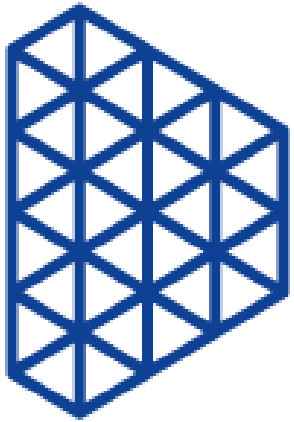
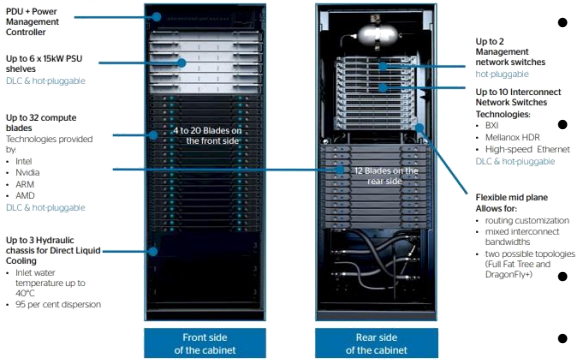


# DISCOVERER

## Sofia Petascale Supercomputer


- **Dicoverer** is a Petascale supercomputer
  - capable of executing:
    - > 4,4 Petaflops Rmax
    - > 6,0 ПетаFLOPS Rpeak
- Ranked at 91st place in the top 500 supercomputers.
- PetaSC Bulgaria is a legal consortium combining the knowledge and 15 years of expertise of Sofia Tech Park, National Center for Supercomputing Applications and the Strategic Center for Artificial Intelligence.
- Discover infrastructure is co-funded by EuroHPC JU (35%) and by PetaSC and the Bulgarian government (65%).
- The objective is to foster better science for society & business and economy and facilitate innovation, cross-boarder collaboration with top institutions and help training the next generation Bulgarian IT talent.

# Discoverer PetaSC System Architecture & Parameters




DISCOVERER
Sofia Petascale Supercomputer

| BullSequana X H2410 AMD blade |  |
|---|---|
| Design | 1U blade comprising 3 compute nodes side-by-side |
| Processors | 3x2 AMD® EPYC Rome® Processor |
| Architecture | 3x1 motherboard |
| Memory | 3x16 DDR4 memory slots (max 2048GB with 128 GB DIMMS) |
| I/O slots | InfiniBand HDR 1 port mezzanine board PCIe gen4 BXI 1 port mezzanine board |
| Storage | 3x1 optional NVMe M2 format |

- **12** Direct Liquid Cooling **BullSequana XH2000 Racks** with up to **32 blades per rack. Discoverer has 376 blades (12x32-8=376)**
- **376 blades** x **3 nodes/blade** = **1128 computing nodes**
  - **2** x **AMD EPYC processors per node** = **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)**
- **2256 CPUs** x **64 cores/CPU** = **144 384 Nodes**
- Total size of the RAM reaches over 300 TB (1128x256+18x(1024-256)=316 416GB)
- **Fast disk storage DDN (>20GBps r/w IO) with total capacity of 2 PB**
- 2 racks with auxiliary (management) infrastructure
- **Internode connection with IB 200Gbps HDR**
- The entire system is backed up against a power failure using an uninterruptible power supply with an output of 1 MW
- The whole system weight is over 30 tons & total power consumption of 1.3MW (incl supporting infrastructure)

# Software & Target Application Areas

**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 Relations / Molecular Discovery
- Digital Formulation & Optimization
- Climate & Whether Forecasting / Environmental Modelling
- Simulated Environments in Automotive & Civil Engineering
- FinTech/MarTech & Big Data (DL/ML/AI)