted)

► **Discoverer's mission & vision:**

  – **T**o foster better science for society

  – **T**o facilitate innovations by establishing deeper collaborations between academic institutions and the business

 – **T**o help training the next generation IT talent

System Architecture & Specs

- **12** Direct Liquid Cooling **BullSequana XH2000 Racks** with up to **32 blades per rack. i.e. Discoverer has 376 blades (12x32-8=376)**

- **376 blades** x **3 nodes/blade** = **1128 computing nodes**

  - **2** x AMD EPYC processors per node i.e. Discoverer has in total of **2256** AMD EPYC CPUs (2.6 GHz normal freq)

  - **256 GB shared memory per node with 18 fat nodes with 1024GB RAM** (3200MT/s DR)
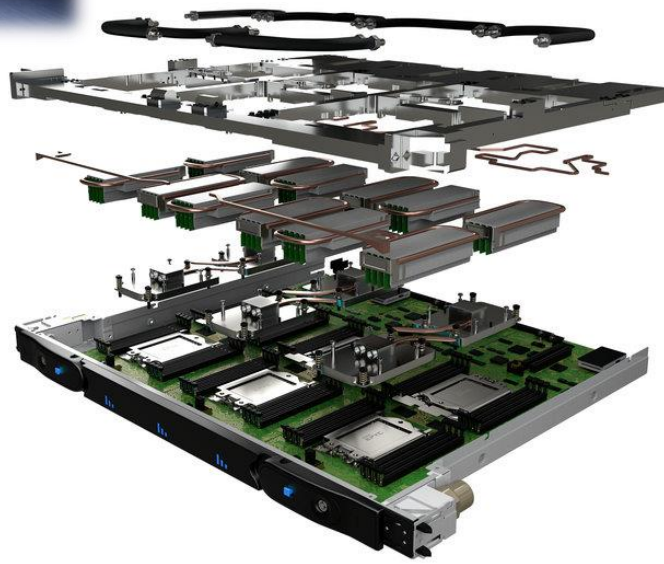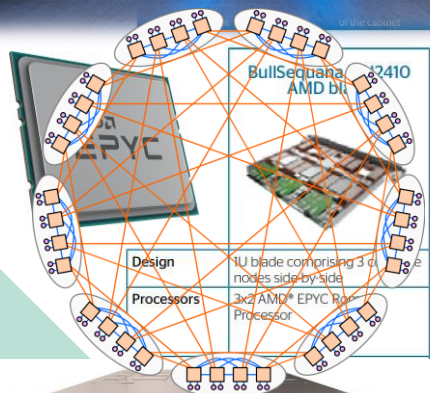
384 Nodes

300 TB (1128x256+18x(1024-256)=316

/w IO) with total capacity of **2 PB**

t, login and storage) infrastructure

Gbps HDR with DragonFly+ topology

inst a power failure using an an output of **1 MW.**

0 tons & total power consumption of ture).

BullSequana ...2410 AMD bl...

| Design | ...1U blade comprising 3 c... nodes side by side |
| Processors | 3x2 AMD® EPYC Ro... Processor |

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AtoS   AtoS

DDN

Software & Target Application Areas

Open-source Software (short list)
- Bioinformatics / Genomics (BLAST/RAY/EXCALATE/(HAD)DOCK/ROSETTA)
- Computational & Quantum Chemistry (CP2K/CPMD/Quantum Expresso/ GAMES)
- Molecular Dynamics & Mesoscale Modelling, Monte Carlo (GROMACS/NAMD/LAMMPS/DL POLY)
- Computational Fluid Dynamic / Finite Elements Methods (Open FOAM/Alya/SALOME)
- AI / Big Data Analytics (Tensor Flow/Python ML Libraries /NEURON)

Application Areas:
- *In-silico* Drug Discovery
- Structure-Property Predictions & Molecular Discovery
- Digital Product Formulation & Optimization
- Climate & Weather Forecasting / Environmental Modelling
- Simulated Environments in Automotive & Civil Engineering
- FinTech/MarkeTech & Big Data (DL/ML/AI)

Discoverer Access Policy

- **EuroHPC has 35% resource share from the Discover's resources, which will be allocated via regular calls for:**
  - <u>Regular HPC projects</u> (~80-90%) (for projects that require significant amount of HPC resources)
  - <u>HPC project benchmarking</u> (few %) (to determine project suitability & scalability, which is prerequisite to apply for a regular project)
  - <u>HPC Software Development & benchmarking</u> (few %)
  - <u>Fast Track applications</u> (~10%) (for example to get extra data quested during the peer-review process of previous project)
- EuroHPC calls will be organised via **PRACE** and are targeting pan-EU HPC projects including academic & industrial applications (with 80:20 split – see bellow)

- **PetaSC's resource share is 65% and it will be allocated using similar to EuroHPC access policy**
- PetaSC calls will be organised by PetaSC's Scientific & Applicant Board and the applications will be assessed by national & international scientific panel.

- For both EuroHPC (35%) and PetaSC (65%) share, there an additional **(min)80:(max)20** split between **free access** for purely scientific/non-profit and **paid access** for industrial/for-profit applications.
  - the distinction between free & paid access will be made on the base of results dissemination, where free access projects have obligation to openly share the all results from the project, while paid access calls can retain (part of) their results and use them for-profit /business proposes.
  - i.e. consortium from academic & industrial partners can qualify for free access to the Discoverer, provided they prepare suitable project proposal, apply for a call and get selected by the panel and after project end to openly share all the data and results from the project.