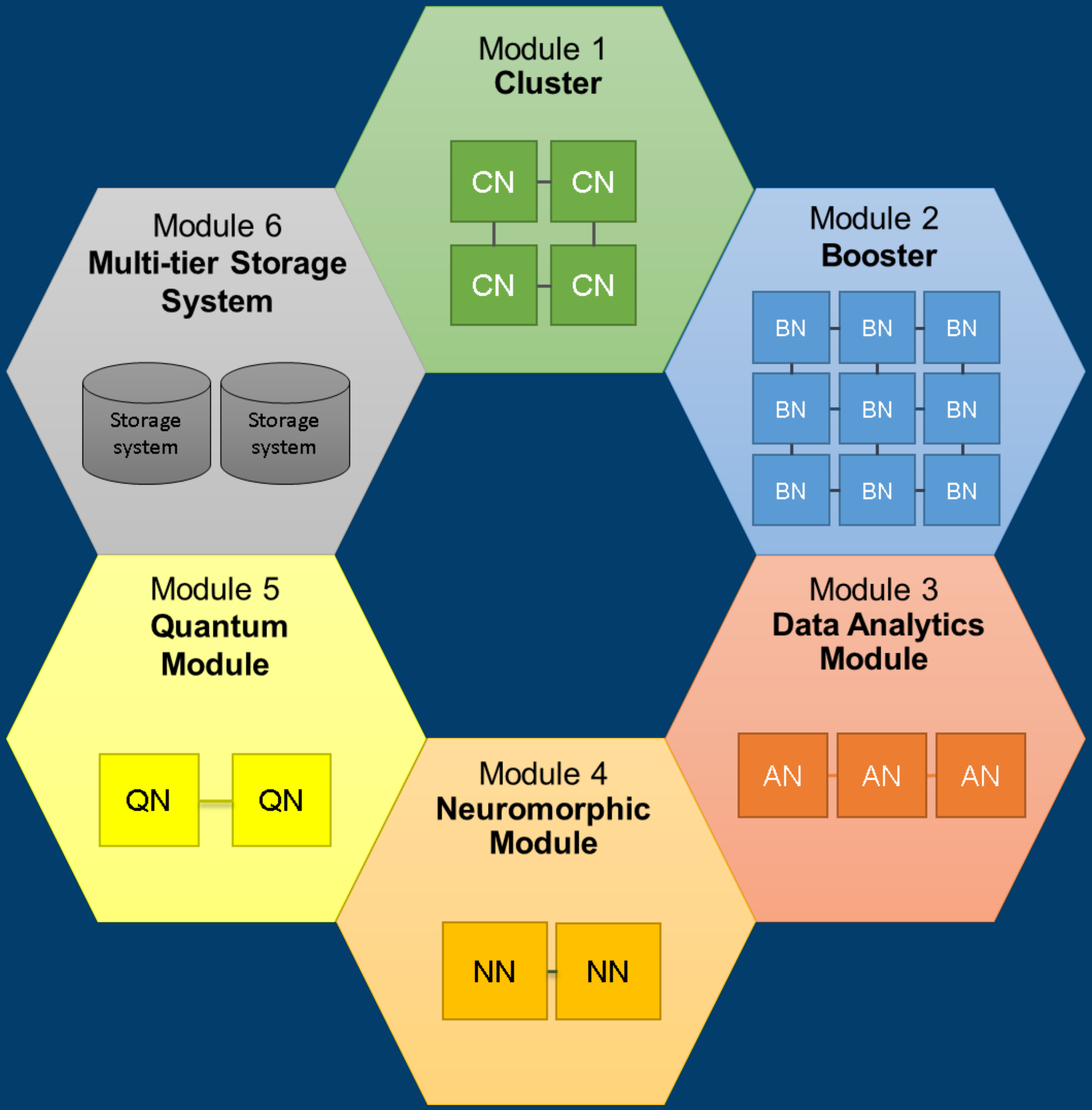
MODULAR SUPERCOMPUTING: a system-wide orchestration of heterogeneous resources

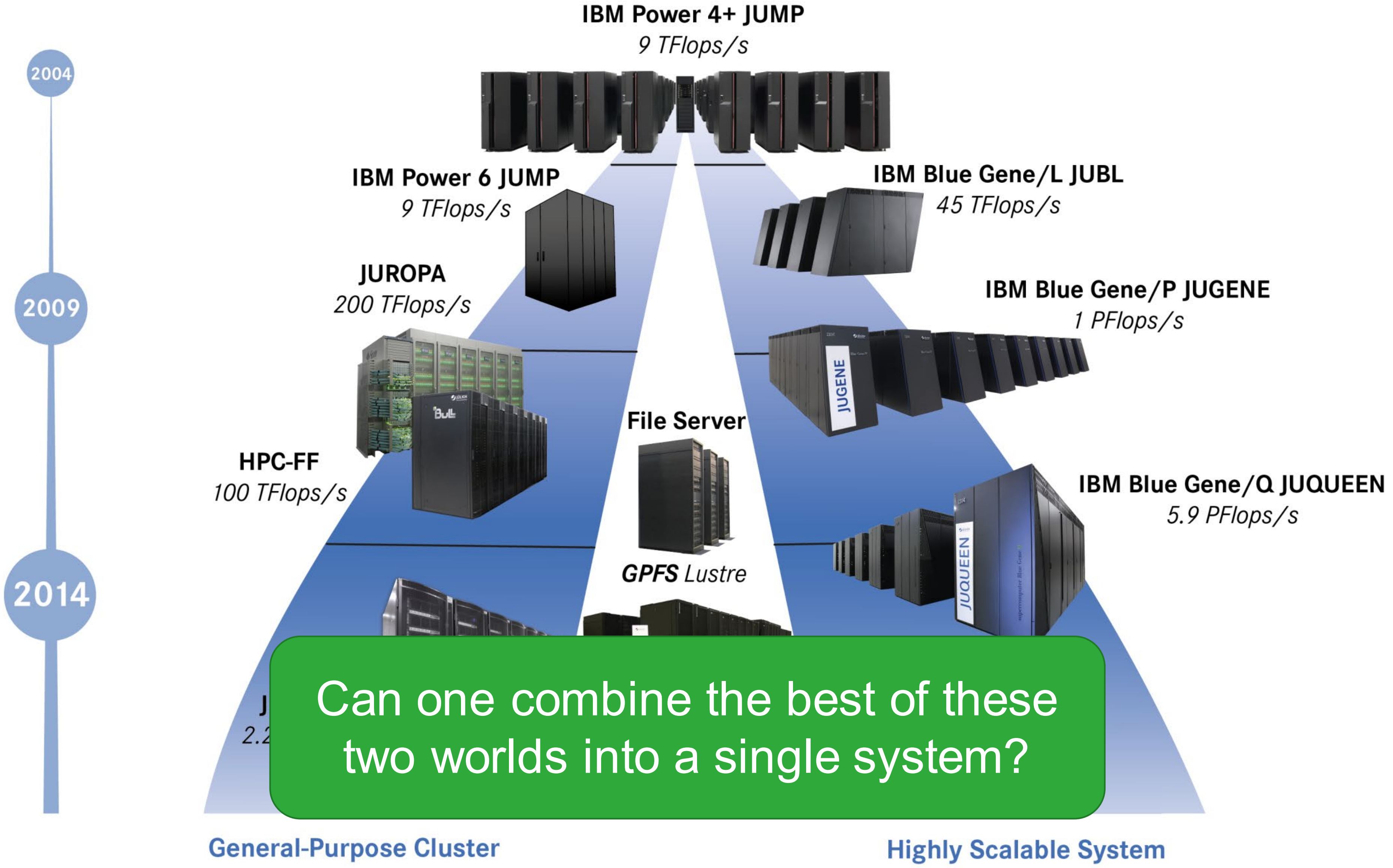
ADAC, 24.01.2022 I Estela Suarez (JSC)

OUTLINE

- **System architecture**
  - From dual architecture to the Modular Supercomputing Architecture (MSA)
  - Hardware implementations of MSA
- **Software**
  - Software stack
  - ParaStation Modulo
  - Scheduler
- **Application experience**
- **Conclusions and next steps**



JSC DUAL APPROACH



Can one combine the best of these two worlds into a single system?

THE DEEP PROJECTS

2011-2021: The DEEP projects

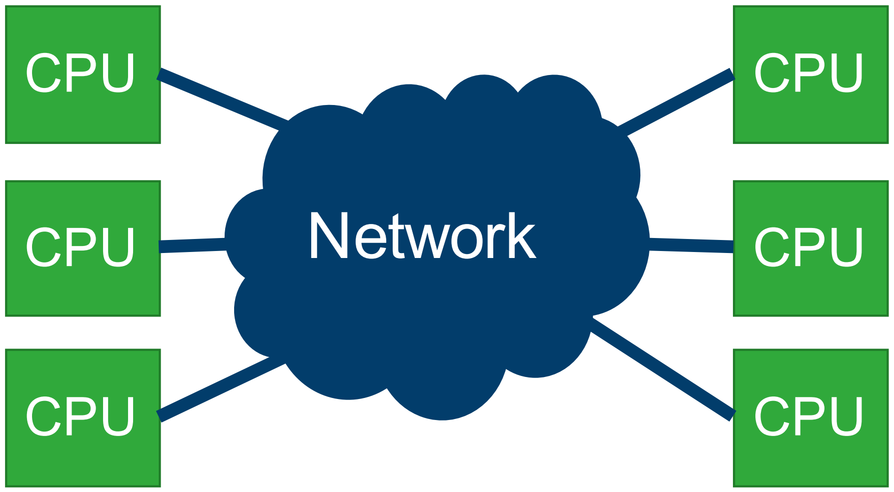
- **DEEP** (2011 – 2015)
  - Introduced Cluster-Booster architecture
- **DEEP-ER** (2013 – 2017)
  - Added I/O and resiliency functionalities
- **DEEP-EST** (2017 – 2021)
  - Modular Supercomputer Architecture

2021-2024 The SEA projects

- DEEP-SEA, IO-SEA, RED-SEA

HOMOGENEOUS

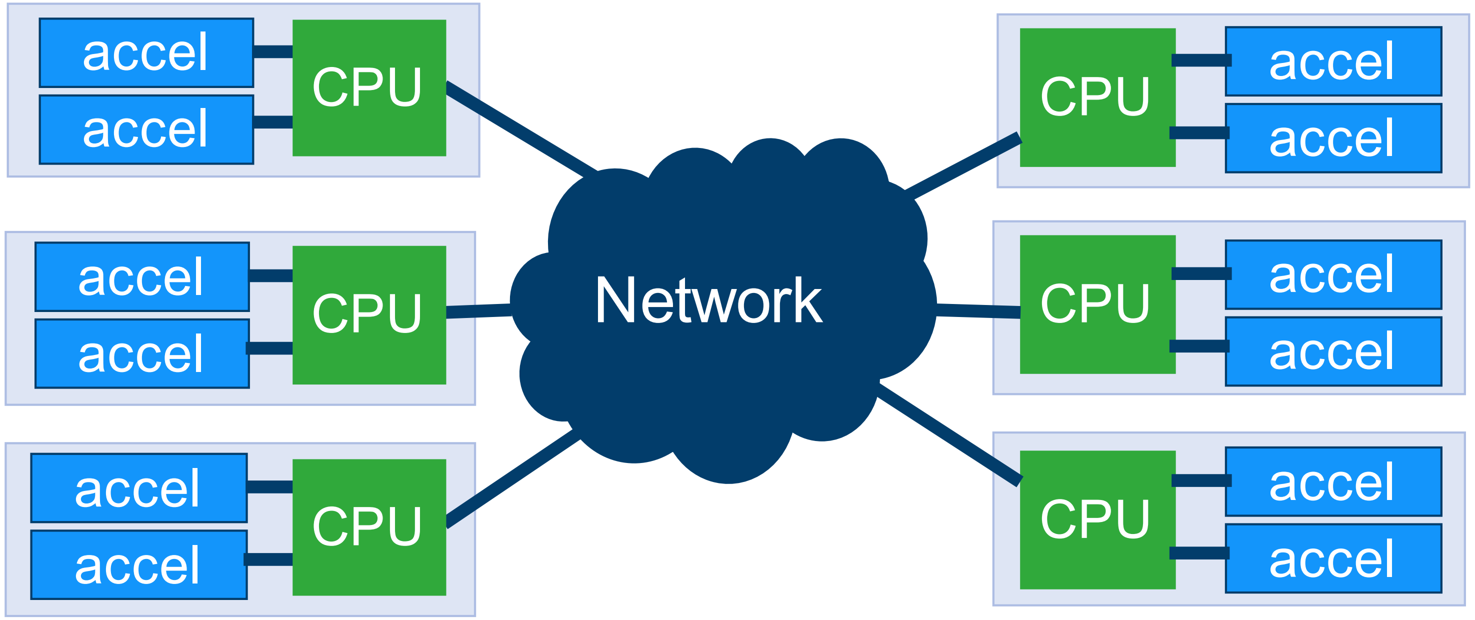
General Purpose Cluster



Nodes contain only CPUs

HETEROGENOUS MONOLITHIC

Every node contains accelerators (e.g. GPUs)

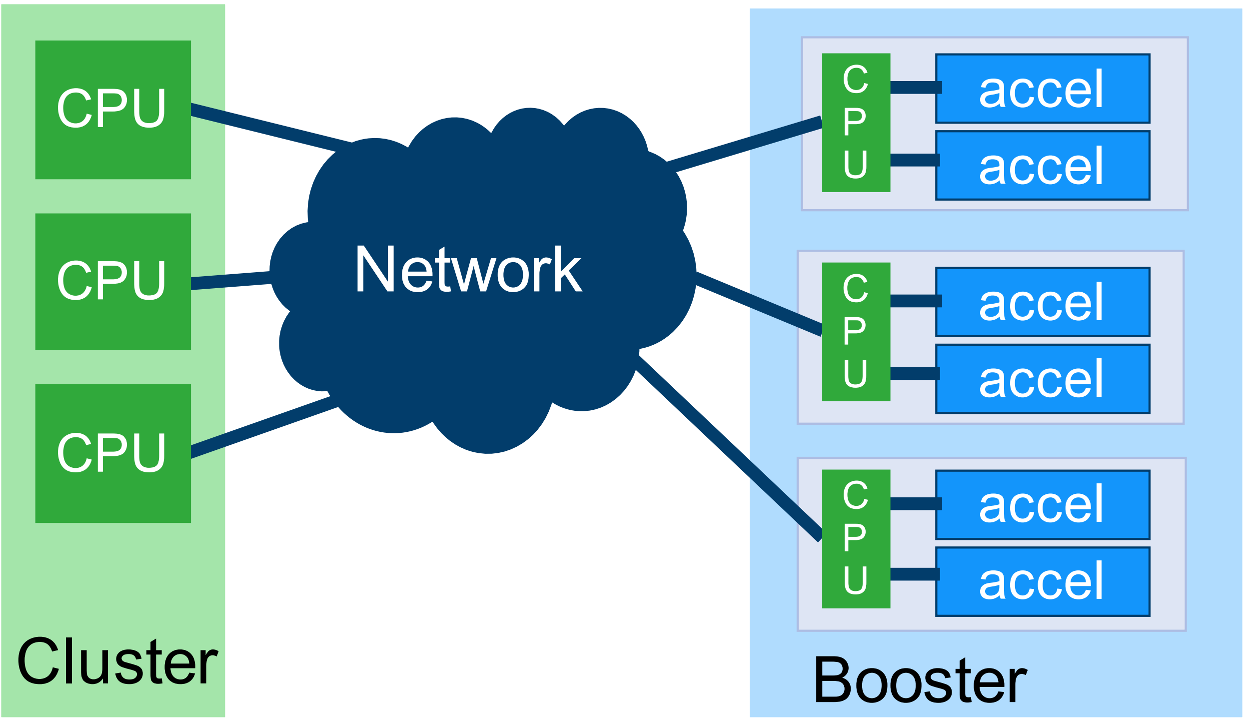


+: Energy efficient
+: Easy management
-: Static assignment of accelerators to CPUs
-: Difficult to efficiently share resources

- Every node contains CPU(s) and some accelerator
- All nodes are equal → "monolithic"

HETEROGENOUS MODULAR

Different nodes are grouped in “modules”



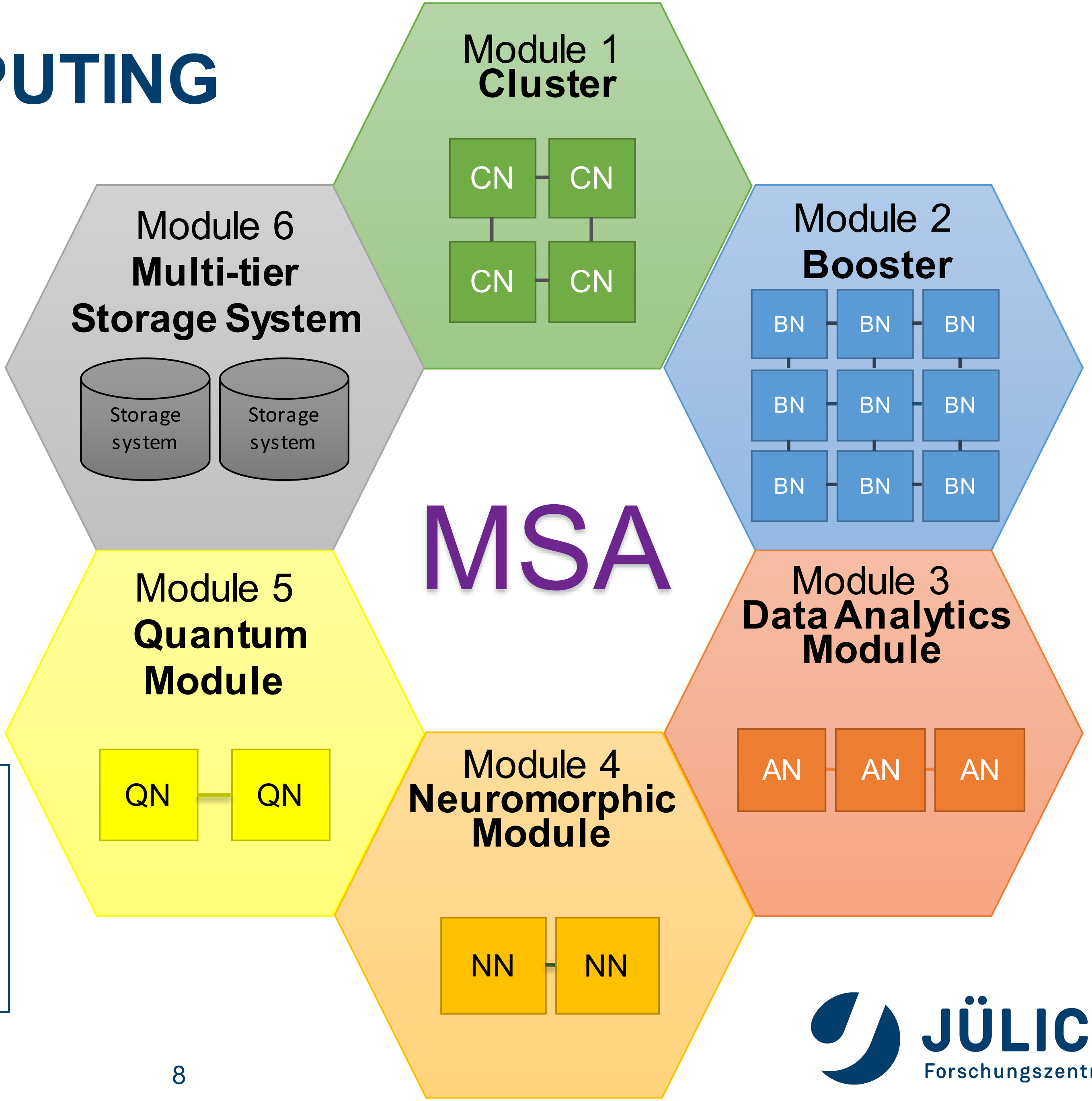
+: *Energy efficient*
+: *Better scalability*
+: *High flexibility*
+: *Dynamic resource assignment*
-: *Complexity*

- All nodes within one module are equal
- Different modules have different configurations → “modular”

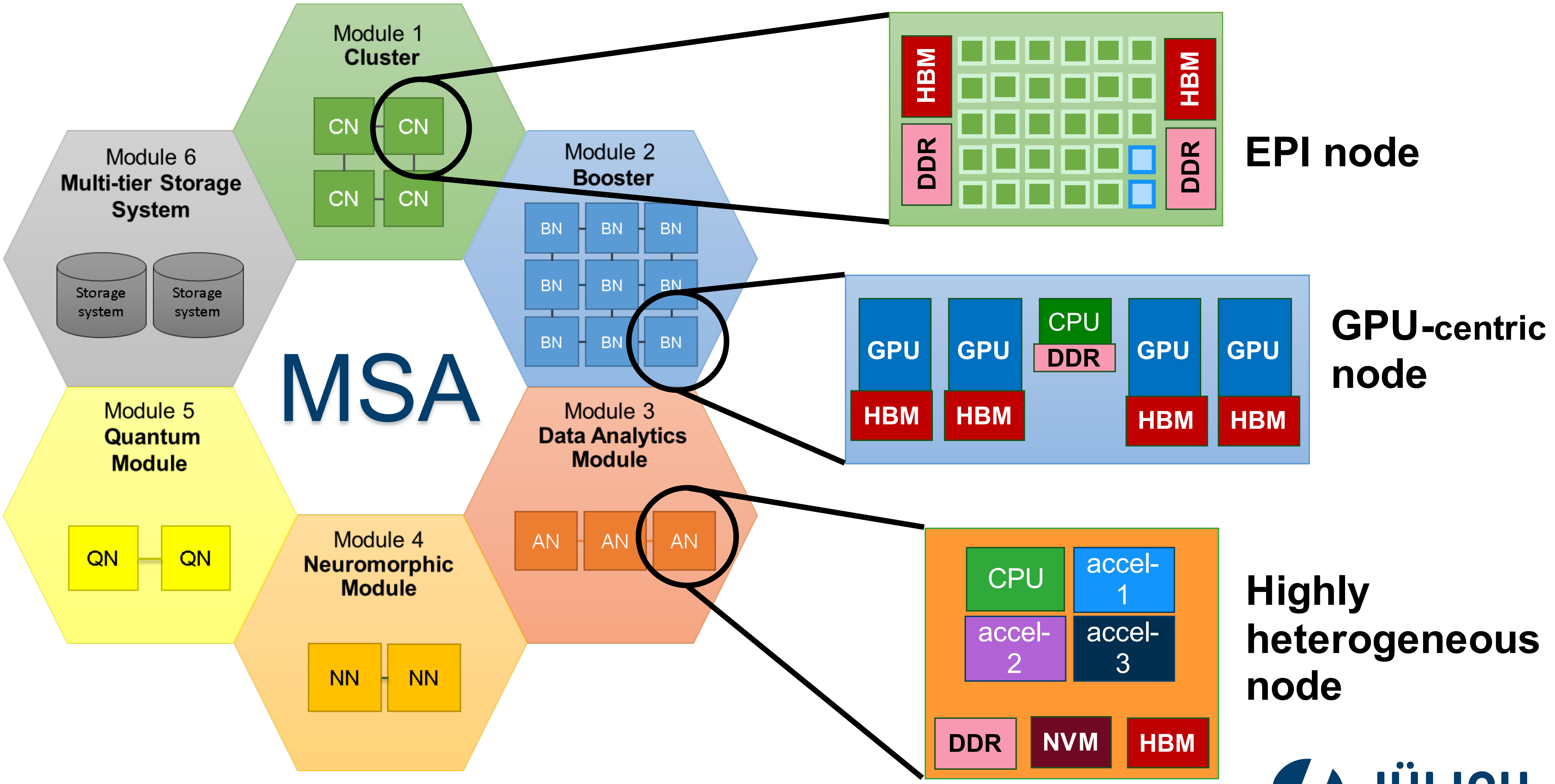
MODULAR SUPERCOMPUTING ARCHITECTURE

Composability of heterogeneous resources

- Cost-effective scaling



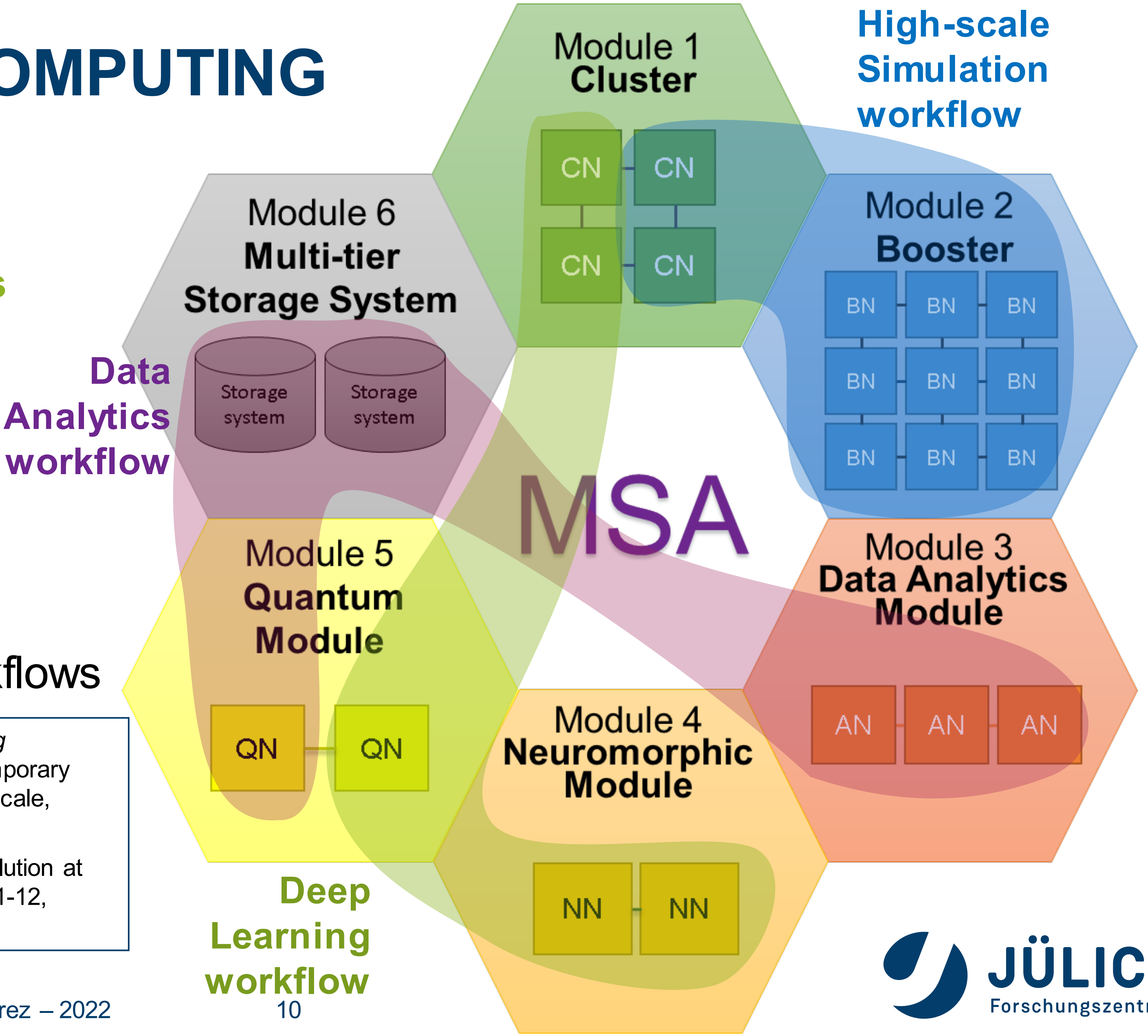
- **E. Suarez**, N. Eicker, Th. Lippert, "*Modular Supercomputing Architecture: from idea to production*", Chapter 9 in Contemporary High Performance Computing: from Petascale toward Exascale, Volume 3, p 223-251, CRC Press. (2019)
- **E. Suarez**, N. Eicker, and Th. Lippert, "Supercomputer Evolution at JSC", Proceedings of the 2018 NIC Symposium, Vol.49, p.1-12, (2018)


Module 1
Cluster
CN
CN
CN
CN
Module 2
Booster
BN
BN
BN
BN
BN
BN
BN
BN
BN
Module 3
Data Analytics
Module
AN
AN
AN
Module 4
Neuromorphic
Module
NN
NN
Module 5
Quantum
Module
QN
QN
Module 6
Multi-tier Storage
System
Storage system
Storage system
MSA
HBM
DDR
HBM
DDR
EPI node
GPU
GPU
CPU
DDR
GPU
GPU
HBM
HBM
HBM
HBM
GPU-centric node
CPU
accel-1
accel-2
accel-3
DDR
NVM
HBM
Highly heterogeneous node

MODULAR SUPERCOMPUTING ARCHITECTURE

Composability of heterogeneous resources

- Cost-effective scaling
- Effective resource-sharing
- Match application diversity
  - Large-scale, complex workflows



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THE HARDWARE PROTOTYPES

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2015

DEEP Prototype
128 Xeon + 284 KNC nodes
InfiniBand + 1.5Gbit Extoll
550 TFlop/s

2016

DEEP-ER Prototype
16 Xeon + 8 KNL nodes
100Gbit Extoll
40 TFlop/s

2020

DEEP-EST Prototype
55 Cluster + 75 Booster + 16 Data Analytics
100 Gbit Extoll + InfiniBand + Eth
800 TFlop/s

MODULAR SUPERCOMPUTER JUWELS

Entry in Nov’20

JUWELS Cluster #44

Intel Xeon (Skylake) processor

InfiniBand EDR network

2,500 compute nodes

10 PFLOP/s peak (CPU-based)

JUWELS Booster #7

Entry in Nov’20

AMD EPYC Rome 7402 processor

3,700 NVIDIA A100 GPUs

InfiniBand HDR DragonFly+

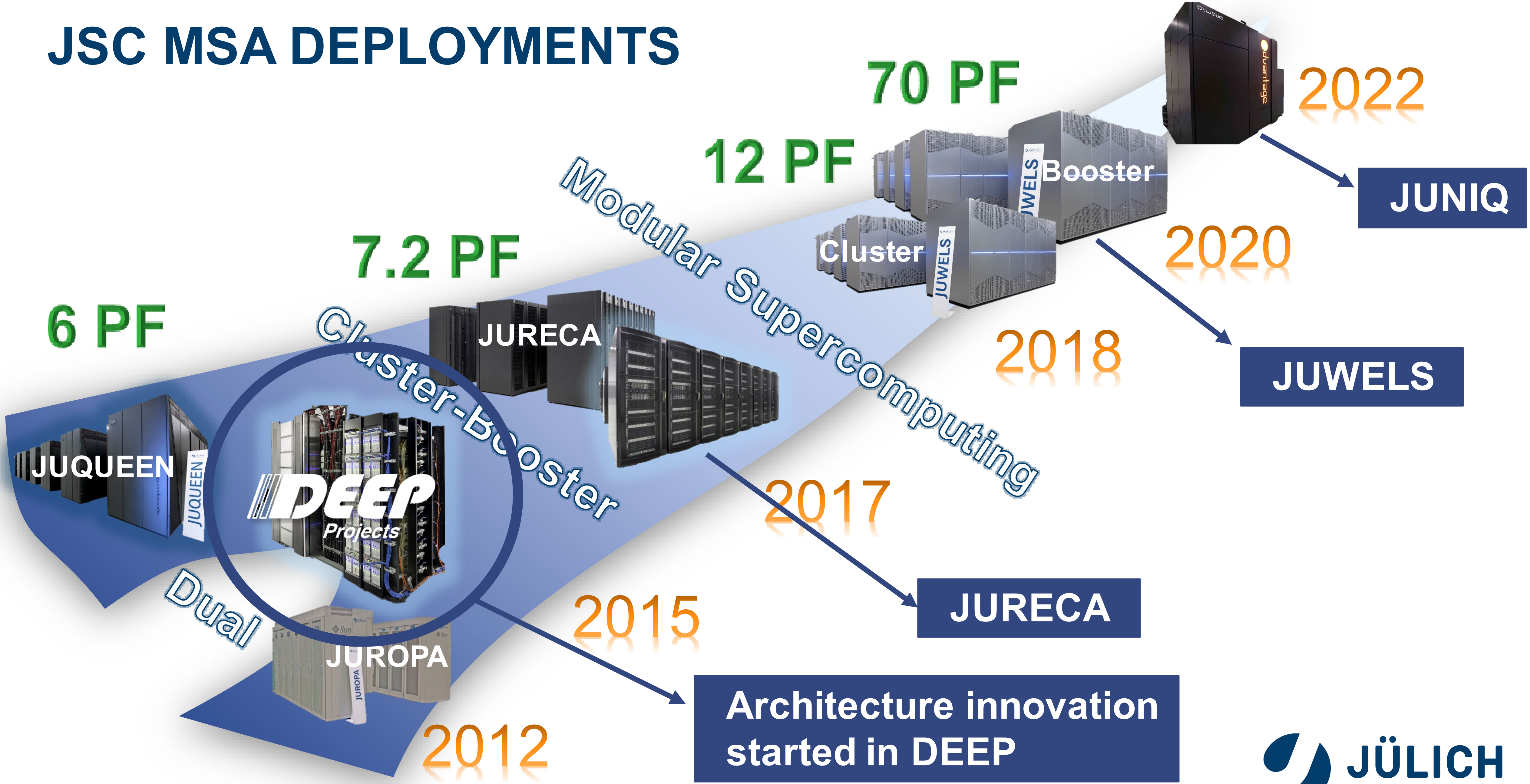
70 PFLOP/s peak (GPU-based)

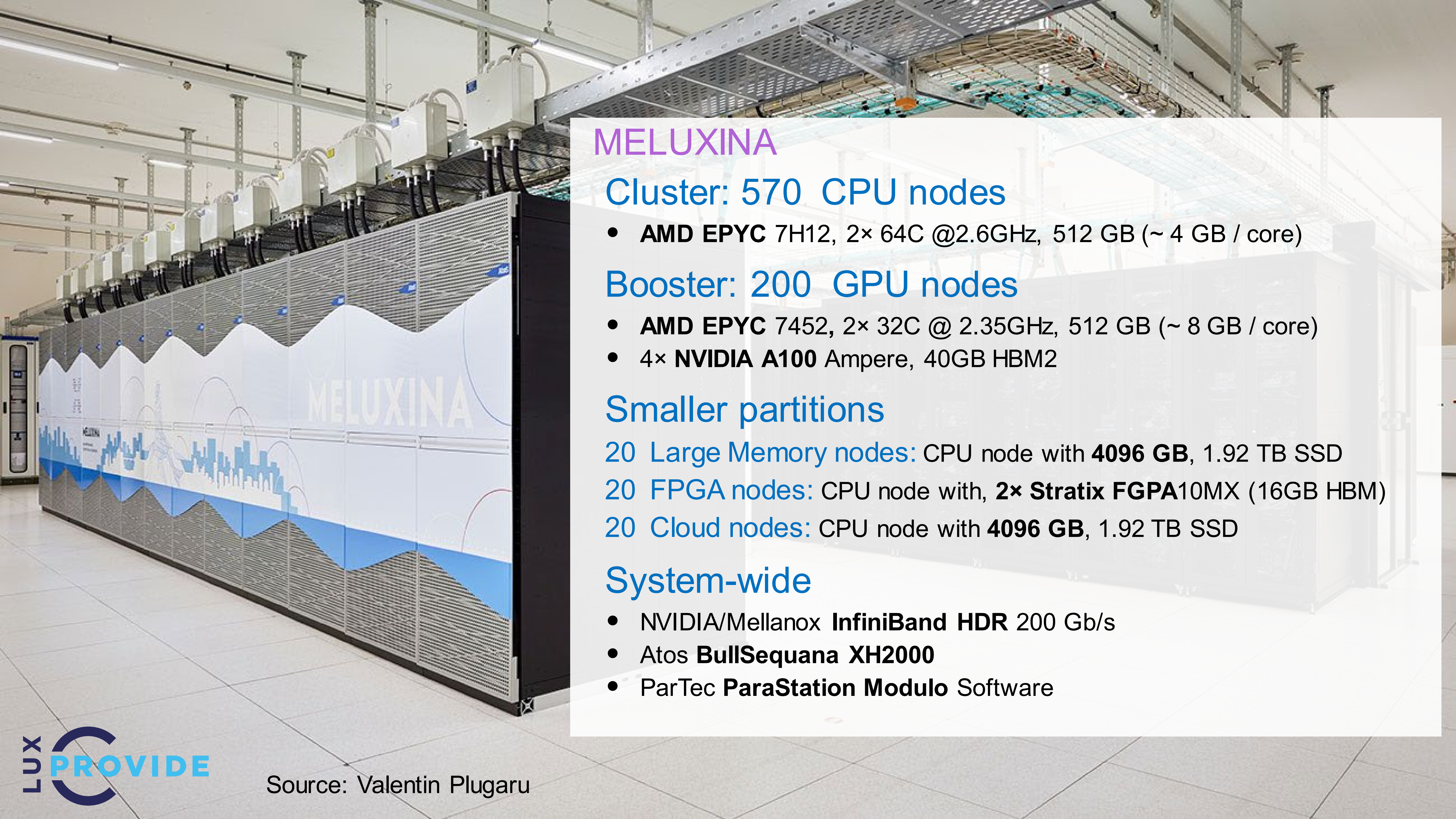
TOP500:	Rank 7 World Rank 1 Europe
Green500:	Rank 1 in TOP250
TOP5 AI:	Rank 4 (3 in 2021)

JUWELS is designed for simulation and large-scale machine learning

Funded through SiVeGCS (BMBF, MWK-NRW)

JSC MSA DEPLOYMENTS





MELUXINA

Cluster: 570 CPU nodes

- **AMD EPYC** 7H12, 2× 64C @2.6GHz, 512 GB (~ 4 GB / core)

Booster: 200 GPU nodes

- **AMD EPYC** 7452, 2× 32C @ 2.35GHz, 512 GB (~ 8 GB / core)
- 4× **NVIDIA A100** Ampere, 40GB HBM2

Smaller partitions

20 Large Memory nodes: CPU node with **4096 GB**, 1.92 TB SSD

20 FPGA nodes: CPU node with, **2× Stratix FGPA**10MX (16GB HBM)

20 Cloud nodes: CPU node with **4096 GB**, 1.92 TB SSD

System-wide

- NVIDIA/Mellanox **InfiniBand HDR** 200 Gb/s
- Atos **BullSequana XH2000**
- ParTec **ParaStation Modulo** Software

LUX PROVIDE

Source: Valentin Plugaru

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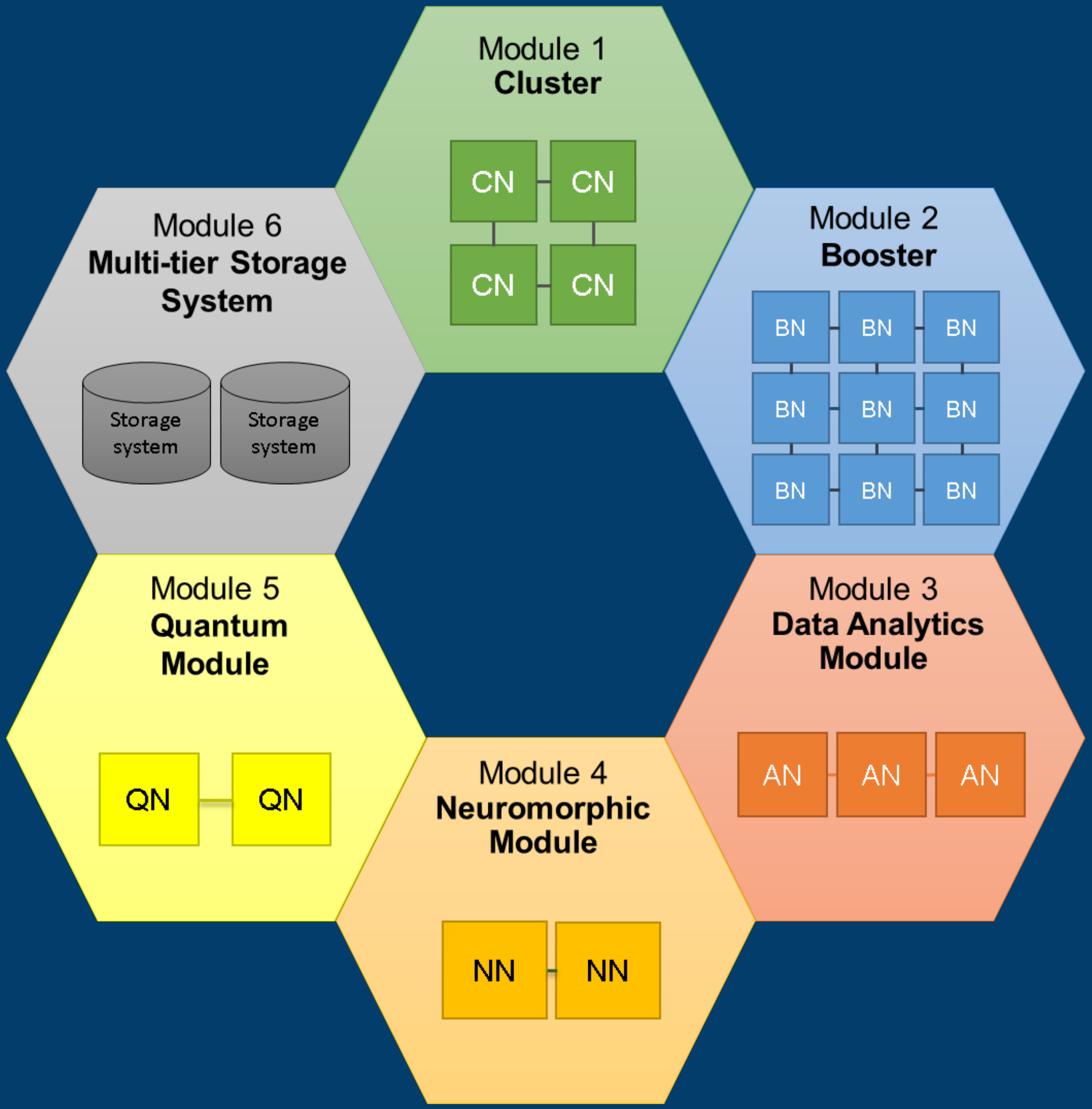
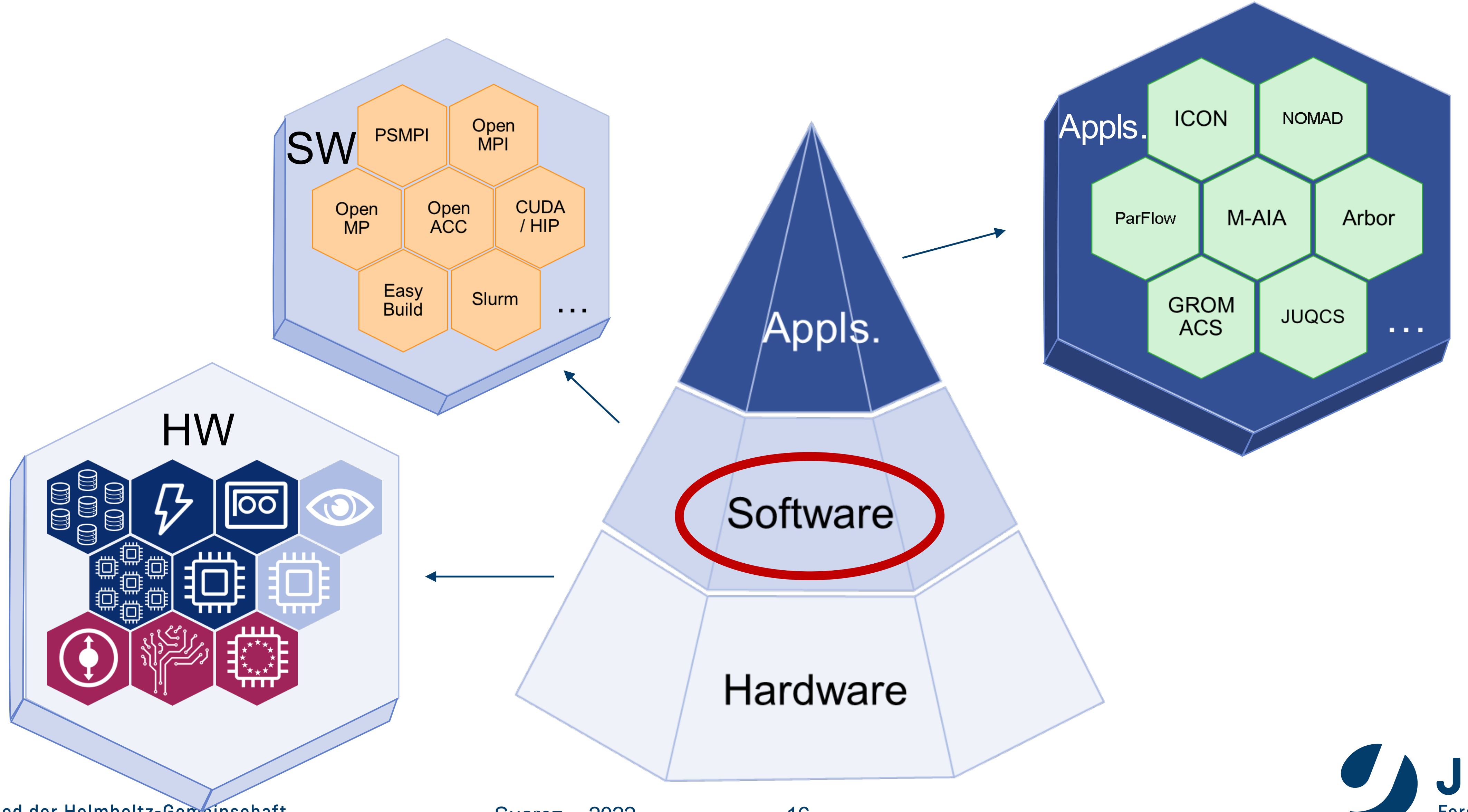


MATCHING APPLICATIONS AND HARDWARE



SOFTWARE ENVIRONMENT

- **Low-level SW:** Inter-network bridging
- **Scheduler**: Slurm, psslurm (ParaStation Modulo)
- **Filesystem**: BeeGFS, GPFS
- **Compilers**: Intel, GCC, NVIDIA HPC SDK
- **Debuggers**: Intel Inspector, TotalView
- **Programming**: ParaStation MPI, OpenMP, OmpSs, CUDA
- **Performance analysis tools**: Scalasca, Score-P Extrae/Paraver, Vampir, Intel Advisor, VTune…
- **Benchmarking tools**: JUBE
- **I/O Libraries**: SIONlib, SCR, HDF5,…

- **Eicker et al.**, *Bridging the DEEP Gap - Implementation of an Efficient Forwarding Protocol*, Intel European Exascale Labs - Report 2013 34-41
- **Clauss et al.**, *Dynamic Process Management with Allocation-internal Co-Scheduling towards Interactive Supercomputing*, COSH@HiPEAC,(2016)

ParaStation Modulo

ParaStation MODULO

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

ParTec Modular Supercomputing

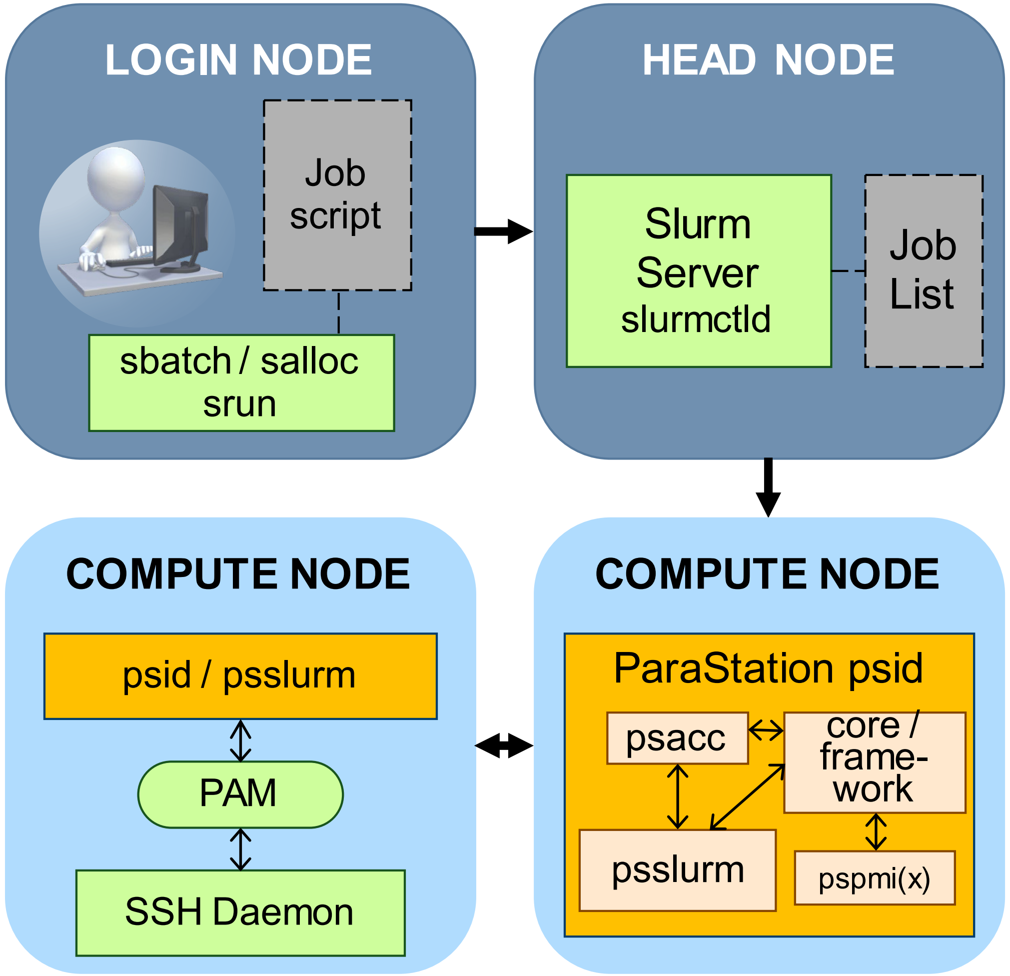
Source: Thomas Moschny

JÜLICH Forschungszentrum

ParaStation Process Manager

ParaStation MODULO

- **Scalable network of process management daemons**
  - Process startup and control, I/O forwarding, …
  - Precise resource monitoring
  - Proper cleanup after jobs
  - Daemons run on the compute nodes
- **psslurm: full integration with Slurm**
  - Plugin to ParaStation Management
  - Reduce number of daemons on compute nodes
    - Replace node-local Slurm daemon
  - Integration with ParaStation HealthChecker
  - Possible to fix problems and add unique features



ParTec Modular Supercomputing

Source: Thomas Moschny

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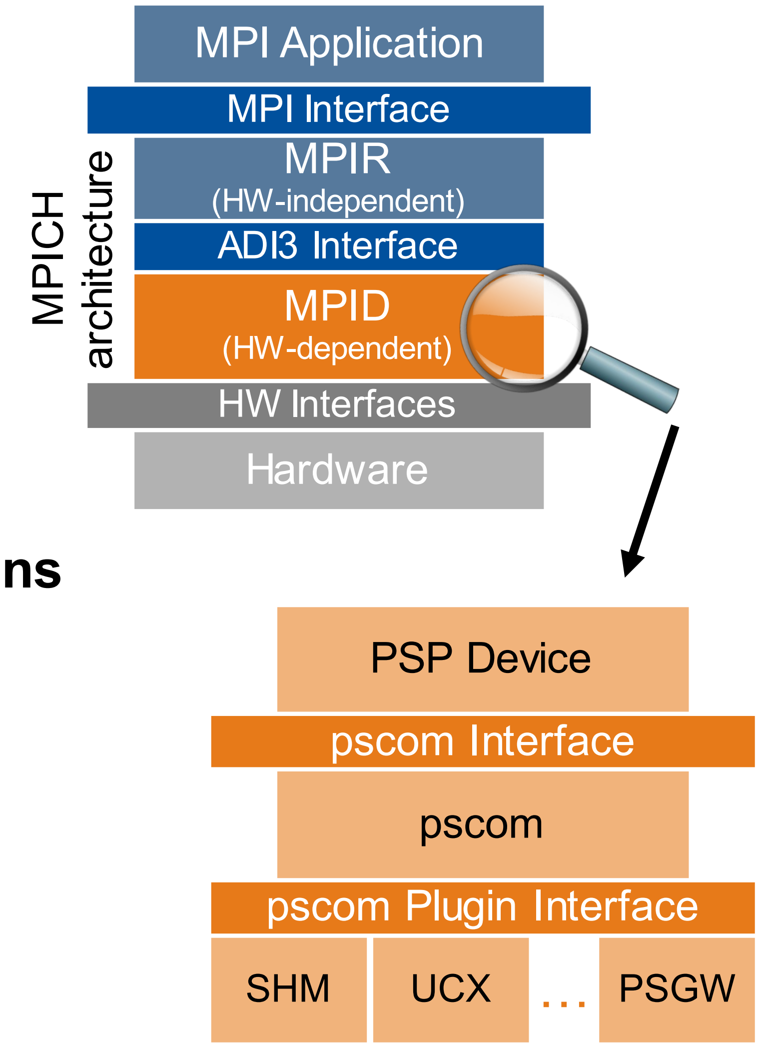
ParaStation MPI Library

- **Based on MPICH 3.4.2** (MPI-3.1 compliant)
  - Supports MPICH tools (tracing, debugging, …)
  - MPICH layers beneath ADI3 replaced by ParaStation PSP Device
  - Powered by pscom low-level communication library
  - Maintains MPICH ABI compatibility
- **Support for various transports and protocols via pscom plugins**
  - Support for InfiniBand, Omni-Path, Extoll, (soon BXI)
  - Multiple transports / plugins can be used concurrently
  - Gateway capability via PSGW plugin
  - CUDA awareness via GPUDirect
- **Proven scaling up to ~3,500 nodes and ~140,000 procs. / job**



Source: Thomas Moschny

ParaStation Global MPI for MSA

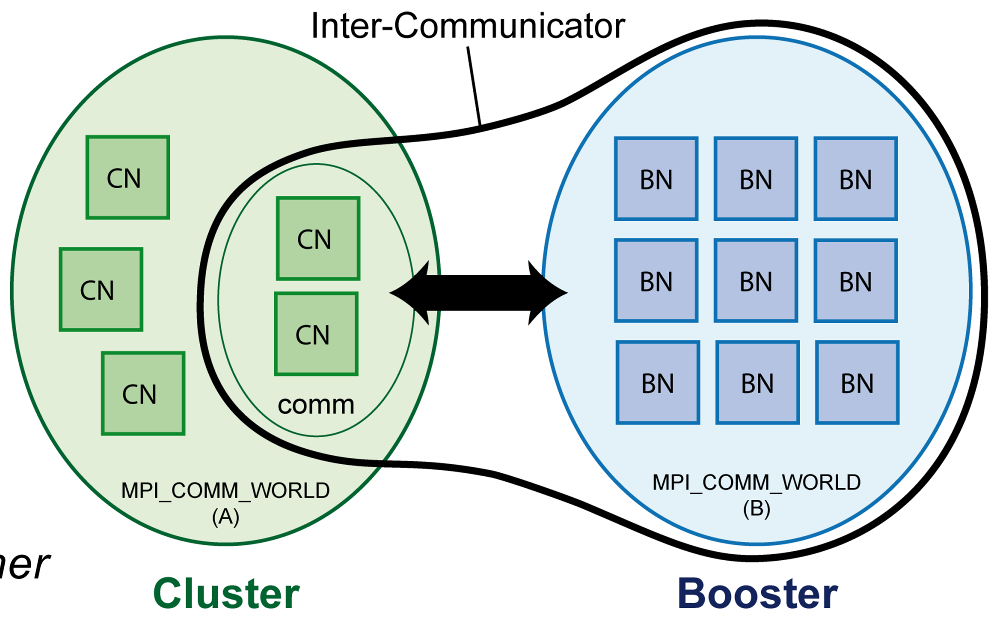
ParaStation MPI

- An MPI application can run:
  - Using only Cluster nodes
  - Using only Booster nodes
  - Distributed over Cluster and Booster
    - *In this case two executables are created*
    - *Collective offload process*
    - *Transparent data exchange via MPI*

- ParaStation Global MPI
  - Uses **`MPI_Comm_spawn()`**
    - *Collective spawn groups of processes from Cluster to Booster (or vice-versa)*
  - Inter-communicator
    - *Connects the 2 MPI_COMM_WORLD*
    - *Contains all parents on one side and all children on the other*
      - *Returned by MPI_Comm_spawn for the parents*
      - *Returned by MPI_Get_parent by the children*

- One can also start two parts of a code and connect them via **`MPI_Connect()`**

- Or have one single common **`MPI_COMM_WORLD`** and split it into subcommunicators via **`MPI_Comm_Split()`**



- **Clauss et al.**, *Dynamic Process Management with Allocation-internal Co-Scheduling towards Interactive Supercomputing*, COSH@HiPEAC, (2016)

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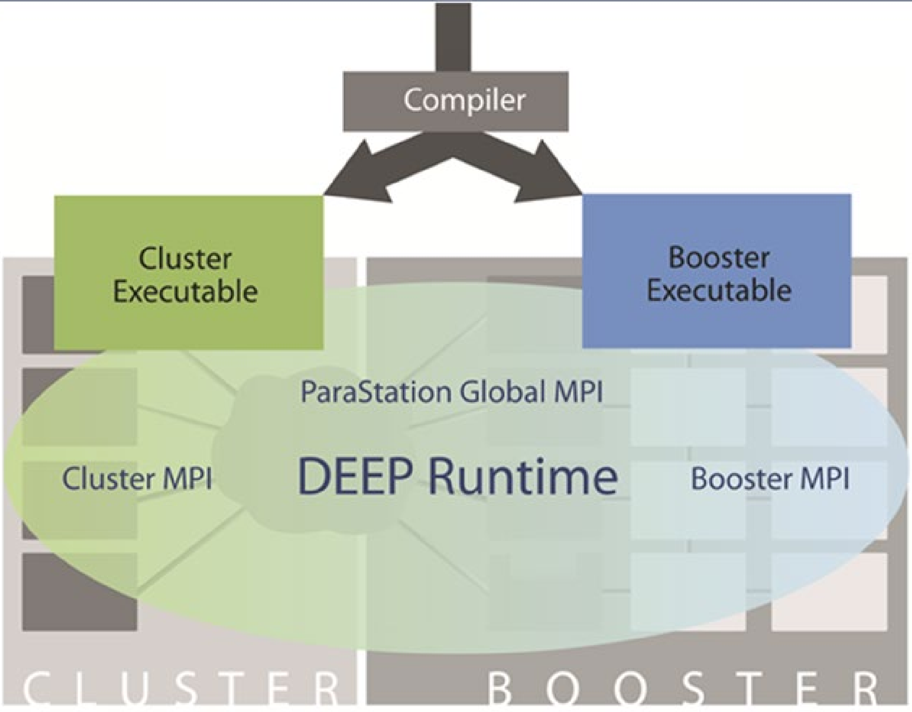
COMPILE AND RUN

- **Compilation**
  - Creates two executables (if different CPU architecture)
    - One for `CLUSTER` code
    - One for `BOOSTER` code
- **Batch system**
  - Reserves required resources
- **Execution**
  - Script starts Booster code
  - This code calls `MPI_Comm_spawn()` with Cluster executable
  - Optional: **xenv** to load suitable environment modules
- **Runtime + Scheduler + FS**
  - Detect ParaStation MPI calls
  - Distribute child binaries

```
salloc --partition=cluster -N 4
       : --partition=booster -N 12
srun --het-group=1 -N 4 -n 8
       ./app_booster
```

```
int main (int argc, char *argv[]){
   /* ... */
   MPI_Comm_spawn("./xPic.Cluster", &argv[1],
      nproc, MPI_INFO_NULL, 0, GRID_COMM_WORLD,
      INTERCOMM, MPI_ERRCODES_IGNORE);
   /* ... */
}
```



Heterogeneity from user's PoV

ParaStation MPI

- **Slurm supports the ability to submit heterogeneous jobs** (since v 17.11)
  - form **job pack (het-job)** allocation using colon notation for salloc, sbatch, srun
  - even allowing different executables

```
$ srun  -N 1 -p part1 ./first \
        : -N 2 -p part 2 ./second
```

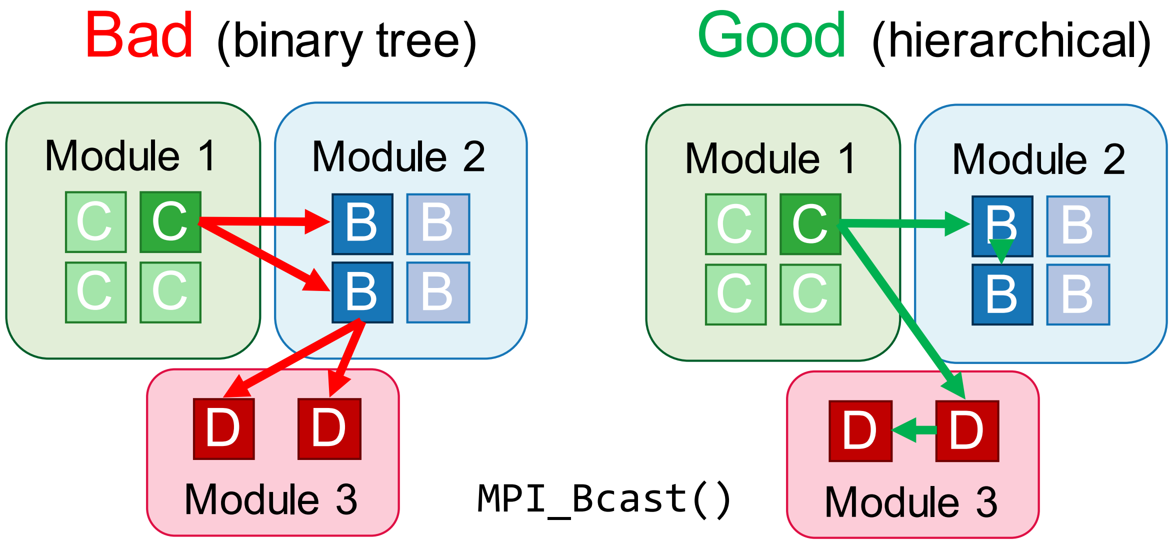
- **Full support for job packs in ParaStation psslurm**, with **unique features** for modular jobs:
  - Support for heterogeneous jobs with common MPI_COMM_WORLD
  - For each job in the job pack, resources can be specified individually
  - Support global resources (e.g. gateways): psgw plugin to psmgmt + spank plugin
    - Compensates for Slurm's inability to handle global resources
    - Extends salloc, srun and sbatch
- **Modular here means: Jobs across heterogeneous hardware**
  - Either with a common MPI_COMM_WORLD, or with separated / interconnected MPI_COMM_WORLDS

Explicit MSA-extensions to ParaStation MPI

- **API additions to retrieve topology information**
  - Querying the module ID: `MPI_Info_get (MPI_INFO_ENV, "msa_module_id", …, value, …);`
  - Splitting communicators according to the topology:

```
MPI_Comm_split_type (oldcomm, MPIX_COMM_TYPE_MODULE, …, &newcomm);
```

- **Modularity-aware MPI collectives**
  - Optimized patterns for collectives that take **topology** of the MSA system into account
  - Assumption: Inter-module communication is the bottleneck
  - Dynamic updates of the communication patterns supported, e.g. for malleable jobs (experimental)

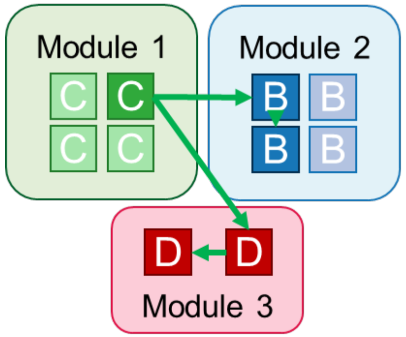


Source: Thomas Moschny

Hiearchical collectives (MSA awareness)

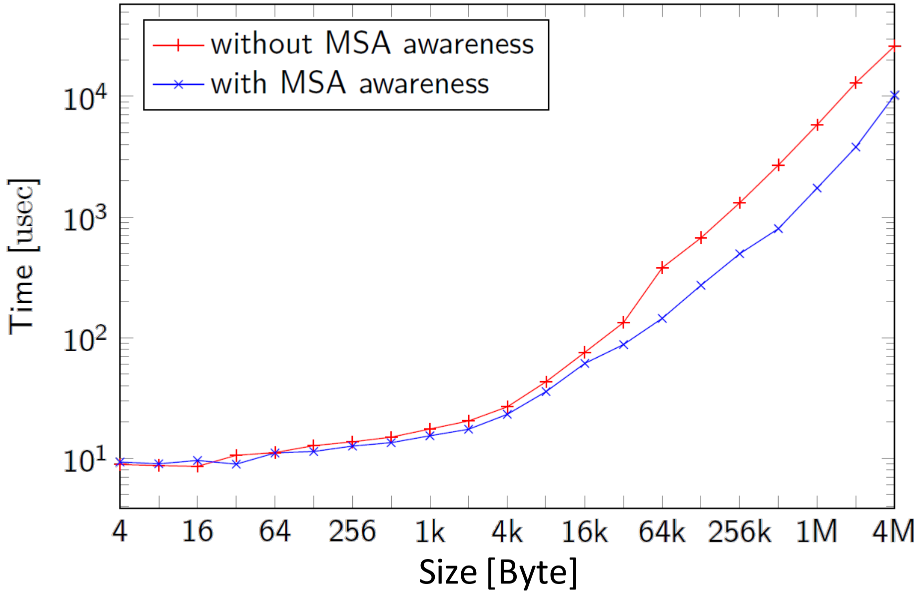
- **General rules to optimize collectives →** execute these steps in order:
  - **1)** Do all **module-internal** gathering and/or reduction operations (if required)
  - **2)** Conduct the **inter-module operation** with a **single process per module**
  - **3)** Perform a strict **module-local data distribution**

Good (hierarchical)



- **Multi-level hierarchy awareness**
  - **Apply this set of rules recursively**, i.e., node level, module level, system level

- **Performance heavily depends on concrete settings**, i.e.:
  - Number of processes / gateway nodes
  - Distribution of the ranks in the communicator
  - Message sizes (and hence the collective communication pattern)

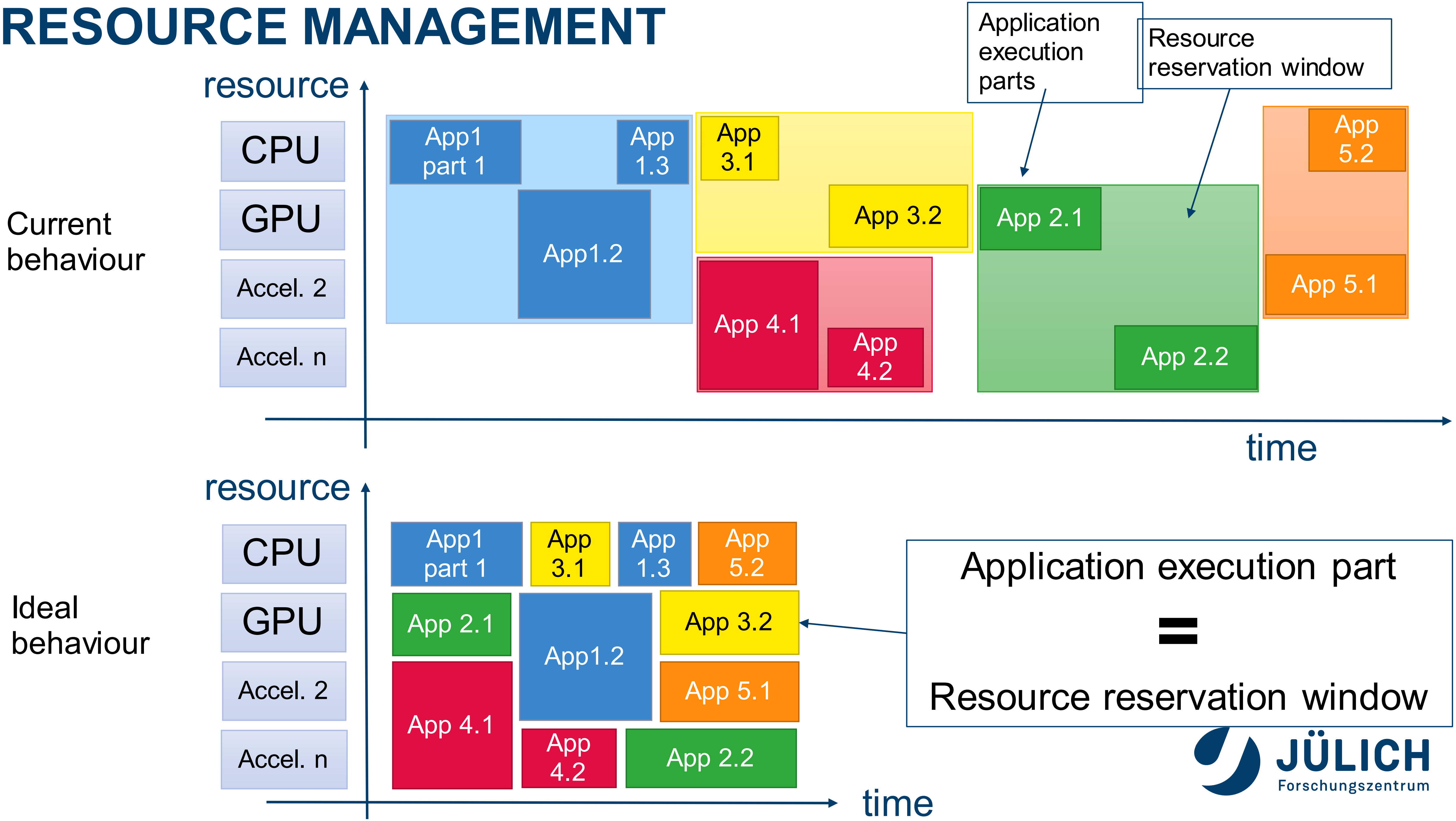


IMB MPI Benchmarks

Allreduce with 8 (CN) + 8 (DAM) nodes, 8 processes per node, and 1 Gateway node

Source: Thomas Moschny

RESOURCE MANAGEMENT



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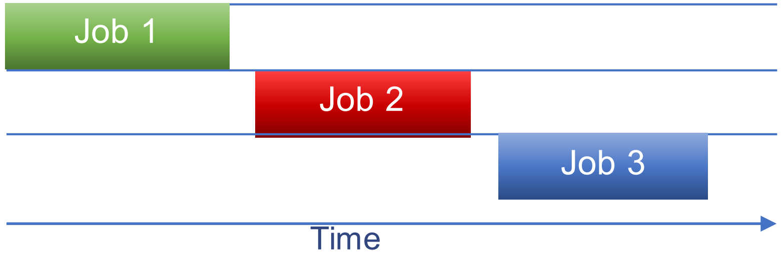
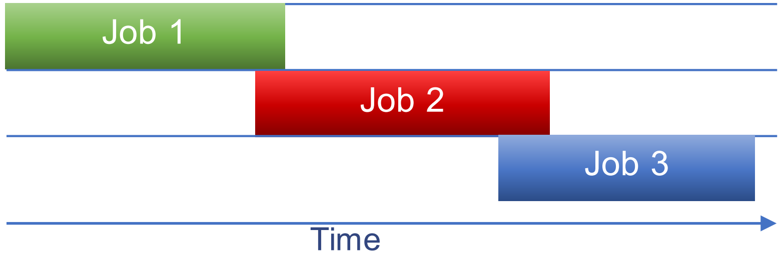
Improved Workflow Support (experimental)

- New parameter `--delay` introduced in sbatch command for job packs
  - Amount of time, the next job should wait after start of the first job in a job pack



Typical Workflow supported by Slurm

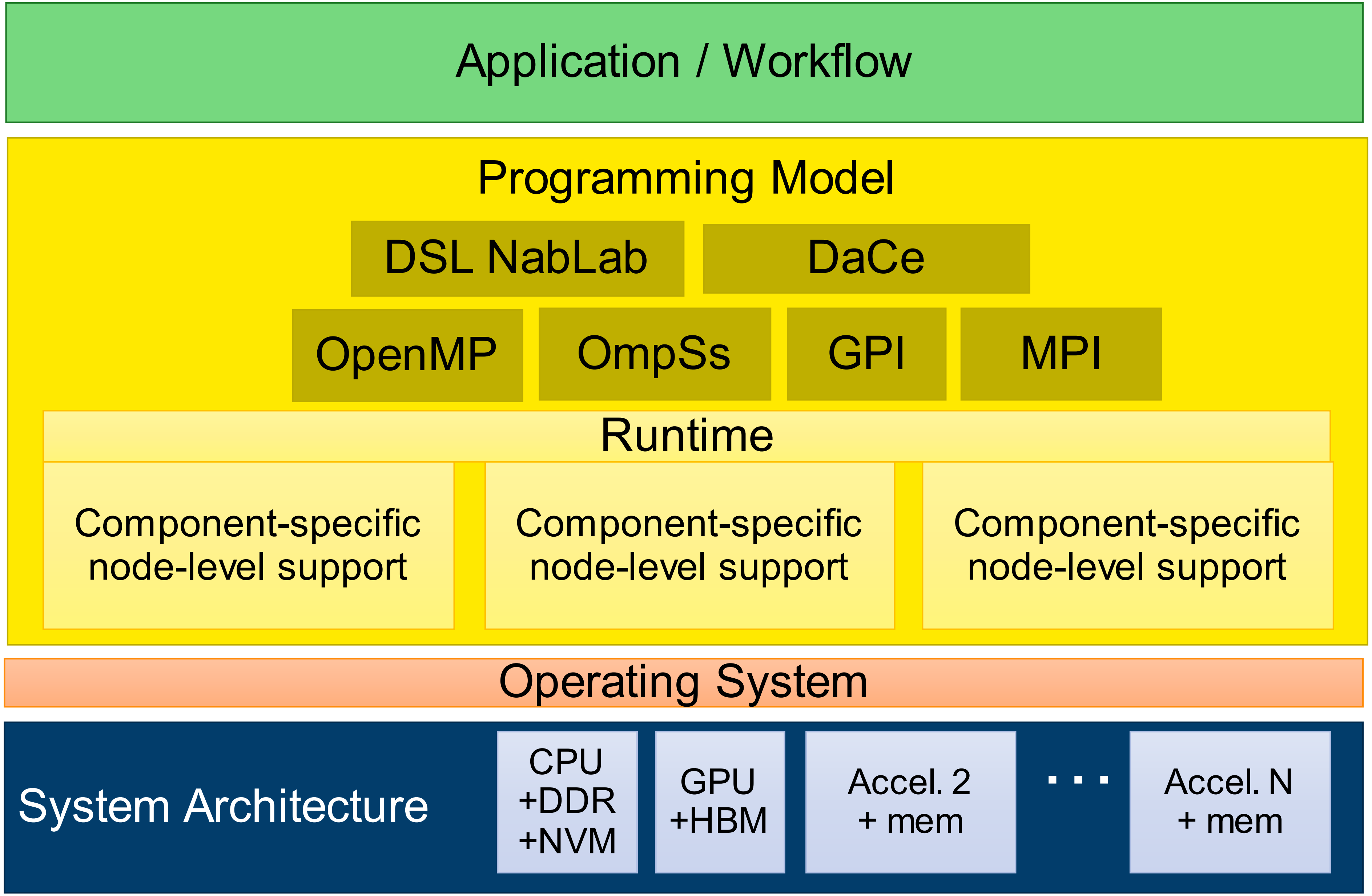
- **Goal**: Overlapping job execution
  - Currently not supported by Slurm
    - Whole job pack either accepted or rejected
    - All jobs allocated and run in parallel
    - All jobs wait for allocation if any of the jobs can not be allocated at the moment



Workflow we are trying to achieve

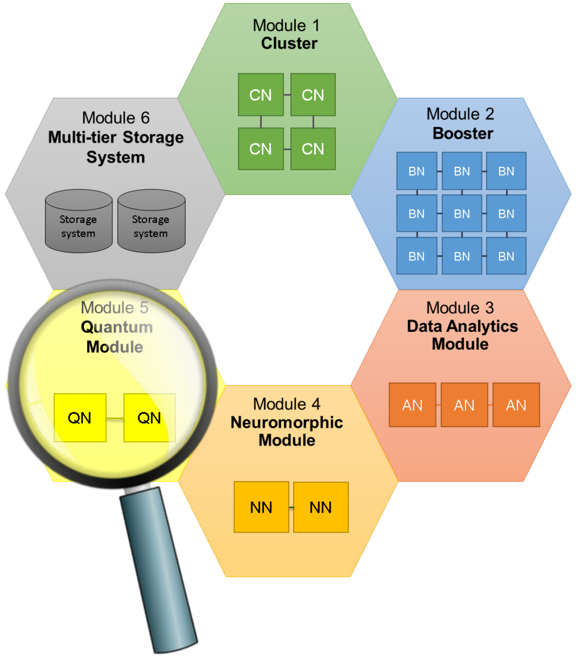
EXTENDING THE SOFTWARE STACK

- **Support for accelerators & memory**
- **Malleability**
- **Interoperability**
- **Composability**
- **Performance portability**
- **Resiliency**



Quantum integration in MSA

- **New usage models**
  - Tightly coupled simulations: benefit from efficient data exchange
  - Hybrid quantum-HPC simulations: combining quantum and classical algorithms
  - Workflows comprising stages on the QPU, with pre- and post-processing on HPC modules
- **Integrate QPU and its front-end into the managements stack**
  - Low-latency connection to other modules via federated, high-speed network
  - Unified environment: Integrated in the user-, SW-, schedule- and resource- mgmt.
    - Provide “direct” access of the QPU via a web-based portal
    - Redirect portal requests through the global scheduler/resource manager
    - Pseudo-shared usage model as prerequisite
- **Exact requirements depend on the use case and are subject to research**



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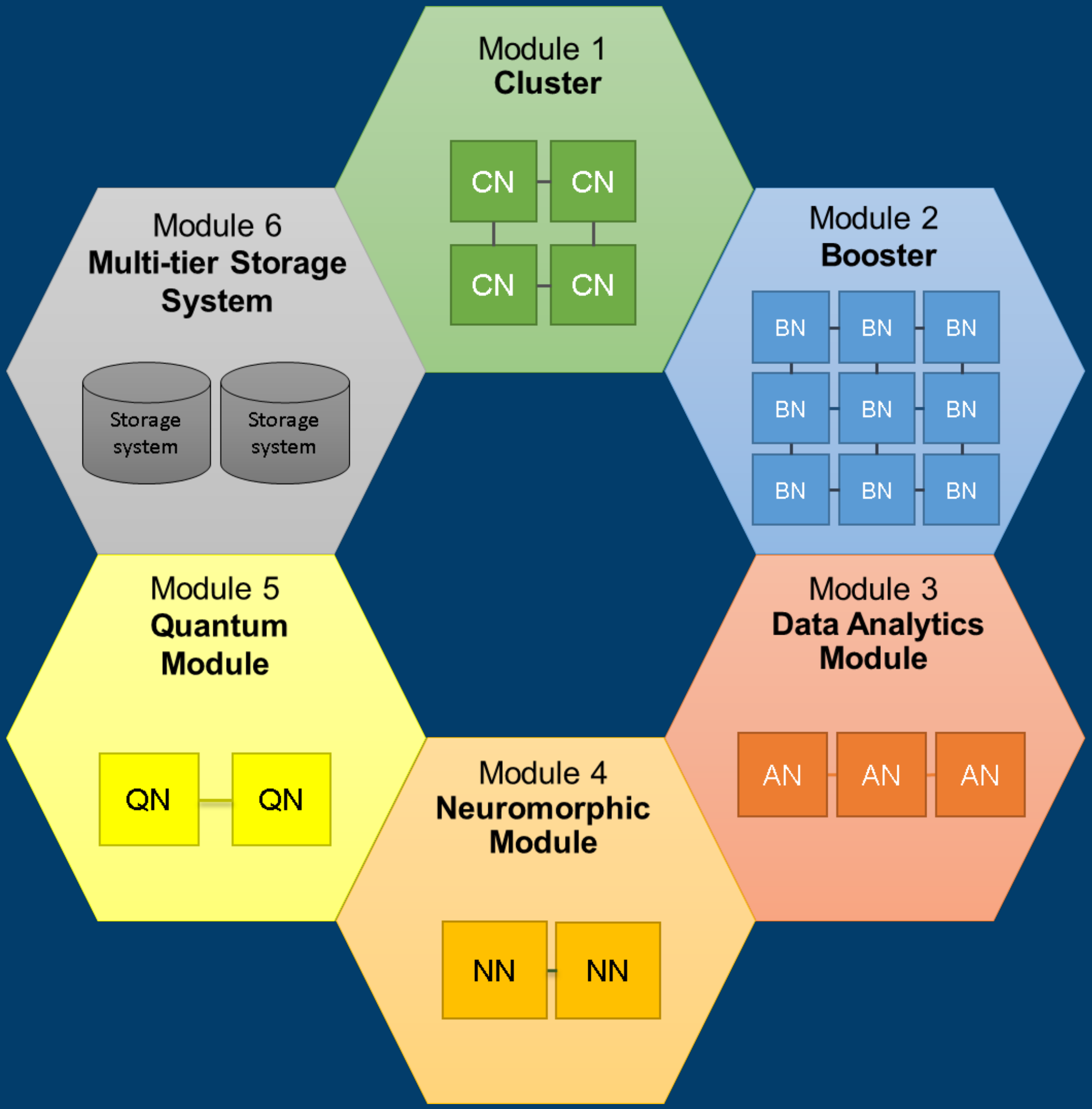
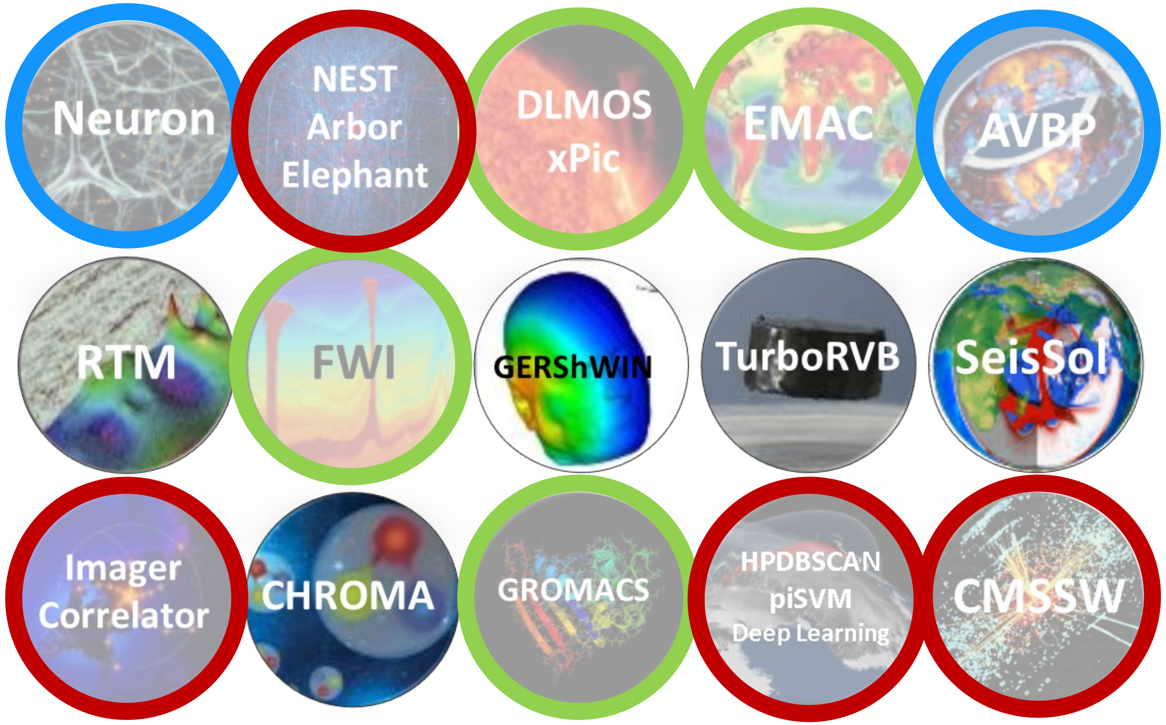


Architecture Use-Modes



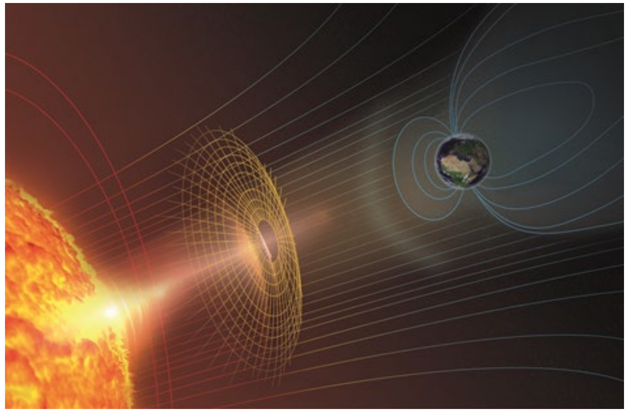
Cluster-Booster
use mode

Code partition
Workflow
I/O forward

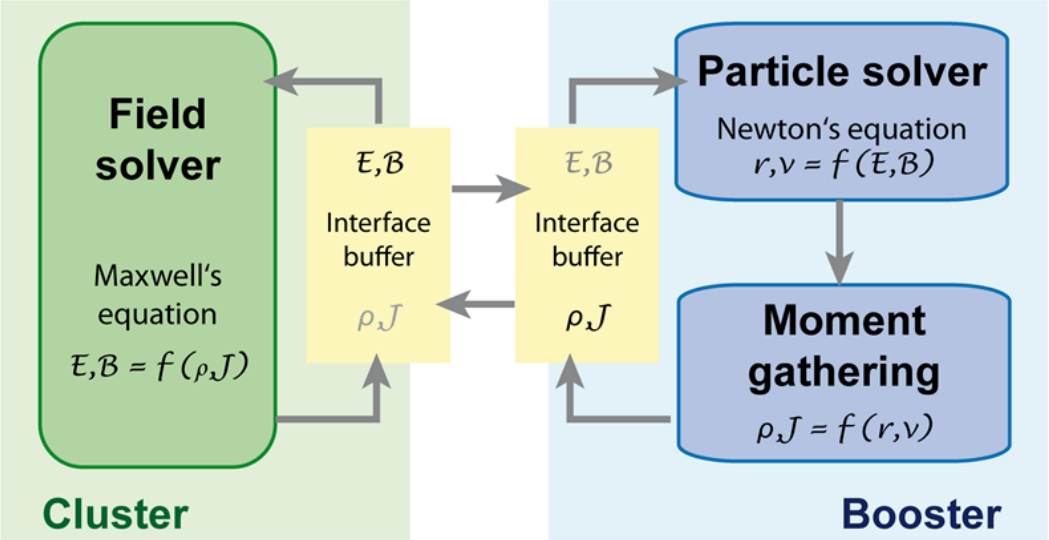
- **Kreuzer, et al.,** *Application Performance on a Cluster-Booster System.* IPDPSW – HCW (2018) [10.1109/IPDPSW.2018.00019]
- **Kreuzer et al.** *The DEEP-ER project: I/O and resiliency extensions for the Cluster-Booster architecture.* HPCC'18 proceedings (*2018)* [10.1109/HPCC/SmartCity/DSS.2018.00046]
- Wolf et al., *PIC algorithms on DEEP: The iPiC3D case study*. PARS-Mitteilungen 32, 38-48 (2015)
- Christou et al., *EMAC on DEEP*, Geoscientific model devel.(2016) [10.5194/gmd-9-3483-2016]
- Kumbhar et al., *Leveraging a Cluster-Booster Architecture for Brain-Scale Simulations*, Lecture Notes in Computer Science 9697 (2016) [10.1007/978-3-319-41321-1_19]
- Leger et al., *Adapting a Finite-Element Type Solver for Bioelectromagnetics to the DEEP-ER Platform.* ParCo 2015, Advances in Parallel Computing, 27 (2016) [10.3233/978-1-61499-621-7-349]

Application use case: xPic

- **Space Weather simulation**
  - Simulates plasma produced in solar eruptions and its interaction with the Earth magnetosphere
  - Particle-in-Cell (PIC) code
  - Authors: KU Leuven



- **Two solvers:**
  - **Field solver**: Computes electromagnetic (EM) field evolution
    - Limited code scalability
    - Frequent, global communication
  - **Particle solver**: Calculates motion of charged particles in EM-fields
    - Highly parallel
    - Billions of particles
    - Long-range communication



A. Kreuzer, J. Amaya, N. Eicker, E. Suarez, *"Application performance on a Cluster-Booster system"*, 2018 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), HCW (20th International Heterogeneity in Computing Workshop), Vancouver (2018), p: 69 - 78. [doi: 10.1109/IPDPSW.2018.00019]

xPic – ORIGINAL CONFIGURATION

```
for (auto i=beg+1; i<=end; i++){
  fld.solver->calculateE();
  fld.cpyToArr_F();



  pcl.cpyFromArr_F();
  for (auto is=0; is<nspec; is++) {
    pcl.species[is].ParticlesMove();
    pcl.species[is].ParticleMoments();
  }
  pcl.cpyToArr_M();



  fld.solver->calculateB();
  fld.cpyFromArr_M();
}
```

`fld`: Field Solver

Copy information between solvers

`plc`: Particle Solver

xPic – CODE PARTITION

```
#ifdef __CLUSTER__
for (auto i=beg+1; i<=end; i++){
  fld.solver->calculateE();
  fld.cpyToArr_F();
  ClusterToBooster();
  // Auxiliary computations
  ClusterWait();
BoosterToCluster();
BoosterWait();
  fld.solver->calculateB();
  fld.cpyFromArr_M();
}
#endif
```

```
#ifdef __BOOSTER__
for (auto i=beg+1; i<=end; i++){
  ClusterToBooster();
  ClusterWait();
  pcl.cpyFromArr_F();
  for (auto is=0; is<nspec; is++) {
    pcl.species[is].ParticlesMove();
    pcl.species[is].ParticleMoments();
  }
  pcl.cpyToArr_M();
  BoosterToCluster();
  // I/O and auxiliary computations
  BoosterWait();
}
#endif
```

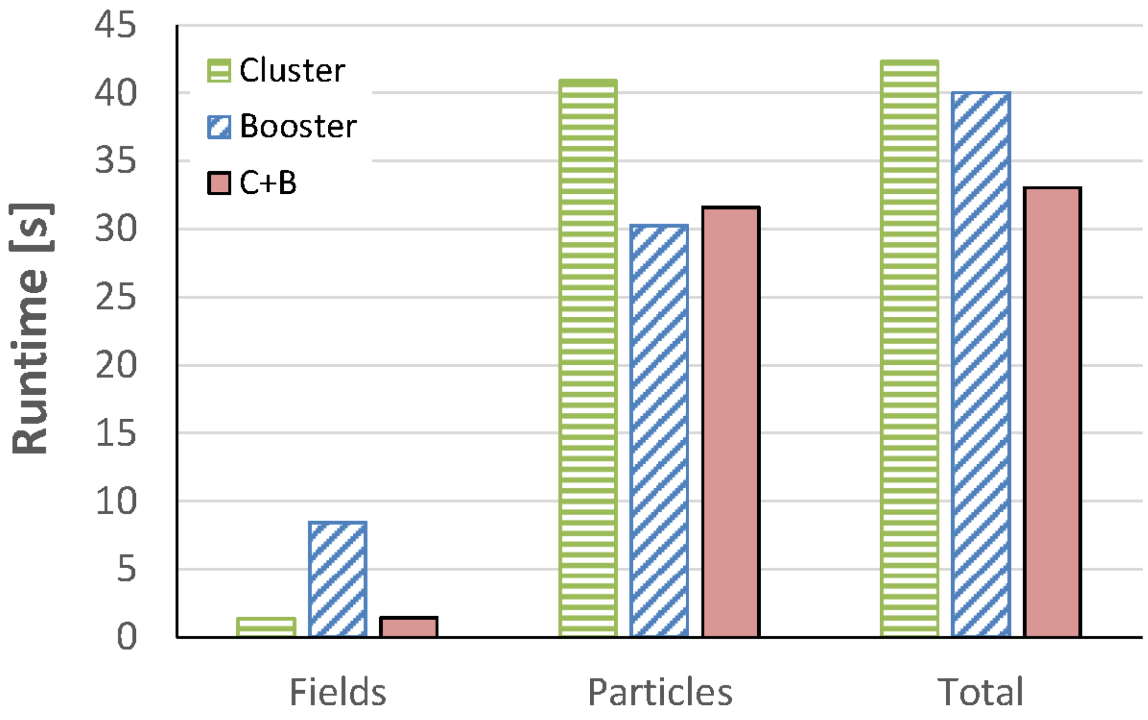
xPic – (1-NODE) PERFORMANCE RESULTS

- **Field solver**: 6× faster on Cluster
- **Particle solver**: 1.35 × faster on Booster
- **Overall performance gain:**

1× node	**28% × gain** compared to Cluster alone **21% × gain** compared to Booster alone

8× nodes	**38% × gain** compared to Cluster only **34% × gain** compared to Booster only

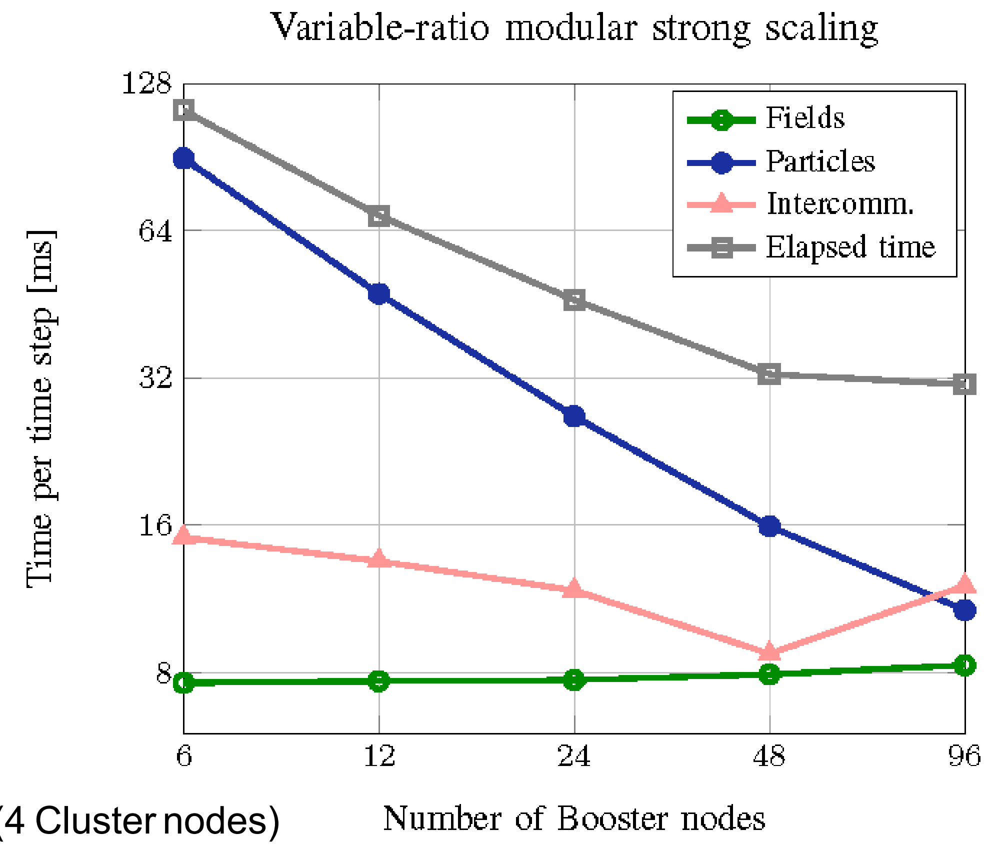
  – 3%-4% overhead per solver for C+B communication (point to point)



#cells per node	4096
#particles per cell	2048
Compilation flags	-openmp, -mavx (Cluster) -xMIC-AVX512 (Booster)

A. Kreuzer et al. "*Application Performance on a Cluster-Booster System*", 2018 IEEE IPDPS Workshops (IPDPSW), Vancouver, Canada, p 69 - 78 (2018) [10.1109/IPDPSW.2018.00019]

xPic – STRONG SCALING on JURECA



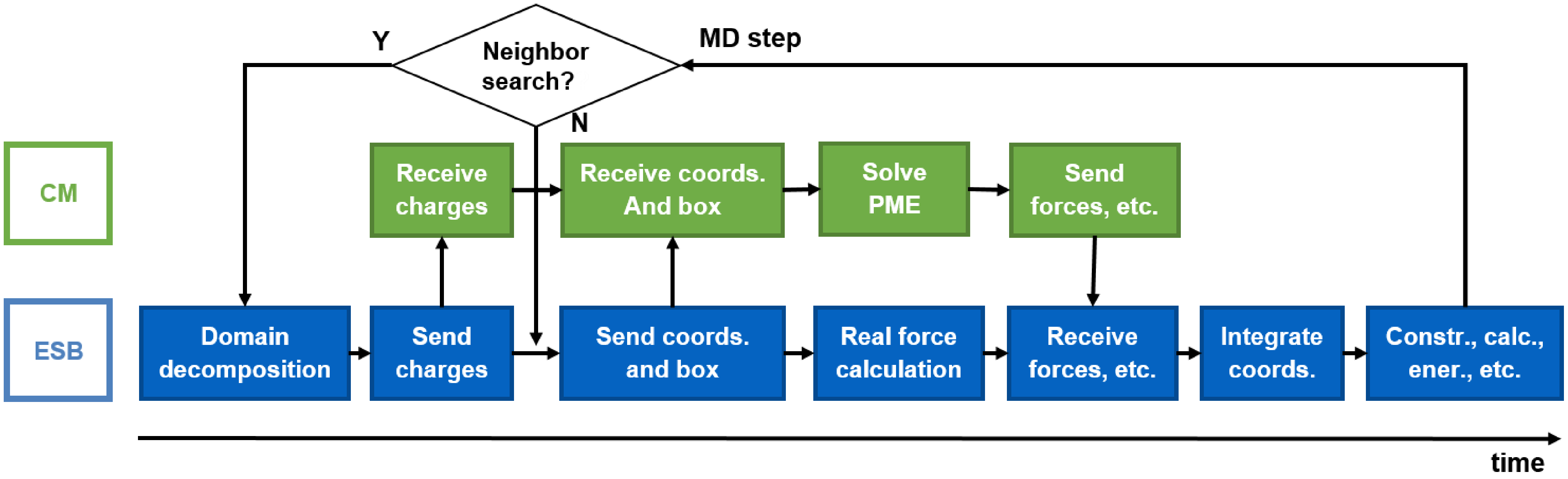
(4 Cluster nodes)

#cells per node	36864
#particles per cell	1024
#blocks per MPI process	12, 32 or 64
Compilation flags	-mavx (Cluster) -openmp, xMIC-AVX512 (Booster)

- Code portions can be scaled-up independently
  - Particles scale almost linearly on Booster
  - Fields kept constant on the Cluster (4CNs)
- A configuration is reached where same time is spent on Cluster and Booster
  - Additional 2× time-saving is enabled via overlapping

GROMACS: multi-module usage in MD simulations

- Best mapping on MSA depends on the problem size and aims at optimizing the computational load
  - $<10^4$ particles: only on Cluster (CPU)
  - ~ 10^5 particles: Booster or DAM (Data Analytics Module)
  - $>10^6$ particles (large macromolecules): pair interactions on GPU, run PME on CPUs



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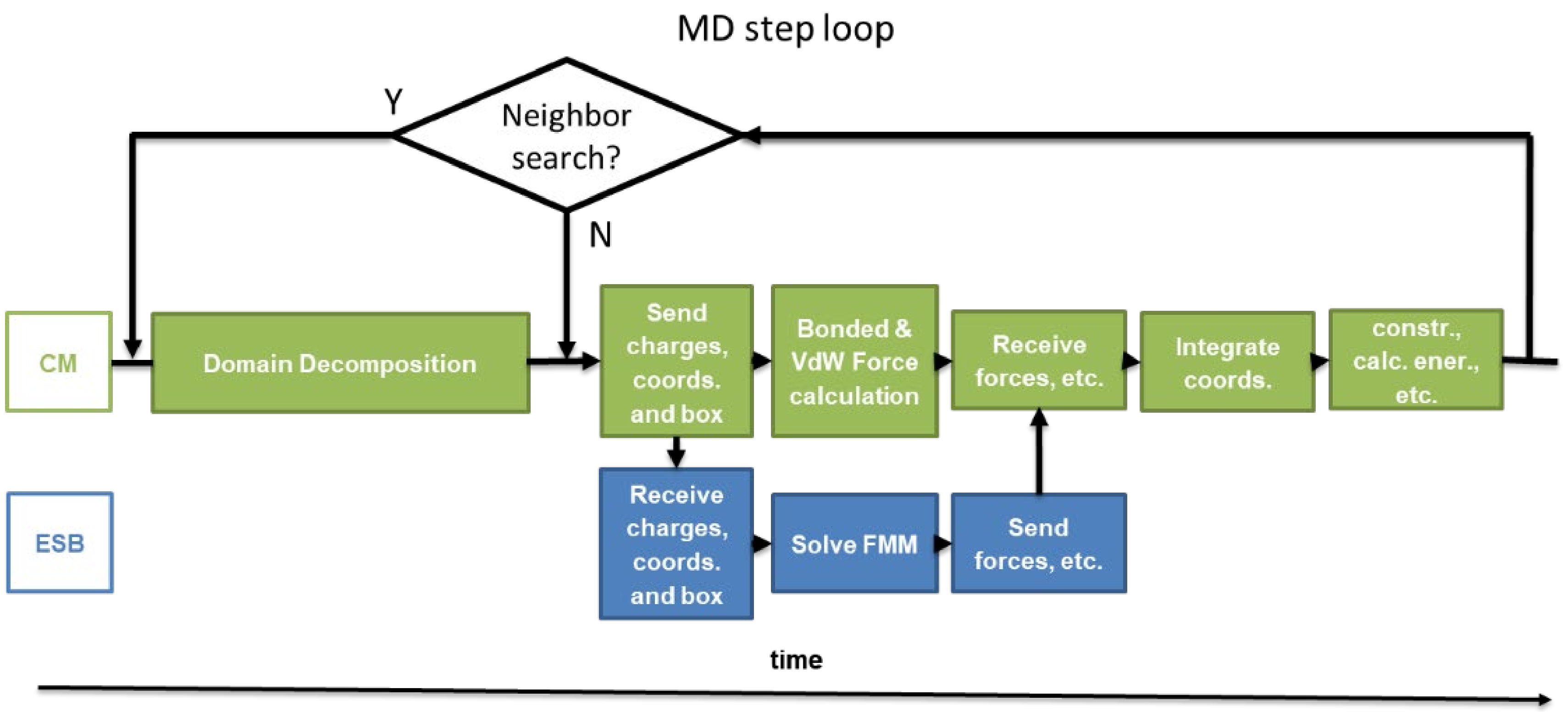
  - Very large volume ($>10^6$ nm^3): Replace PME with FMM (Fast Multipole Method) running on ESB



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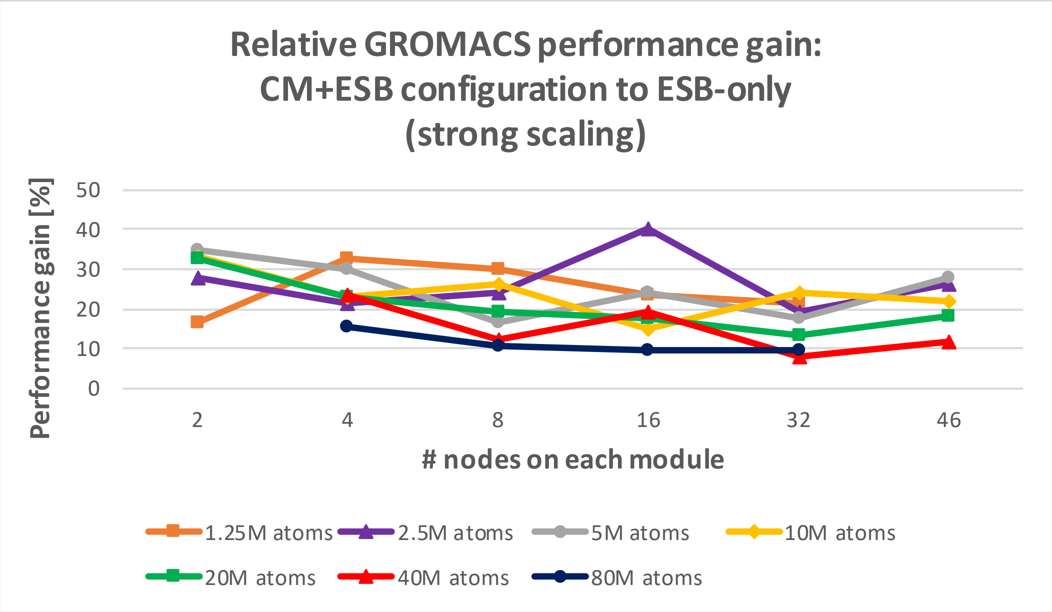
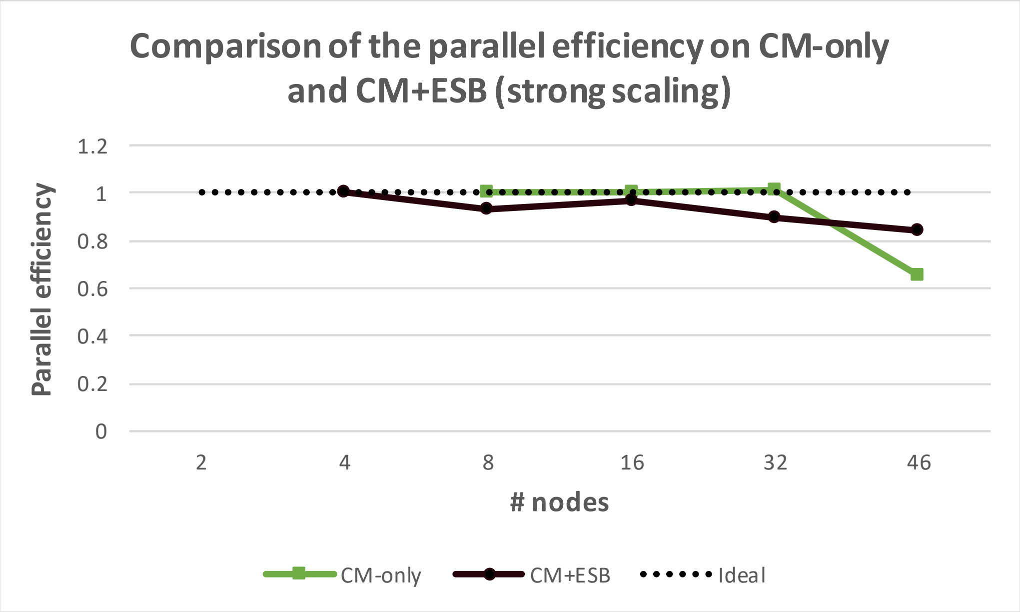




NextDBSCAN: multi-module usage in ML

- Parallel algorithm for density-based clustering of arbitrary data sets
  - Performance and flexibility gain by running on multiple modules

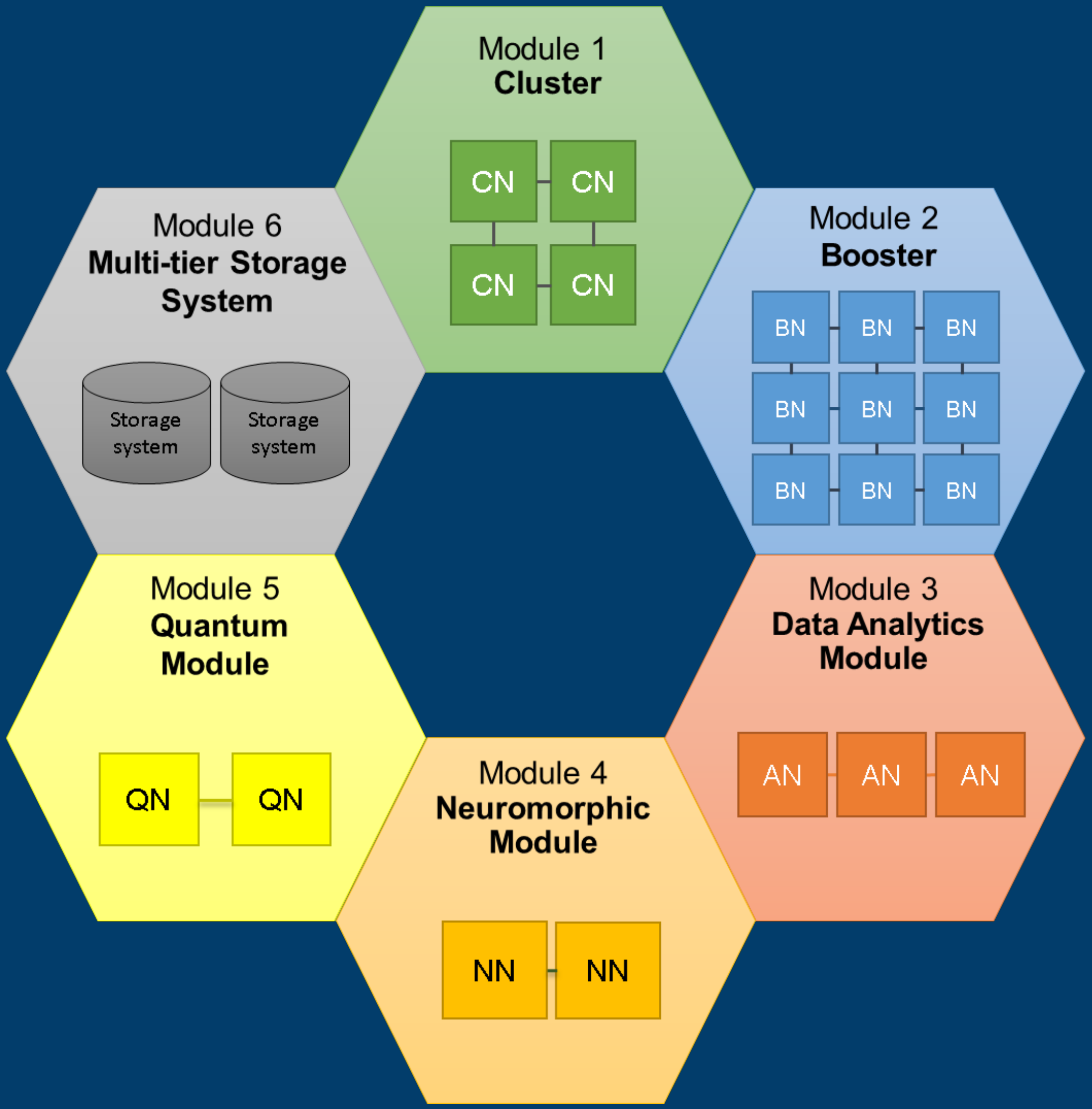
See presentation in
ADAC applications group:

DBSCAN Clustering and Modular Supercomputing: Lessons Learned

Ernir Erlingsson (University of Iceland)

OUTLINE

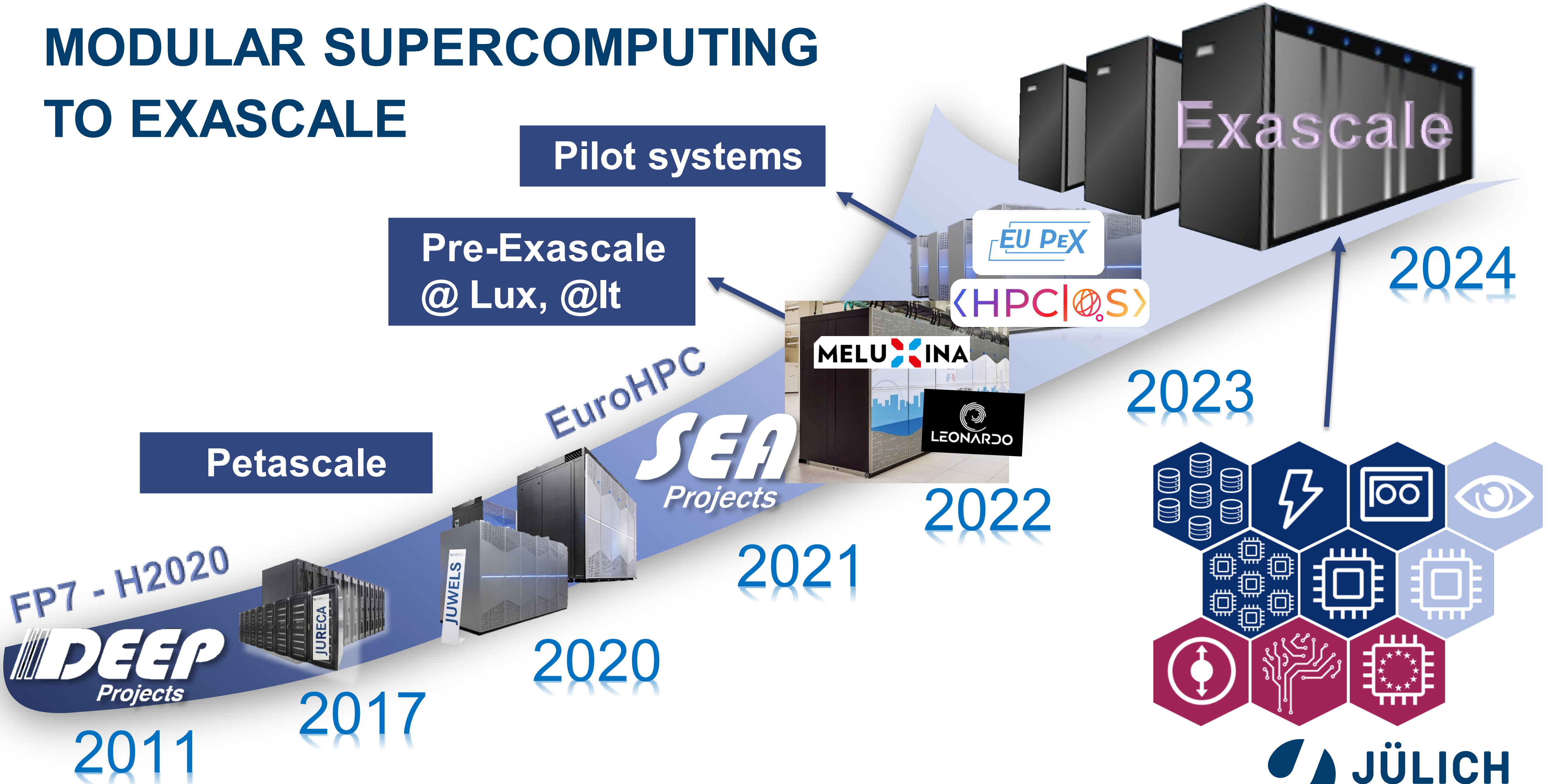
- **System architecture**
  - From dual architecture to the Modular Supercomputing Architecture (MSA)
  - Hardware implementations of MSA
- **Software**
  - Software stack
  - ParaStation Modulo
  - Scheduler
- **Application experience**
- **Conclusions and next steps**



CONCLUSIONS

- **The Modular Supercomputing Architecture (MSA)**
  - Orchestrates heterogeneity at system level
  - Allows scaling hardware in economical way (Booster → Exascale)
  - Serves very diverse application profiles
    - Maximum flexibility for users, without taking anything away (still can use individual modules)
- **Distribute applications on the MSA give each code-part a suitable hardware**
  - Straight-forward implementation for workflows
  - Partition at MPI-level interesting for multi-physics / multi-scale codes
  - Monolithic codes do not need to be divided
- **Current / Upcoming implementations of MSA**
  - DEEP system, JURECA, JUWELS
  - MELUXINA (Luxembourg EuroHPC Petascale system)
  - EUPEX and HPCQS pilots
  - … Exascale !

MODULAR SUPERCOMPUTING TO EXASCALE



THANK YOU!

www.deep-projects.eu
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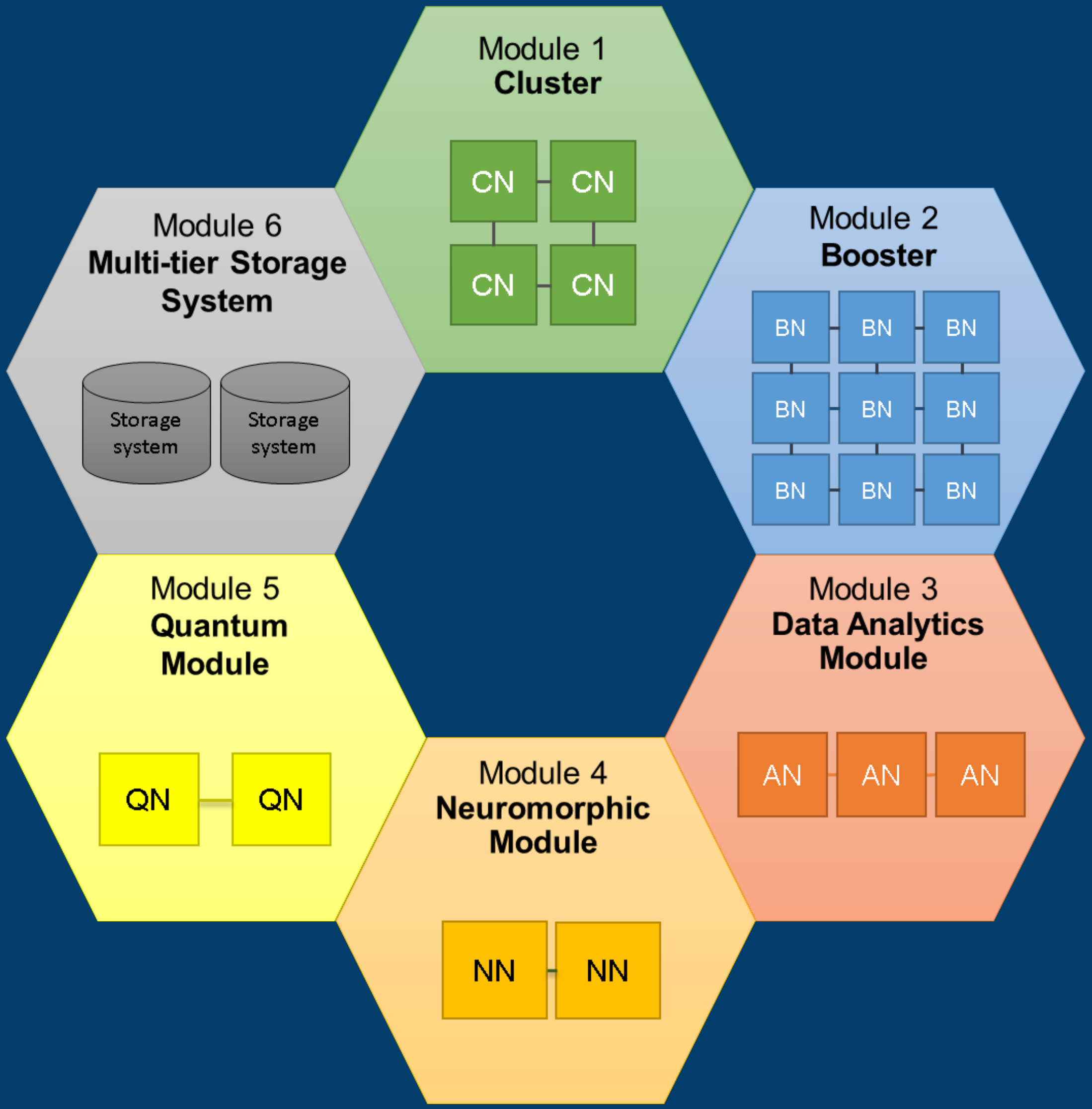

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