

JUPITER - THE ARRIVAL OF EXASCALE IN EUROPE

ETP4HPC Webinar

2024-06-14 I ANDREAS HERTEN, BENEDIKT VON ST. VIETH | JÜLICH SUPERCOMPUTING CENTRE













WHAT TO EXPECT FROM TODAYS WEBINAR

- Describe the whole JUPITER *journey*
 - Design decisions
 - Procuring JUPITER
 - Current Status, including JEDI
- Users!
 - During the procurement
 - Recent research on Grace-Hopper
 - Future plans with JUREAP







JÜLICH SUPERCOMPUTING CENTRE



Develop the supercomputing facility towards Exascale (2024)

Complement the Exascale by the **quantum computer** facility JUNIQ





Develop **federated data infrastructures** and advanced data science

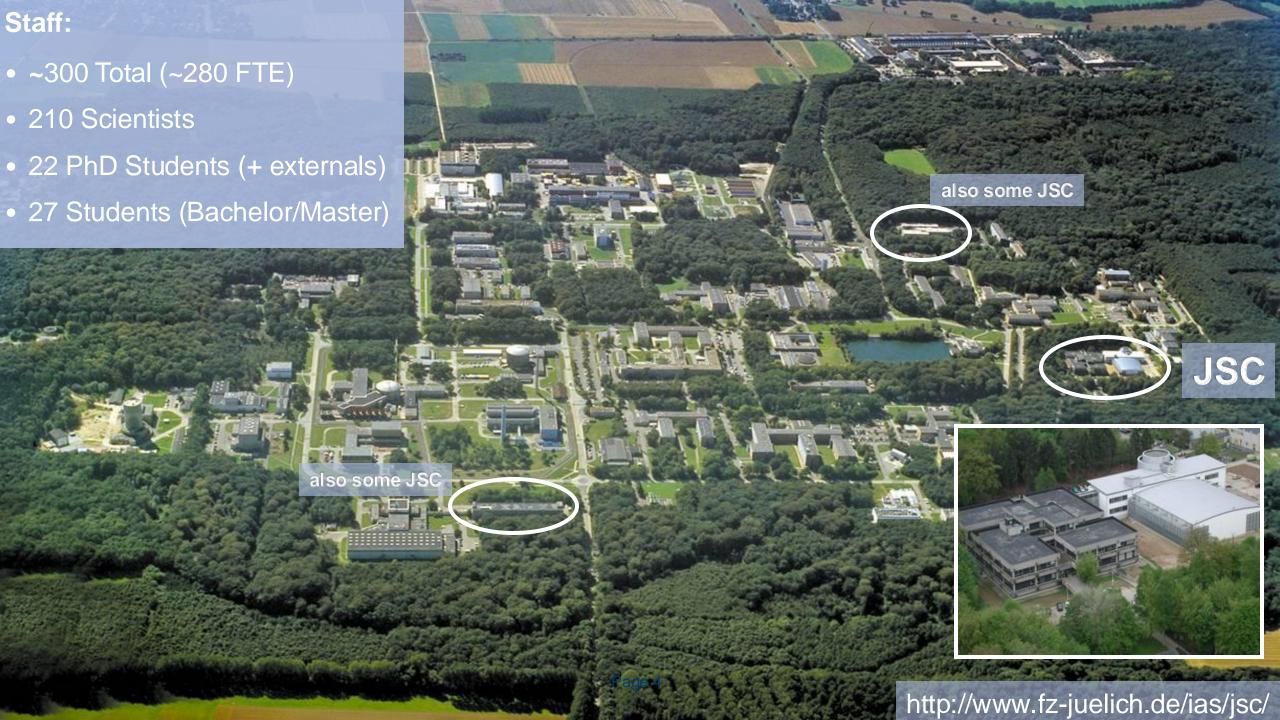
Provide most innovative support structures, tools, algorithms and methods





Educate a new generation of simulation and data science specialists





DESIGN DECISIONS

THE PATHFINDER Implementing the Modular Supercomputing Architecture 2× MSA pilots **MSA** EU PEX **Pre-Exascale** @Lux, @It KHPC @S EuroHPC Modular MELUIN 2023 Supercomputing **Architecture** (MSA) 2022 **Projects** FP7 - H2020 2021



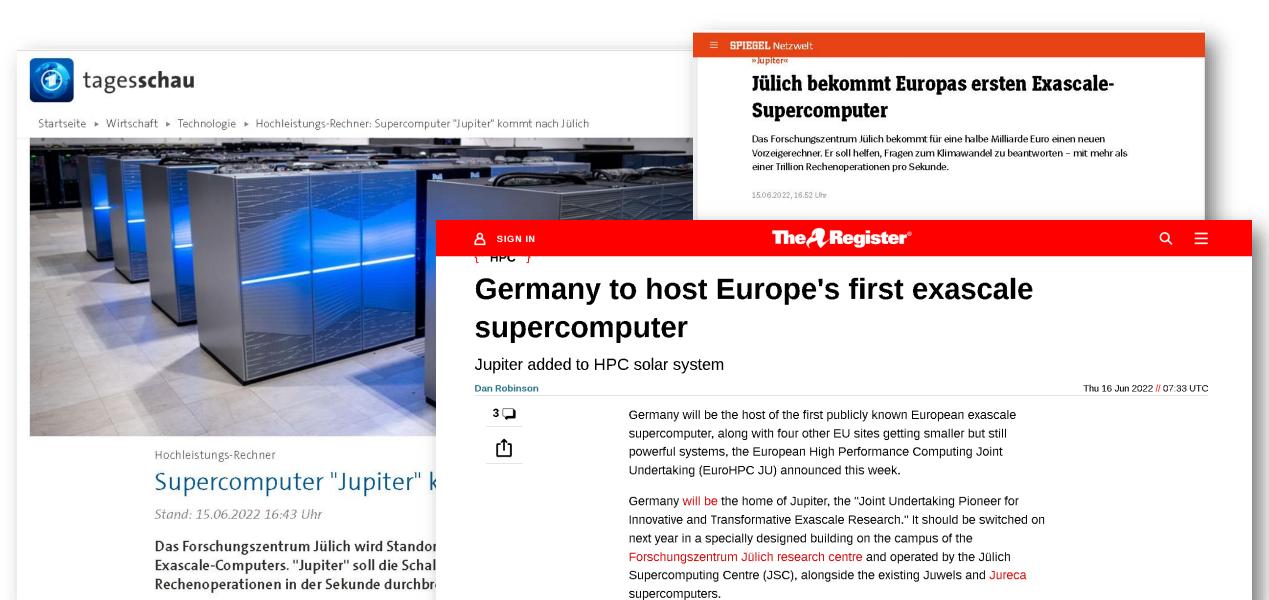
Projects





JUPITER - HOSTING ENTITY DECISION

15.06.2022



PREPARING FOR LAUNCH

- Mission planning
 - Preparing descriptions, conditions, requirements, evaluation
 - Regular meetings
 - Started already early in year
 - Location: Earth
- Target: JUPITER
 - Booster
 - Cluster
 - Storage
 - (Machine Hall)







READY FOR TAKE OFF

Competitive Dialogue - Descriptive Document

- Description of procurement procedure
- Overall budget, 273 M€
- High-level description of targeted system
 - Implementing the MSA
 - Booster to achieve 1 EF
 - Cluster, preferably based on European IP
 - Flash storage module
 - Interconnect expectations
 - Login system sizing
 - System management



European High Performance Computing Joint Undertaking

GENERAL INVITATION TO TENDER EUROHPC/2023/CD/0001

Descriptive Document

Acquisition, delivery, installation and hardware and software maintenance of JUPITER Exascale Supercomputer for the European High Performance Computing Joint Undertaking (EuroHPC)





16. Jan 2023: Publish Call (Descriptive Document)

17. Feb 2023: Deadline for Request for Participation

22. Feb - 17. Mar 2023: Evaluation, Notification

4. Apr 2023: First Dialogue

3.-5. May 2023: Second Dialogue

1. June 2023: Invitation to Tender

3. July 2023: Deadline for final Tender

3.-7. July 2023: Evaluation by Technical Experts until 20. Aug 2023: Governing Board Decision

23. Aug 2023: Notification to Tenderers

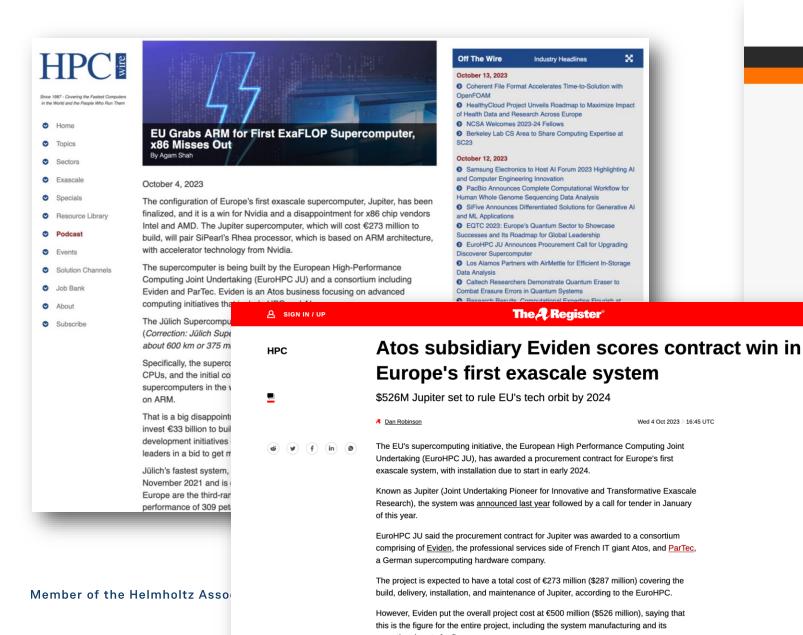
> 12. Sep - 02. Oct 2023: Contract Negotiations

> > 3. Oct 2023: Contract Signature



JUPITER CONTRACT ANNOUNCEMENT

3.10.2023





THENEXTPLATFORM

Q =

ich Supercomputing Center in Germany in 2024. There has been a lot of speculation about what Jupiter l include for its compute engines and networking and who will build and maintain the system. We now by some of this and can infer some more from the statements that were made by the organizations ticipating in the Jupiter effort.

fune 2022, the Forschungszentrum Jülich in Germany, which has played host to many supercomputers ice it was founded in 1987, was chosen to host the first of three European exascale-class uters to be funded through the EuroHPC Joint Undertaking and through the European national d state governments countries who are essentially paying to make sure these HPC and AI clusters are ere they want them. With Germany having the largest economy in Europe and being a heavy user of C thanks to its manufacturing focus, Jülich was the obvious place to park the first machine in Europe to ak the exaflops barrier.

at barrier is as much an economic one as it is a technical one. The six-year budget for Jupiter weighs in at 00 million, which is around \$526.1 million at current exchange rates between the US dollar and the ropean euro. That is in the same ballpark price as what the "Frontier" exascale machine at Oak Ridge tional Laboratory and the "El Capitan" machine that is being installed right now at Lawrence Livermore onal Laboratory - both of which are based on a combination of AMD CPUs and GPUs and Hewlett kard Enterprise's Slingshot variant of Ethernet with HPE as the prime contractor.

erybody knows that Jupiter was going to use SiPearl's first generation Arm processor based on the verse "Zeus" VI core from Arm Ltd, which is codenamed "Rhea" by SiPearl and which is appropriate

JUPITER - OVERALL TIMELINE











- 17.12.2021: Call for Expression of Interest (EoI) for Hosting Entity
- 14.02.2022: Deadline Eol Submission
- Q2 2022: Hearings & Hosting site decision and announcement
- Q1-Q3 2023: Procurement (Competitive Dialogue)
- 03.10.2023: Contract Signature
- Q3/Q4 2023: Installation Planning
- Q1/2024: Start installation of JUPITER
- Beg. of 2025: Put in operation JUPITER

The acquisition and operation of the EuroHPC supercomputer is funded jointly by the EuroHPC Joint Undertaking, through the European Union's Digital Europe programme, as well as by Germany through the BMBF and the MKW.







JUPITER ARCHITECTURE





DISCOVERING JUPITER

- First Exascale system in Europe (HPL); modular system
- Procured/funded by: EuroHPC JU, BMBF/NRW-MKW
 - Contract signed end of 2023
 - Installation starting soon
- JUPITER Booster: High scalablibty; 1 EFLOP/s HPL, >70 EFLOP/s FP8
 JUPITER Cluster: High versatility; 0.5 B/FLOP balance
- Network: InfiniBand NDR; Storage: 20 PB NVMe, 200 PB HDD
- Deployed in Modular Datacenter
- Building on: MSA (JUWELS); DEEP, EPI; ThunderX2, Ampere; ...
- About 1.936.000 Arm cores













JUPITER MODULES

JUPITER Booster

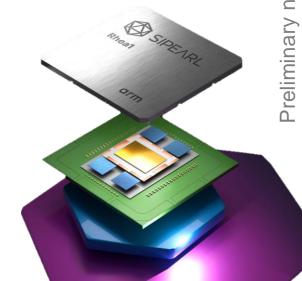
- Node design
 - ~6000 nodes
 - 4× NVIDIA CG1 per node
- CG1: Grace-Hopper
 - 72 Arm Neoverse V2 cores (4×128b SVE2); 120 GB LPDDR5
 - H100 (132 SMs); 96 GB HBM3
 - NVLink C2C (900 GB/s)





JUPITER Cluster

- Node design
 - ~1300 nodes
 - 2× SiPearl Rhea1 per node
- Rhea1
 - 80 Arm Neoverse V1 cores (2×256b SVE)
 - 256 GB DDR5,
 64 GB HBM2e



BOOSTER NODE DESIGN

• 4× NVIDIA **Grace-Hopper** in SXM5 Board (4× 680W)

Node Specs

- 4x NVIDIA InfiniBand NDR200
- 480 GB LPDDR5X / 360 GB HBM3 (usable)
- NVLink 4
 - GPU-GPU 150 GB/s per dir
- Links: CPU-GPU 450 GB/s per dir, CPU-CPU 100 GB/s per dir
- ARM Neoverse V2

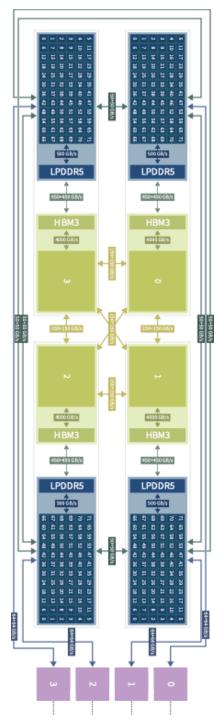
CPU Specs

- SVE2/NEON (4x 128 bit vector op)
- 72 cores @ ~2.4GHz (~3.2 GHz turbo)
- 120 GB LPDDR5X (8 channels)
 - ≥450 GB/s
 - ~150 ns latency

• H100

GPU Specs

- ~50 TFLOP/s (HPL single GPU)
- 96 GB HBM3
 - ~4 TB/s



JUPITER - LOGIN/VISUALIZATION

EVIDEN an atos business







Login Partition and Visualization Capabilities

- Login Nodes
 - Booster: 12 nodes, 1x CG1
 - Cluster: 5 nodes, 2x Rhea1
- Visualization Nodes
 - Booster: 3 nodes, 1x CG1
 - Cluster: 3 nodes, 2x Rhea1 and 2x NVIDIA A40
- 2x 100 Gbit Ethernet for external connectivity



JUPITER - INTERCONNECT

an atos business



One Network to Rule Them All

- NVIDIA Mellanox InfiniBand NDR/NDR200
 - NVIDIA Quantum-2 switches
 - NVIDIA Connect-X7 HCAs
- Dragonfly+ topology
 - 27 Dragonfly groups
 - Within each group: full fat tree
- Approximately 51000 links, 102000 logical ports, 25400 endpoints, 867 switches
- Adaptive Routing
- In-network processing on switch level (SHARPv3), tentatively

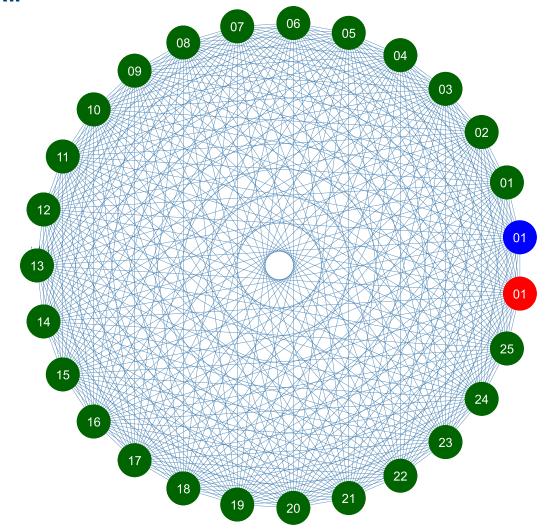


JUPITER - INTERCONNECT





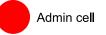
One Network to Rule Them All







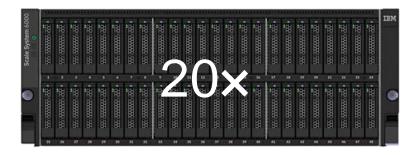




JUPITER - STORAGE (SCRATCH)



- Gross Capacity: 29 PB; Net Capacity: 21 PB
- Bandwidth: 2.1 TB/s Write, 3.1 TB/s Read
- 20x IBM SSS6000 Building Blocks (40 servers)
 - 2x NDR400 per server
 - 48× 30 TB NVMe drives per block
 - IBM Storage Scale (aka Spectrum Scale/GPFS)
- Manager and Datamover Nodes
- Exclusive for JUPITER
 - Integrated into InfiniBand fabric



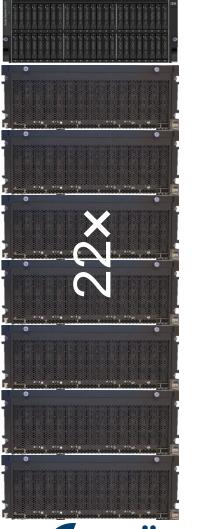
JUPITER - STORAGE (EXASTORE)





In kind contribution from JSC, not part of the JUPITER procurement

- Gross Capacity: 308 PB; Net Capacity: 210 PB
- Bandwidth: 1.1 TB/s Write, 1.4 TB/s Read
- 22× IBM SSS6000 Building Blocks (44 servers)
 - 2x NDR200 per server
 - 7× JBOD enclosures, each with 91x 22 TB Spinning Disks per block
 - IBM Storage Scale (aka Spectrum Scale/GPFS)
- Manager and Datamover Nodes
- Exclusive for JUPITER
 - Integrated into InfiniBand fabric



JUPITER MANAGEMENT STACK

"Power is nothing without control"

- Eviden SMC xScale
- ParaStation Modulo
 - Resource management
 - ParaStation MPI
- Ansible as provisioning system
- SLURM as scheduler
- EasyBuild as scientific software package management
- RedHat Enterprise Linux 9































DATA CENTER FOR JUPITER





DATA CENTER FOR JUPITER





CAMPUS INFRASTRUCTURE PREPARATIONS

- Upgrade of campus power supply 110 kV / 35 kV from 2x 40 MVA to 2x 60-80 MVA
- Upgrade of 110 kV power line to next electric power transformation substation
- New powerline 2x 35 kV from campus power transformation substation to Exascale site
- Construction of new weather tower further away from Exascale site
- Construction of concrete slab 85 m x 42 m x 0.5 m
- Connection to campus cooling loop, river water, potable water, process water, wastewater, network
- Connection to heating network for heat reusage



CAMPUS ELECTRIC POWER TRANSFORMER SUBSTATION

• Upgrade of transformers 110 kV / 35 kV from 2 × 40 MVA to 2 × 60-80 MVA









CAMPUS ELECTRIC POWER TRANSFORMER SUBSTATION

- Upgrade of 110 kV power line to next
- electric power transformation substation







EXASCALE SITE

Construction of concrete slab 85 m × 42 m × 0.5 m









MODULAR DATA CENTER FOR JUPITER







nary numbers, might change during installati

MODULAR DATA CENTER FOR JUPITER

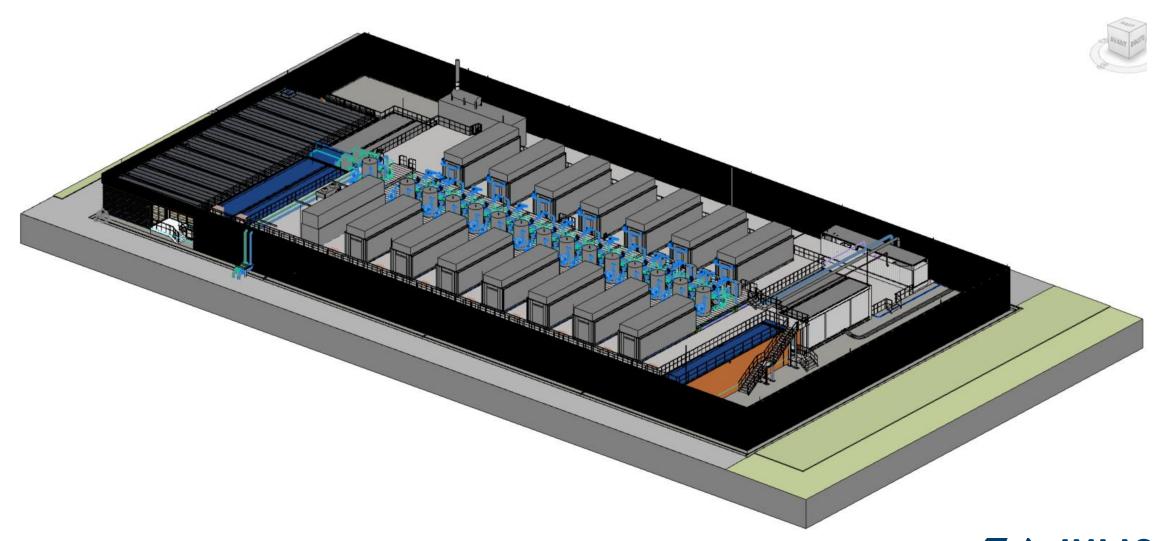
MDC provided by Eviden

- Base area: 2300 m2
- 7 IT modules (2 containers each)
 - Each container can be equipped with 10 Sequana XH3000 racks
- Data hall (4 containers) for standard racks with RDHx in 4 rows, electrical power max. 1 MW
- 15 energy supply modules with transformer 35 kV / 400 V, 2.5 MVA
 - 14 IT containers + data hall
- Logistic part with entrance area, control room, workshop, warehouse, restroom
- 1 glycol free hybrid cooling unit on the roofs for each IT container ~ 36°C / 48°C
- Redundancy by modules



MODULAR DATA CENTER FOR JUPITER

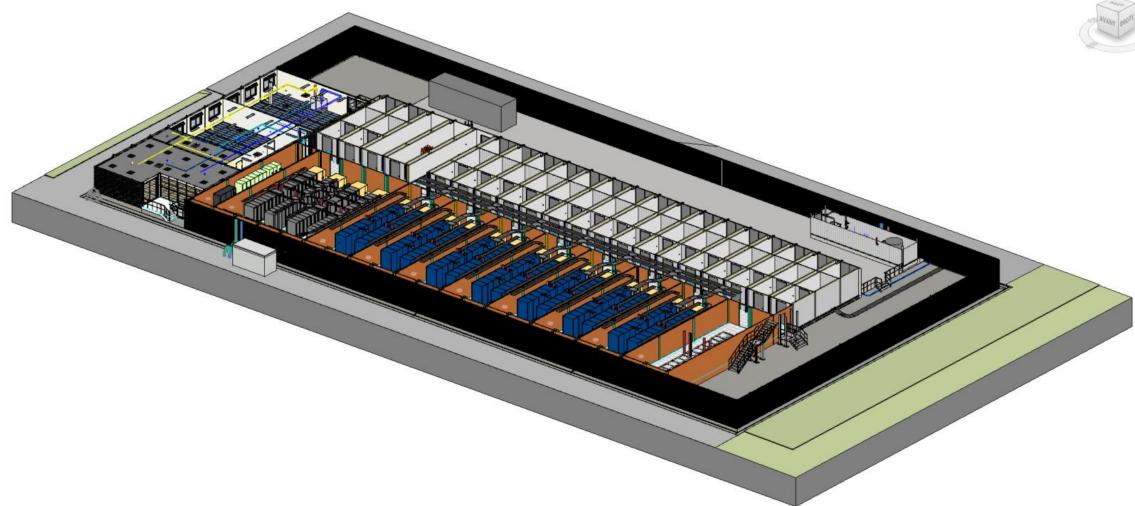




MODULAR DATA CENTER FOR JUPITER













JUPITER EXASCALE DEVELOPMENT INSTRUMENT

EuroHPC / Forschungszentrum Jülich

- Eviden BullSequana XH3000
 - 48× compute nodes (24× blades)
 - NVIDIA quad-GH200 96 GB Grace-Hopper Superchip
 - Memory: 480 GB on CPUs + 384 GB on GPUs
 - NVIDIA quad-rail InfiniBand NDR200
- Usage
 - System management preparations
 - JUREAP
 - Application porting
- Also: GH200 COTS test nodes





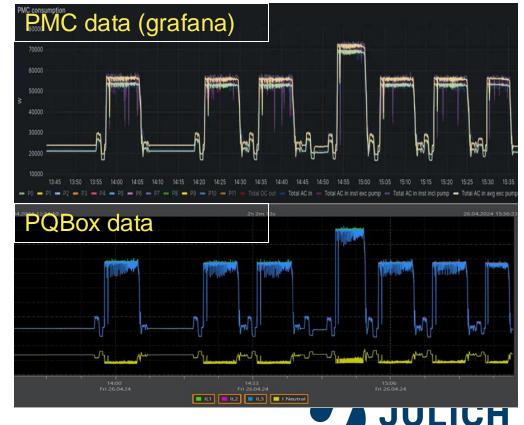
POWER MEASUREMENT

Choice of Source

- XH3000 rack sensors vs Power meter
 - Similar measurements
 - In all tests, variation between 0.5 and 1.3%
 - 73.17 GF/W vs 72.73 GF/W
- Choice to use data from power meter:
 - More conservative measurement results



Sensor	Measurement	Difference
Rack sensors	51838.4 W	0.0%
Power meter	52154.3 W	+0.6%



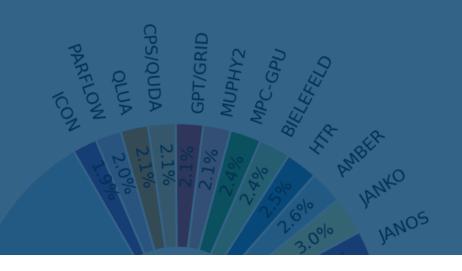
Forschungszentrum

GREEN500 – JUNE 2024

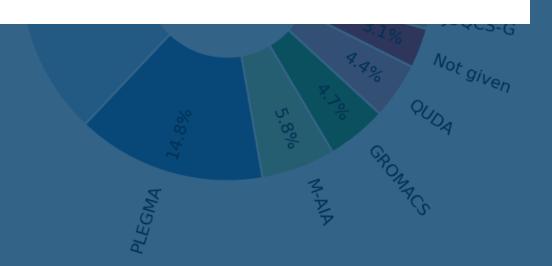
Green500 Data

Rank	TOP500 Rank	System	Cores	Rmax (PFlop/s)	Power (kW)	Energy Efficiency (GFlops/watts)
1	189	JEDI - BullSequana XH3000, Grace Hopper Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, ParTec/EVIDEN EuroHPC/FZJ Germany	19,584	4.50	67	72.733





APPLICATIONS





ASSESSING WITH APPLICATIONS

- Theoretical FLOP/s and GB/s are nice; but building machines for <u>users</u>
- > Applications core of procurement assessment
- Define representative benchmarks, *ExaBench*
 - 1. Analyze workload (JSC, de, eu, 🔵)
 - 2. Select fitting applications
 - Benchmarkize them
 - 4. Submit as part of specification
 - → Get best machine

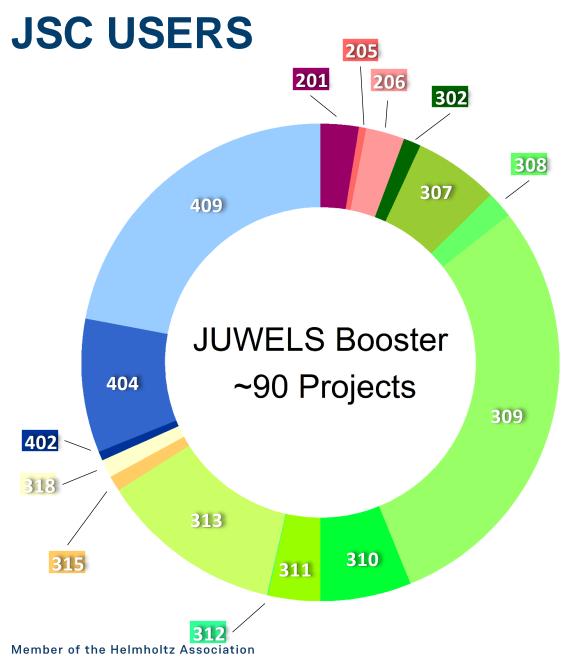


EVALUATION

- Criteria
 - Requirements to project planning, etc.
 - Technical requirements to overarching design and details
 - Performance of applications, benchmarks
 - Total cost of ownership (TCO): How much science for money
 - Further categories (Synthetic Benchmarks, High-Scaling Applications)
- Quantified evaluation







Reseach Fields

- 201 Basic Biological and Medical Research
- 205 Medicine
- 206 Neurosciences
- 302 Chemical Solid State and Surface Research
- 307 Condensed Matter Physics
- 308 Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
- 309 Particles, Nuclei and Fields
- 310 Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
- 311 Astrophysics and Astronomy
- 312 Mathematics
- 313 Atmospheric Science, Oceanography and Climate Research
- 315 Geophysics and Geodesy
- 318 Water Research
- 402 Mechanics and Constructive Mechanical Engineering
- 404 Heat Energy Technology, Thermal Machines, Fluid Mechanics
- 409 Computer Science

→ Define Benchmarks



SUB-BENCHMARKS, VARIANTS

- Type of benchmarks
 - Applications benchmarks
 - Synthetic benchmarks
- Execution targets
 - JUPITER Booster (GPU, CPU)
 - JUPITER Cluster (CPU)
 - MSA
- Application benchmark categories
 - TCO
 - High-Scaling

		Booster			Cluster	MSA
Before Dialogue	After Dialogue	GPU	GPU High-Scale	CPU	CPU	
Amber	Amber	4				
Arbor	Arbor	\checkmark	\checkmark			
Chroma	Chroma	\checkmark	\checkmark			
Gromacs	Gromacs (2)	\checkmark				
ICON	ICON (2)	\checkmark				
JUQCS	JUQCS	\checkmark	\checkmark			\checkmark
nekRS	nekRS	\checkmark	\checkmark			
ParFlow	ParFlow	\checkmark				
PIConGPU	PIConGPU	\checkmark	\checkmark			
Quantum	Quantum	\checkmark				
ESPRESSO	ESPRESSO					
SOMA	SOMA	4				
AI-MMoCLIP	AI-MMoCLIP	\checkmark				
AI-NLP	AI-NLP	\checkmark				
Al-ResNet	Al-Resnet	4				
dynQCD	dynQCD				\checkmark	
NAStJA	NAStJA				\checkmark	
Graph500	Graph500			\checkmark		
HPCG	HPCG	\checkmark			✓	
HPL	HPL	✓			\checkmark	
IOR	IOR			\checkmark	✓	
LinkTest	LinkTest			\checkmark	✓	✓
Multi-Flow IP	Multi-Flow IP			✓		
OSU	OSU (2)	✓		\checkmark	✓	
STREAM	STREAM	\checkmark			✓	



TCO APPLICATIONS

Total Cost of Ownership

- Traditional benchmark category
- How much of benchmark suite can be run in lifetime of system? Also: energy
- Key: same metric for each benchmark
 - Unit: time / s
 - Needed to convert rate → time
- One reference run for formula (e.g. 8 nodes); additional strong-scaled runs (e.g. 4, 16)
- Weights per individual benchmark



HIGH-SCALING APPLICATIONS

- Novel category for us
- Give benchmarks a focus on large-scaleness of system
- Compare execution on full* JUWELS Booster to full* JUPITER Booster
 - *: Use 50 PFLOP/sth. peak part of JUWELS Booster
 - → compare to 1000 PFLOP/s^{th. peak} part of JUPITER Booster
- Challenging design, challenging commitments
 - Design for unknown system, unknown device, unknown memory size Introduce 3 memory variants: small (2/4), medium (3/4), high (4/4 JWB A100 memory)
 - Many tests on scale at JUWELS Booster
 - Some internal extrapolations to JUPITER scale

- Arbor tiny (1/4), small, medium, large
- Chroma small, medium, large
- JUQCS small, large
- nekRS small, medium, large
- PIConGPU small, medium, large



JUREAP

Seeding Exascale in Europe!



Mitglied der Helmholtz-Gemeinschaft

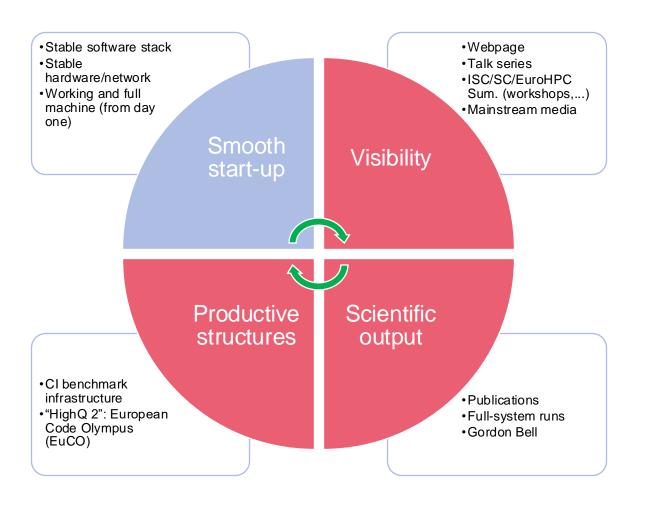
Foto von Robert Wiedemann auf Unsplash

JUPITER Research and Early Access Program



JUREAP OVERVIEW

One necessary goal – and three sufficient goals for success of JUREAP with ~20 applications



~20 participating teams with codes/applications

EXA: Exascale Applications

LAX: Large Applications with X

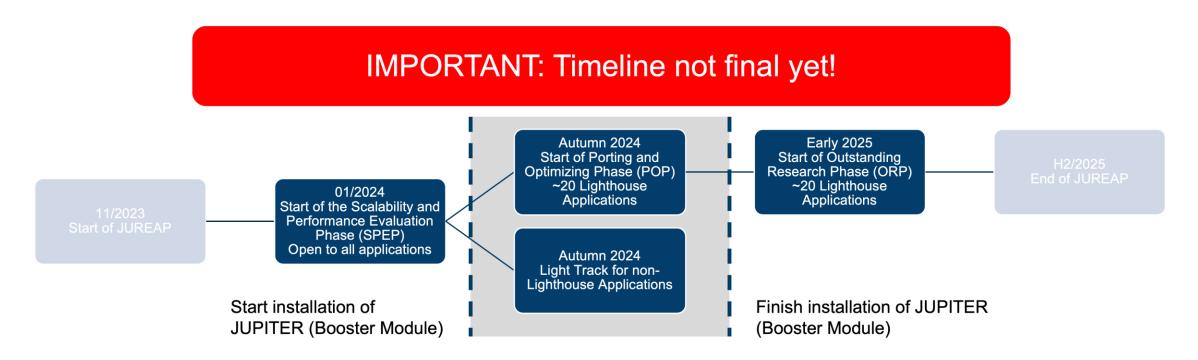
Balanced in terms of simulation, AI, and scientific domains

Computing time via GCS and EuroHPC



JUREAP

JUPITER Research and Early Access Program



Phase 1: Scalability and Performance Evaluation Phase (SPEP)

Phase 2: Porting and Optimizing Phase (POP)

Phase 3: Outstanding Research Phase (ORP)

JUREAP call open since Jan'2024 https://events.hifis.net/event/1239/





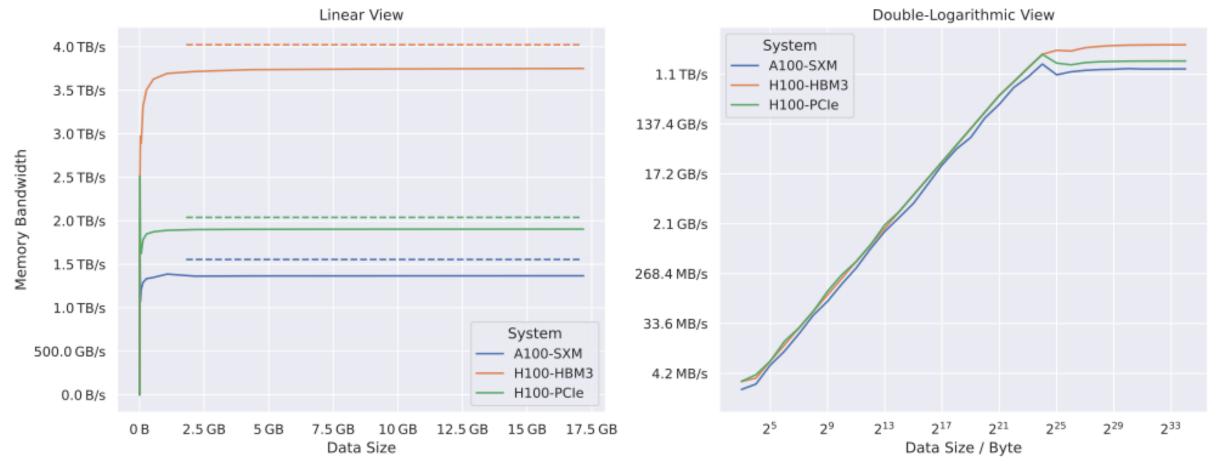
GH200 TEST NODES

- GH200 Prototype
- 2× Grace-Hopper superchips
 - 1 Grace CPU (72 cores), 480 GB LPDDR5X RAM
 - 1 H100 GPU
 - TDP 700-1000 W
- Slightly different variant compared to JUPITER node design



GPU STREAM

GPU STREAM Variant Scan for GPU Generations/Flavors



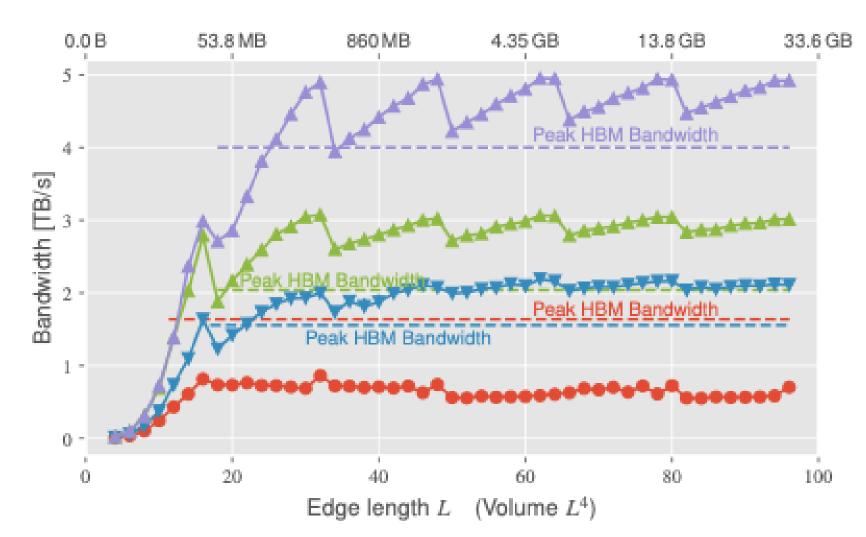
https://github.com/AndiH/CUDA-Cpp-STREAM



KOKKOS LQCD BENCHMARK

By Simon Schlepphorst / JSC

- Simplified Staggered
 Fermion Dirac Operator
- MI250
- A100
- H100 (PCIe)
- H100 (GH200)

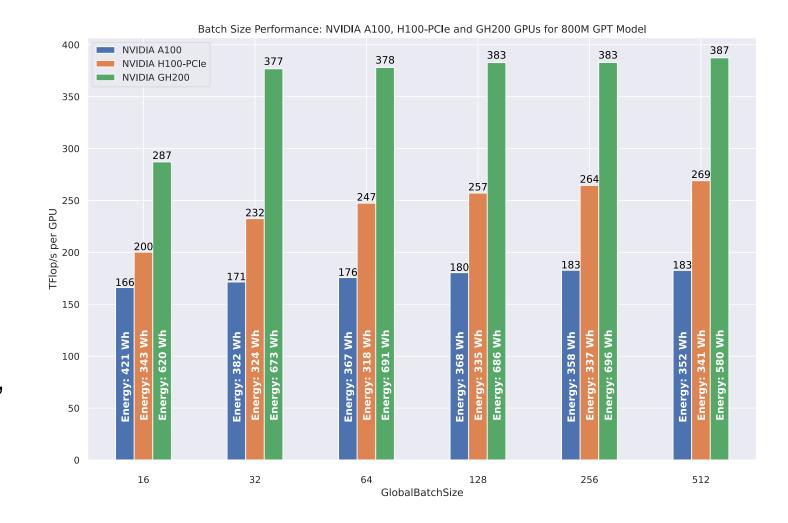




MEGATRON-LM

By Chelsea John / JSC

- OpenGPT-X: BMWK project for LLM with EU languages, Open
- 1 node benchmark:
 800M GPT Model
- Increasing Batchsizes
- Excellent performance on H100, especially GH200 variant (HBM3, TDP)

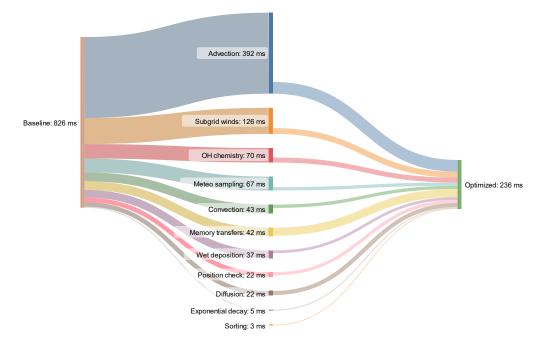


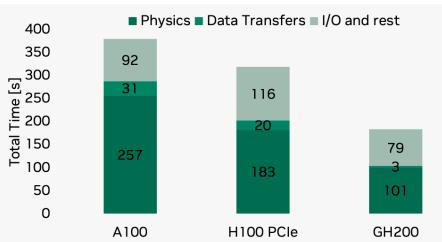


MPTRAC

By Lars Hoffmann / JSC

- Lagrangian particle dispersion model: atmospheric transport processes (troposphere/stratosphere)
 - → volcanic emissions
- Continuously optimized for GPUs Recently: Significant speedup on A100
- First test on GH200





See also GTC talk by Mathias Wagner

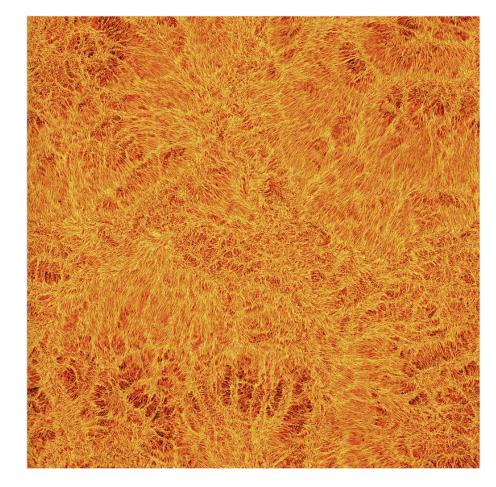


OTHER GH200 RESULTS

JUWELS Booster A100 vs. GH200

- ICON:
 - R2B4 Benchmark: 563 s vs. 343 s → 1.62×
 - By Manoel Römmer / JSC
- nekRS
 - Rayleigh

 Bénard Convection: 2.16x
 - By Mathis Bode / JSC
- Arbor
 - Busyring Benchmark: 330 s vs 167 s → 1.97×
 - By Thorsten Hater / JSC

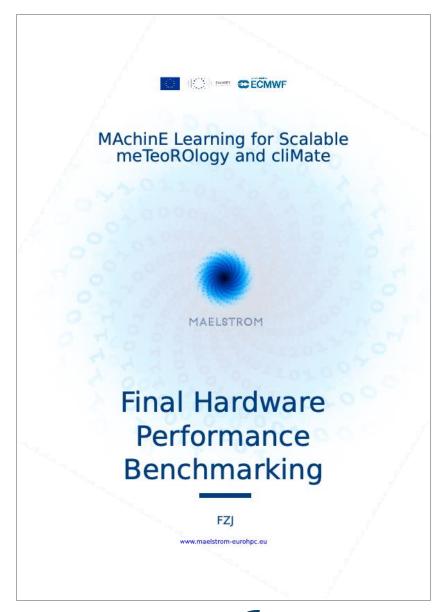


RBC Visualization (M. Bode)



MAELSTROM TESTS

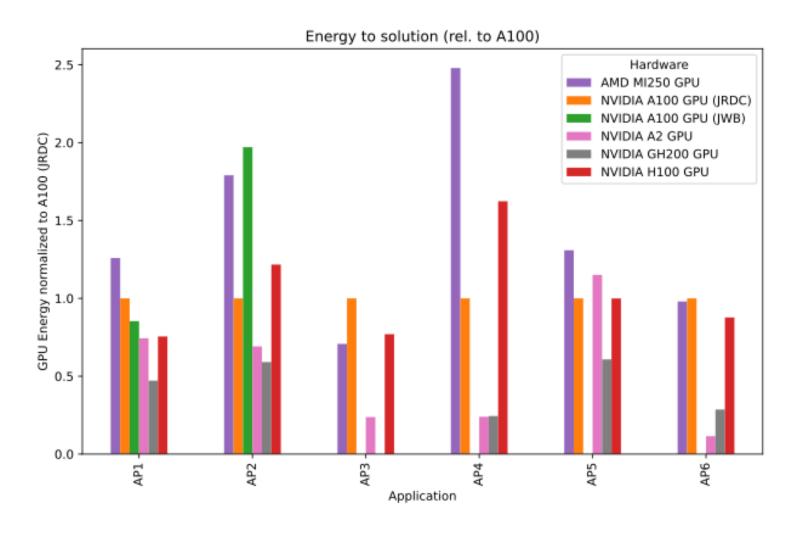
- MEALSTROM: EuroHPC-JU-funded project, ended in March 2024
- Enablement/optimization of 6 weather & climate applications using ML
- D3.7 (Feb 2024): Benchmarking of final applications on diverse hardware
- → www.maelstrom-eurohpc.eu





MAELSTROM TESTS

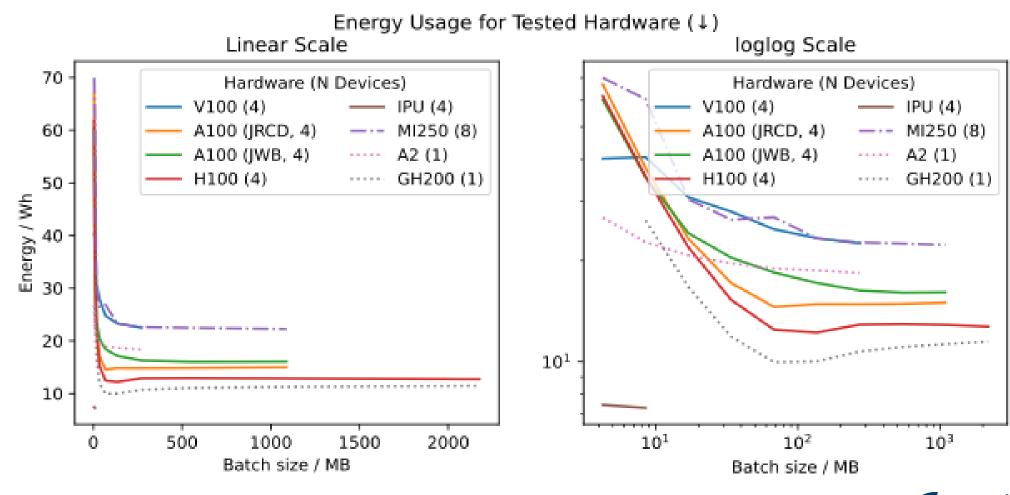
Energy-to-Solution Application Overview





MAELSTROM TESTS

AP1: MetNor





FIRST CPU INVESTIGATIONS (GRACE)

- Focus mostly on GPU currently
- Some first results on Grace hardware
- → Very competitive performance, especially wrt TDP (but still early)

DynQCD: 1.5× vs. EPYC Rome 7742 (2×64 cores)

- · Best: Grace-Clang, ACfL
- Slightly worse: GCC
- Investigating FMLA instructions
- (Auto-Vectorization works well!)

NAStJA:

- 2.3x vs. EPYC Rome 7402 (2x24 cores)
- 5.6x vs Intel Skylake 8168 (2x24 cores)

JUQCS: 1.35× vs. EPYC Rome 7402 for 31 Qubits (2×24 cores)

FLEUR:

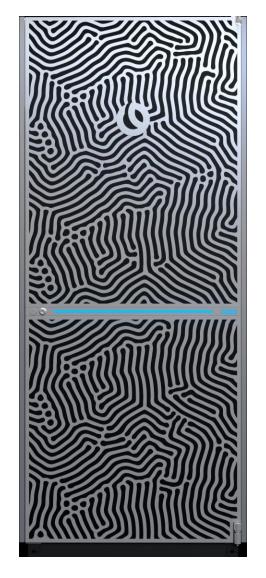
- 1.2x vs. Intel Skylake 8168 (2x24 cores, 400 W TDP)
- 0.8x vs. EPYC Rome 7742 (2x64 cores, 450 W TDP)
- 1.5× vs. Intel SPR-HBM (2×32 cores, 700 W TDP)



MISSION BRIEFING OVERVIEW

- En route to JUPITER: EuroHPC JU system hosted at JSC
- Launched with focus on applications
- ~6000 nodes,
 24 000 H100 GPUs, 1 728 000 Arm cores, 24 000 NDR200 endpoints
- Landing in Modular Data Center
- Preparing for descent:
 - JUREAP
 - GH200 test systems
- → <u>jupiter.fz-juelich.de</u>







JUPITER

The Arrival of Exascale in Europe

fz-juelich.de/jupiter | #exa_jupiter











