



Scaling Innovation

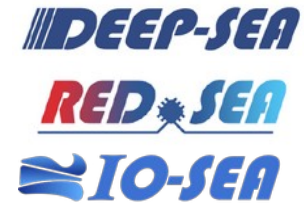
Modular Computing & QPUs

Forum Teratec

June 22, 2021

Thomas Moschny
CTO, ParTec AG

- Strong general purpose cluster specialist for more than two decades
 - *ParaStation research project: 1995 (Univ. of Karlsruhe)*
 - *ParTec founded as a spin-off in 1999*
 - *HPC full service provider since 2004*
- Cooperation with Jülich Supercomputing Centre since 2004
 - *ParaStation Consortium founded in 2005*
- Pioneering and enabling Modular Supercomputing
 - *Since 2010: DEEP Projects*
 - *ParaStation Modulo Software Suite*
- Significant contributions in European research projects
 - *Exascale-related: *-SEA Projects, EUPEX*
 - *Quantum- and AI-related: HPCQS, CoE RAISE*



- **ParaStation Modulo Software Suite**
 - *Software for HPC Systems developed for >20 years*
 - *Pioneering the Modular Supercomputing Architecture (MSA) for >10 years*
 - *Extensively used in production environments*
 - *Platform for research projects*
- **ParTec Support: on-site (or remote) system operations**
 - *System setup and installation*
 - *System maintenance and administration*
 - *General 1st and 2nd level support*
- **Co-design and co-development**
 - *Transferring results from research projects into production*
 - *Enhancing production systems over their lifetime*

ParaStation
MODULO



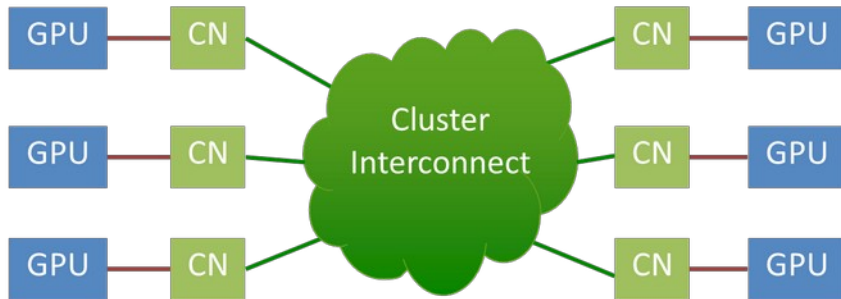
MELU  **INA**



- **ParaStation ClusterTools**
 - *Tools for provisioning and management*
- **ParaStation HealthChecker & TicketSuite**
 - *Automated error detection & error handling*
 - *Ensuring integrity of the computing environment*
 - *Keeping track of issues*
 - *Powerful analysis tools*
- **ParaStation MPI & Process Management**
 - *Runtime environment specifically tuned to the largest distributed memory supercomputers*

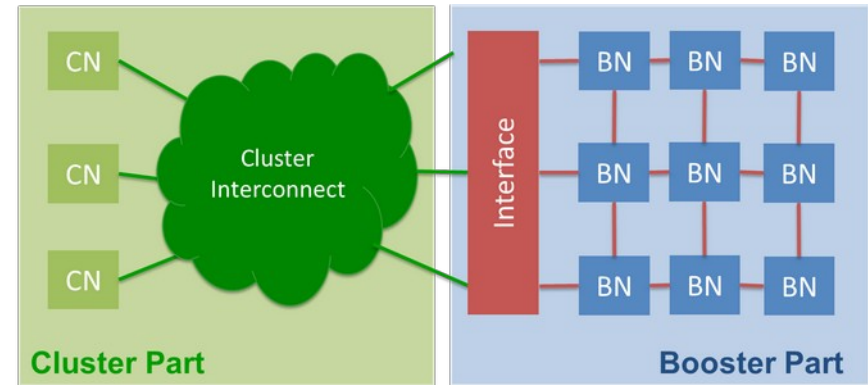
ParaStation
MODULO

**Maximize job throughput –
Minimize administration effort**



Accelerated Cluster

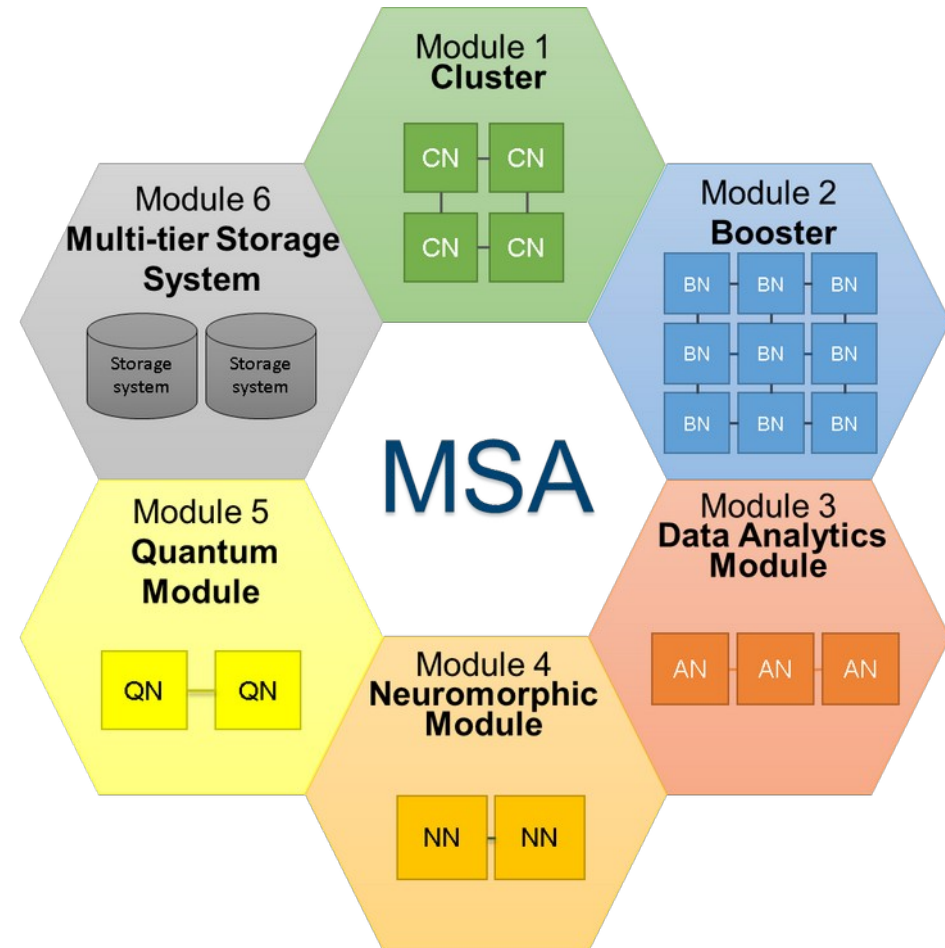
- *Fixed, static ratio and assignment of accelerators to CPUs*
- *Static management of resources*
- *Accelerators do not act autonomously*
- *General-purpose Cluster interconnect*
- *Programming via local offload interfaces*



Cluster-Booster Architecture

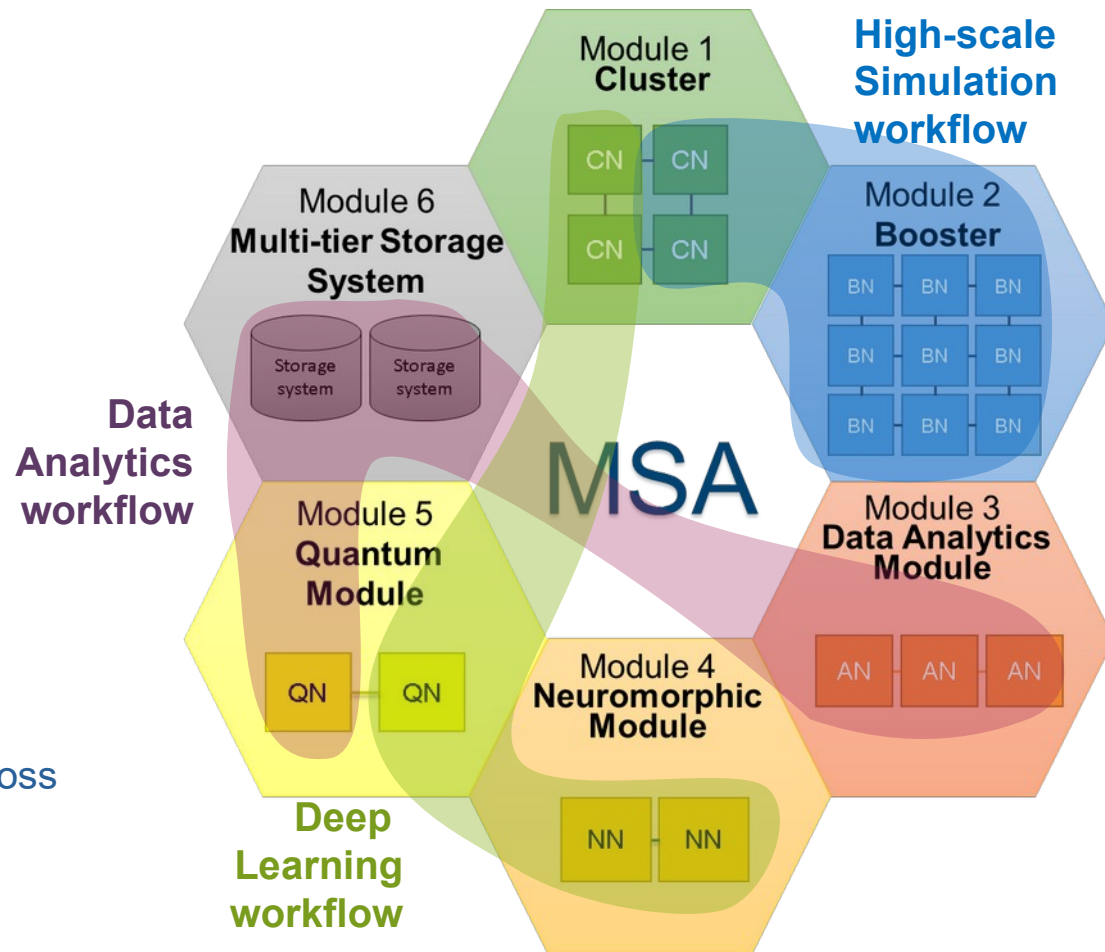
- *No fixed ratio or assignment between resources (multicore & manycore nodes)*
- *Dynamic management and association of resources*
- *High-throughput network in the Booster*
- *Programming via MPI and “global” tasking interfaces*

- **Generalization of the Cluster-Booster Concept**
 - *Composability of heterogeneous resources*
 - *Effective resource-sharing*
- **Any number of (specialized) modules possible**
 - *Cost-effective scaling*
- **Fit application diversity**
 - *Large-scale simulations*
 - *Data analytics*
 - *Machine/Deep Learning, AI*
 - *Hybrid Quantum Workloads*
- **Achieve leading scalability & energy efficiency**
→ Exascale
- **Unified SW environment to run applications across all modules**
 - *ParaStation Modulo providing a Slurm-based Scheduler*



Modular Supercomputing Architecture

- Generalization of the Cluster-Booster Concept
 - Composability of heterogeneous resources
 - Effective resource-sharing
- Any number of (specialized) modules possible
 - Cost-effective scaling
- Fit application diversity
 - Large-scale simulations
 - Data analytics
 - Machine/Deep Learning, AI
 - Hybrid Quantum Workloads
- Achieve leading scalability & energy efficiency
→ Exascale
- Unified SW environment to run applications across all modules
 - ParaStation Modulo providing a Slurm-based scheduler



JUWELS – A Modular Supercomputer

Cluster Module



© Forschungszentrum Jülich

Booster Module



© Forschungszentrum Jülich/Ralf-Uwe Limbach



JÜLICH
SUPERCOMPUTING
CENTRE

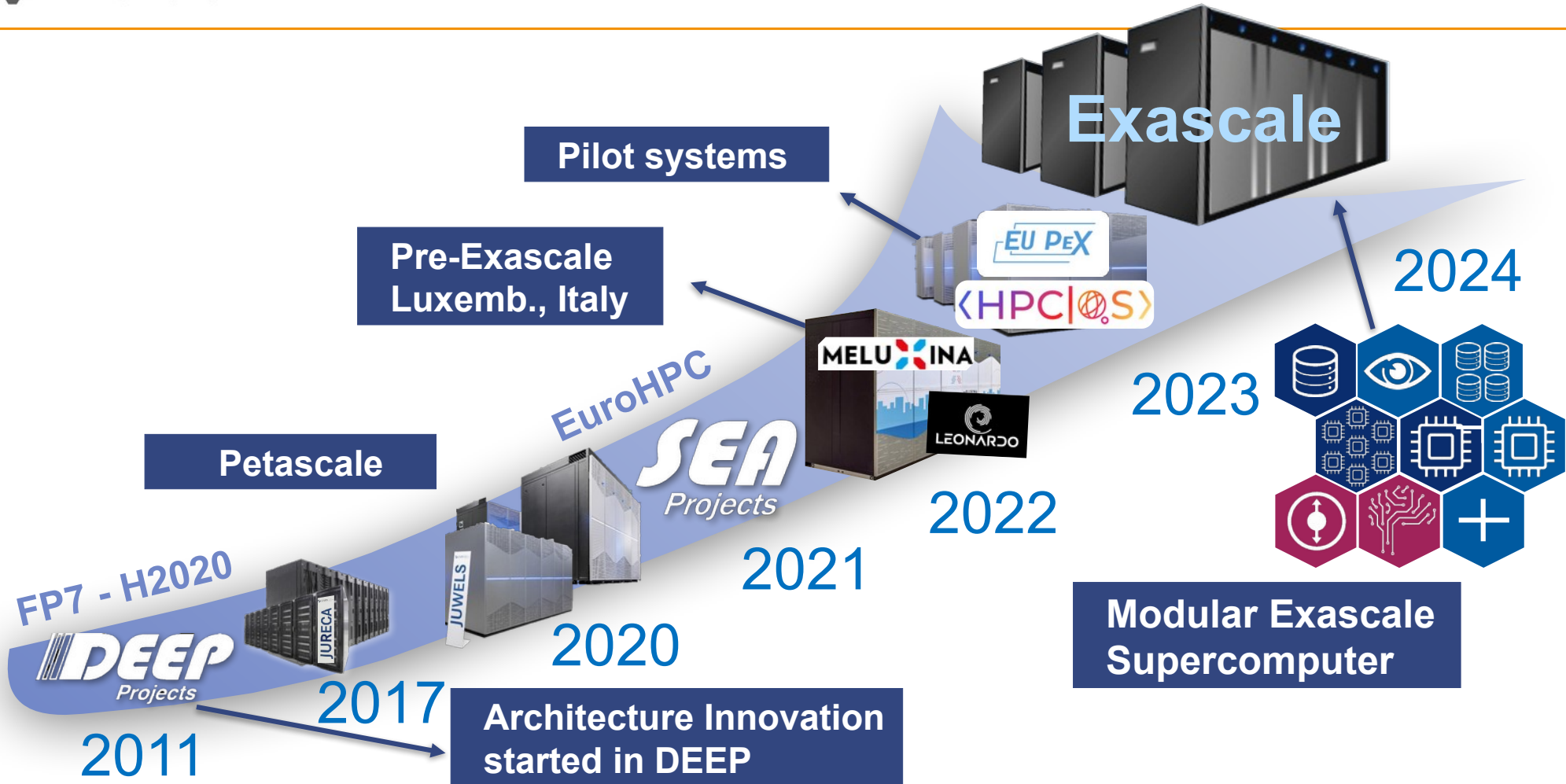
- 12 PFlop/s peak
- #23 on Top500 list (June 2018)
- 2575 nodes (Bull Sequana X1000)
- Intel Xeon Platinum 8168 / Gold 6148
- Mellanox EDR, ParaStation MPI



- GPU-accelerated module, 70 PFlop/s peak
- #7 on Top500, #3 on Green500 (Nov. 2020)
- 936 nodes (Bull Sequana XH2000)
- 4x NVIDIA A100 GPUs per node
- Quad-rail Mellanox HDR200, ParaStation MPI

Operated as one Modular System with ParaStation Modulo and Slurm

Modular Supercomputing to Exascale

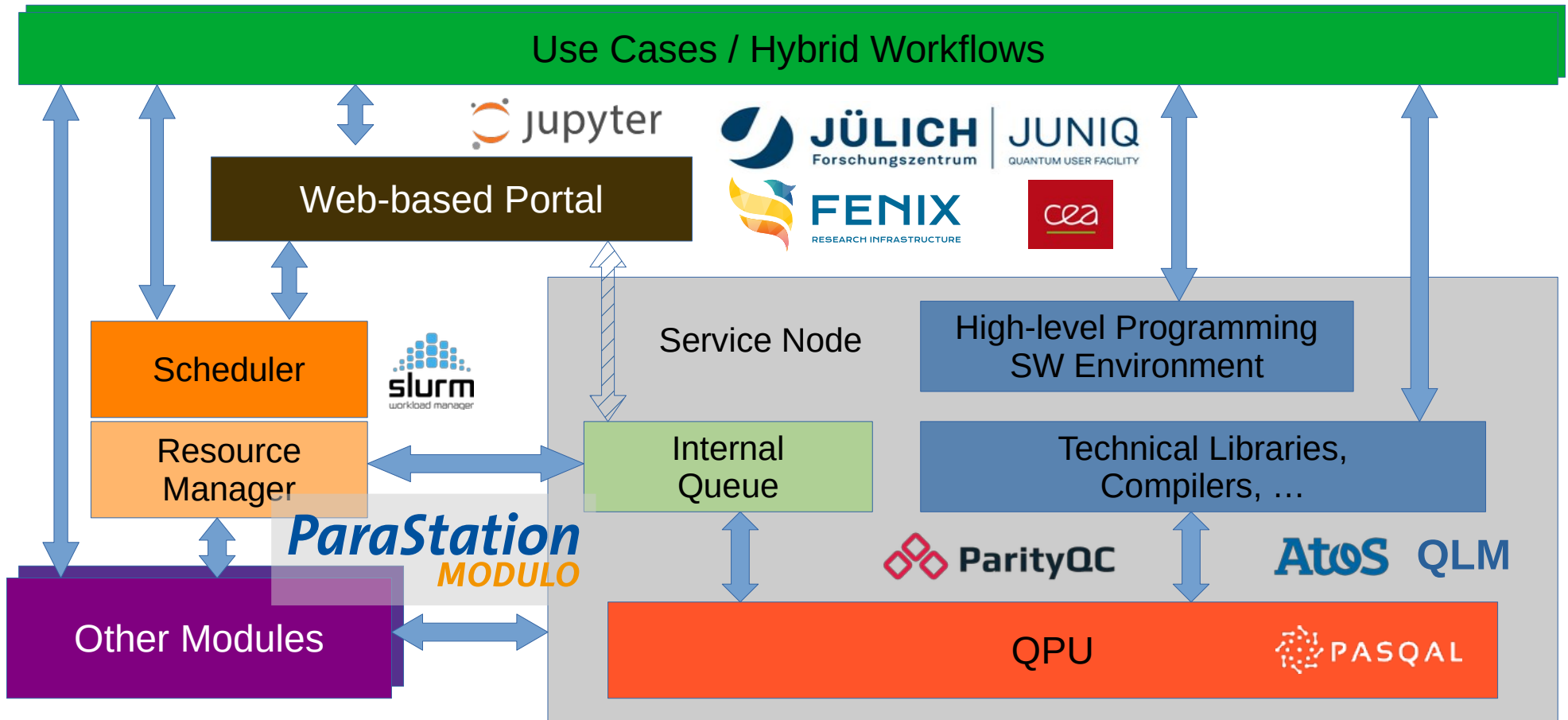


- **Applying the MSA approach**
 - *Integrate the QPU as a new module type into the supercomputer*
- **Implementation aspects**
 - *Integration of the QPU and its front-end into the full management stack of the modular supercomputer, including user and SW management, storage access, provisioning, and more*
 - *Low-latency connection to other modules via federated, high-speed network*
 - *Integration in the scheduling and resource management on the system level*
- **Benefit: New usage models**
 - *Tightly coupled simulations: benefit from efficient data exchange*
 - *Workflows exhibiting one or more stages on the QPU and doing pre- and post-processing tasks on other modules*
 - *Unified environment (due to the tight integration: user and SW management, storage, ...)*



- The QPU is a scarce resource: it cannot be used concurrently by multiple users
 - *Implement a pseudo-shared usage model, e.g., based on time slices*
 - *Enable communication between the internal queue of the QPU and the system-wide scheduler/resource manager via well-defined interfaces*
- Provide “direct” access of the QPU via the web-based portal
 - *Redirect portal requests through the global scheduler/resource manager*
 - *Pseudo-shared usage model as prerequisite*
- Exact requirements/timings depend on the use case and are subject to research



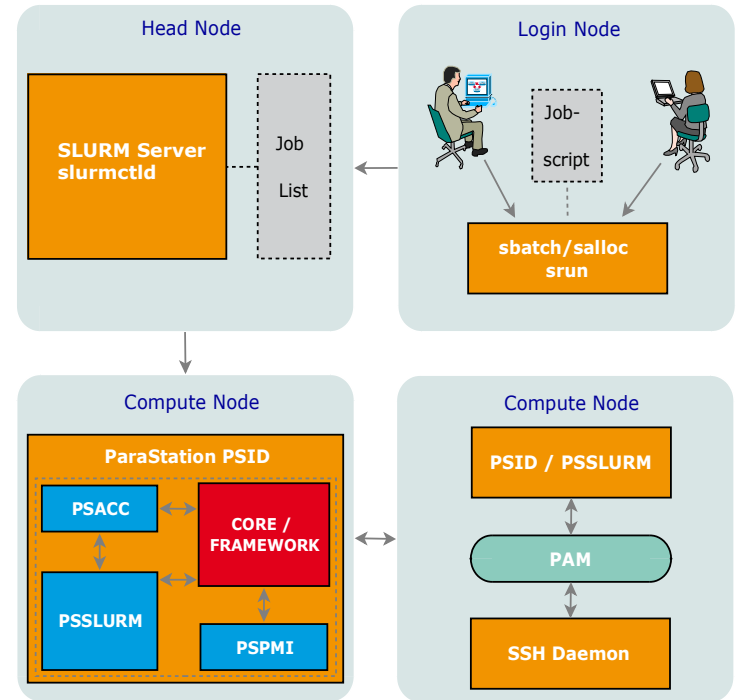


Thank you for your attention!

Questions?

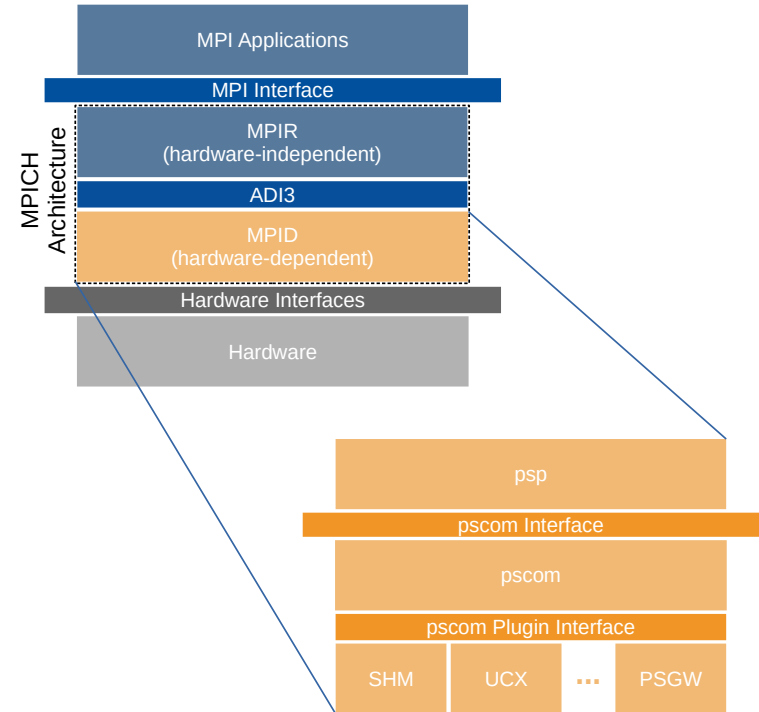
moschny@par-tec.com

- Scalable network of MPI process management daemons
 - *Running on the computational nodes*
 - *Process startup and control, I/O forwarding, ...*
 - *Precise resource monitoring*
 - *Proper cleanup after jobs*
- **PSSLURM: Full integration for Slurm**
 - *Plugins to the ParaStation Management daemons*
 - *Replace node-local Slurm daemons (also reduces number of daemons)*
 - *Enforces resource limits*



ParaStation
MPI

- Based on MPICH 3.3.2 (MPI-3.1 compliant)
 - Maintains MPICH ABI compatibility
 - Supports MPICH tools (tracing, debugging, ...)
 - MPICH layers beneath ADI3 are replaced by ParaStation PSP Device
 - Powered by pscom low-level communication library: non-blocking p2p semantics
- Support for various transports and protocols via pscom plugins
 - Support for InfiniBand, Omni-Path, Extoll, ...
 - Applications may use multiple transports / plugins at the same time
 - Gateway capability via PSGW plugin to bridge transparently between different networks
 - CUDA awareness for all transports / CUDA optimization via GPUDirect for UCX, and Extoll
- Proven to scale up to ~3,500 nodes and ~140,000 processes per job



ParaStation
MPI