The DEEP Projects:
10 years turning heterogeneity into modularity

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The DEEP projects

2011-2021: The DEEP projects

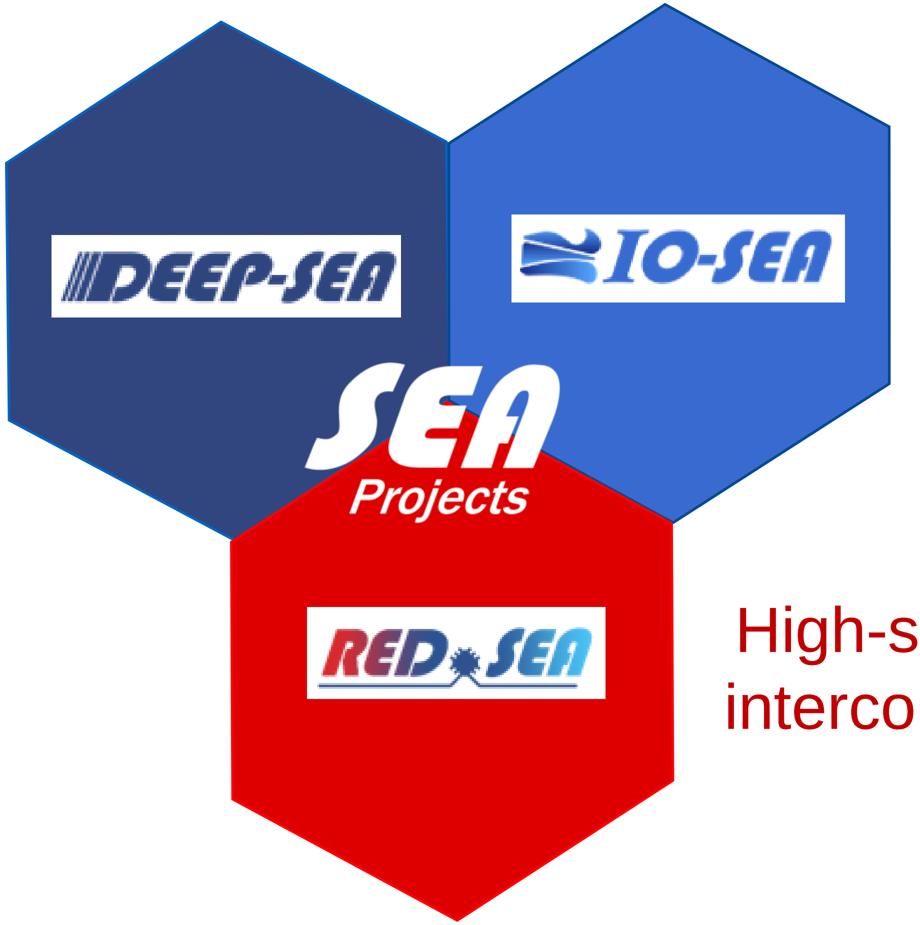
- **DEEP** (2011 – 2015)
  - Introduced Cluster-Booster architecture
- **DEEP-ER** (2013 – 2017)
  - Added I/O and resiliency functionalities
- **DEEP-EST** (2017 – 2021)
  - Modular Supercomputer Architecture

2021-2024 The SEA projects

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

SEA Projects family

Provide solutions for Modular Supercomputers of Exascale performance



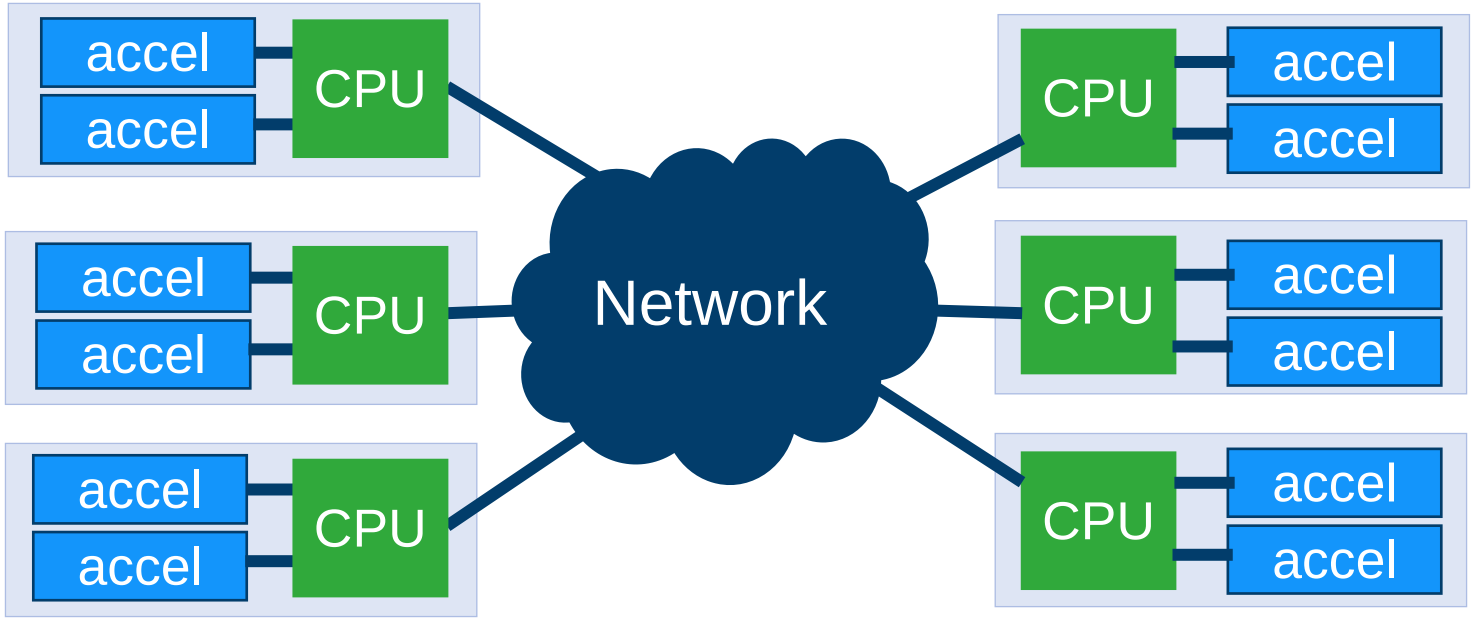
Software stack for heterogeneous compute and memory systems

I/O and data management

High-speed interconnect

Heterogenous Monolithic

Every node contains accelerators (e.g. GPUs)



+: Energy efficient

+: Easy management

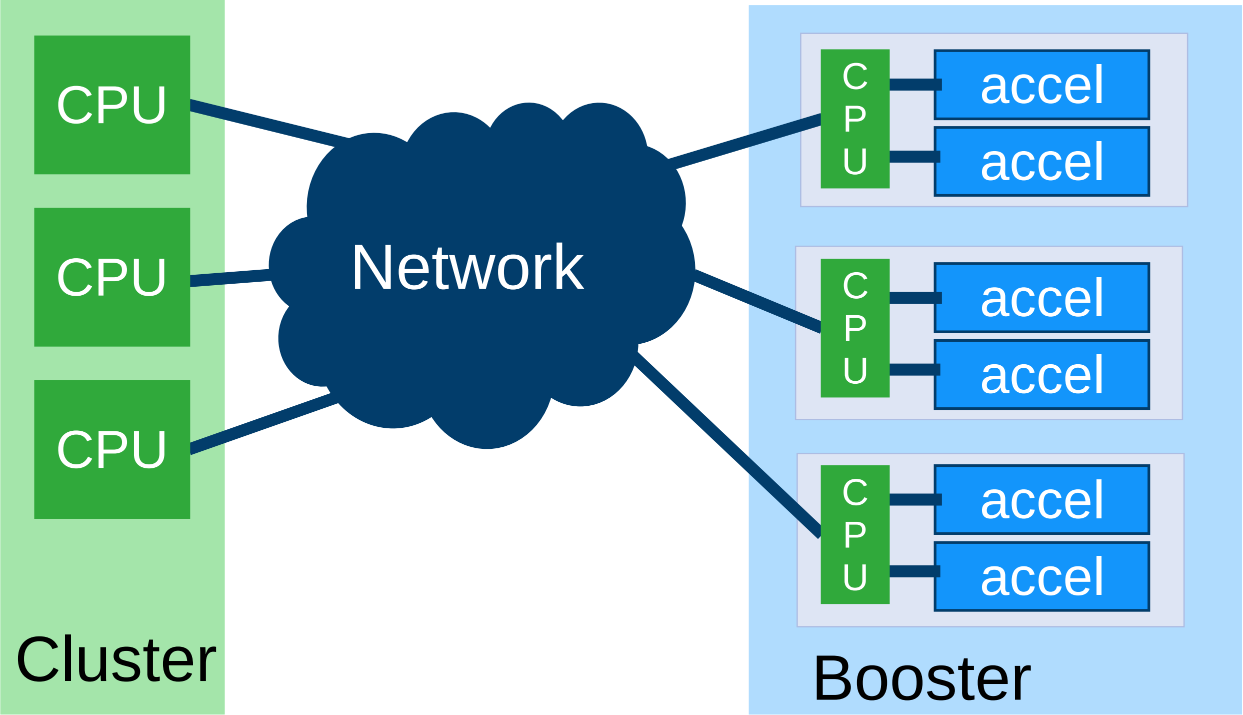
-: Static assignment of accelerators to CPUs

-: 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"

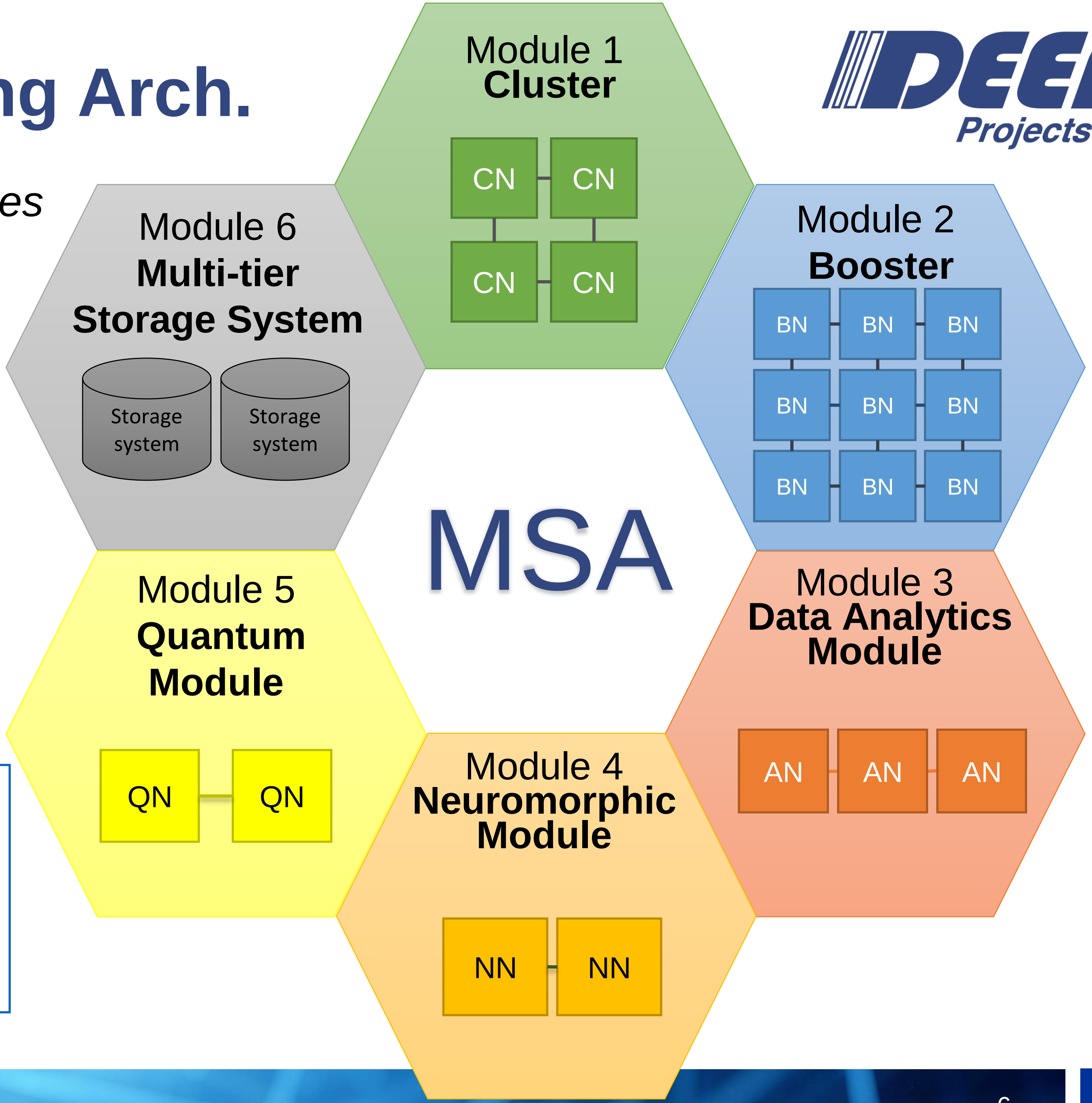


+: Energy efficient
+: Better scalability
+: High flexibility
+: Dynamic resource assignment
-: Complexity

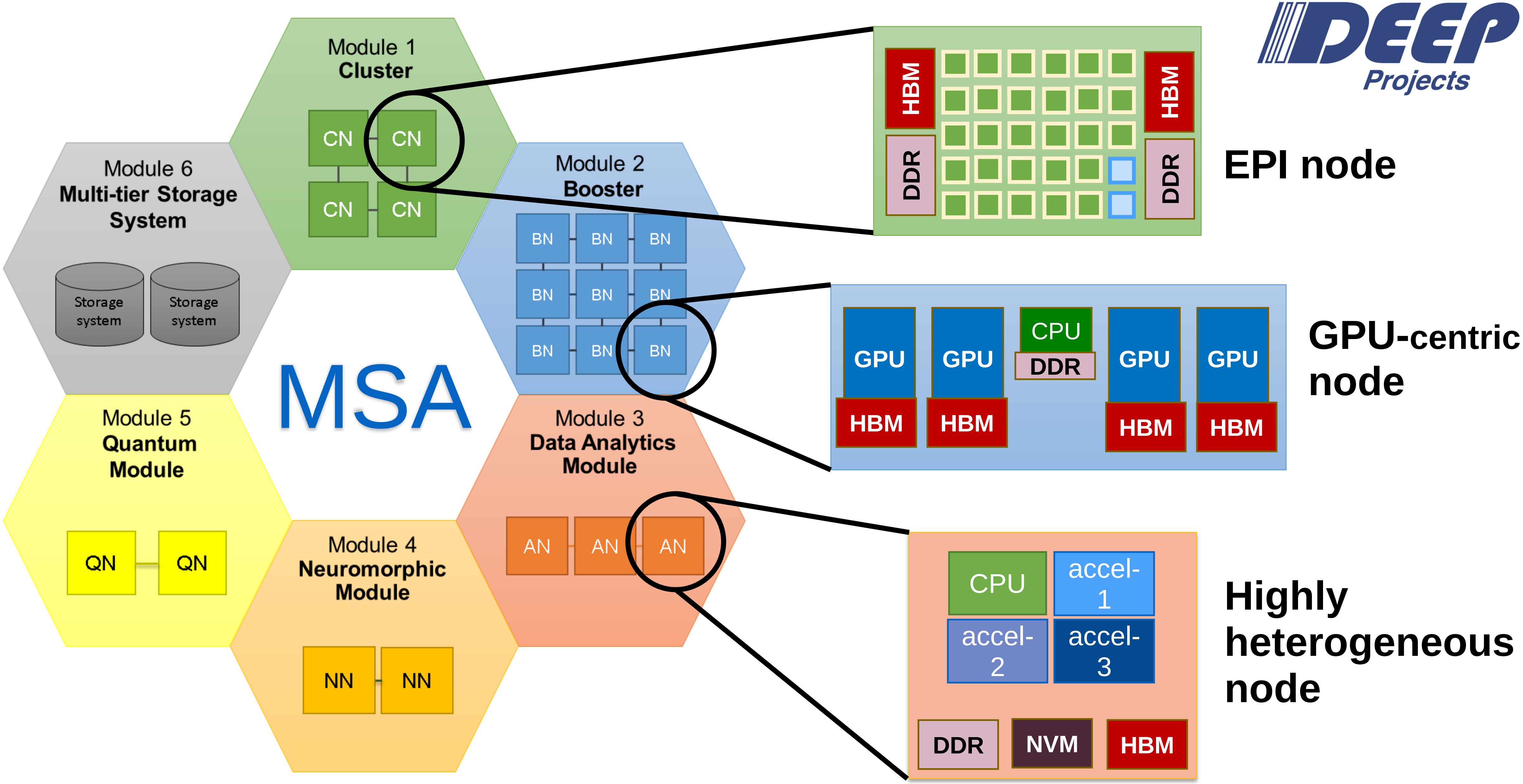
- All nodes within one module are equal
- Different modules have different configurations → "modular"

Modular Supercomputing Arch.

Composability of heterogeneous resources



- **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)



MSA

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

EPI node

HBM DDR HBM DDR

GPU-centric node

GPU GPU CPU DDR GPU GPU
HBM HBM HBM HBM

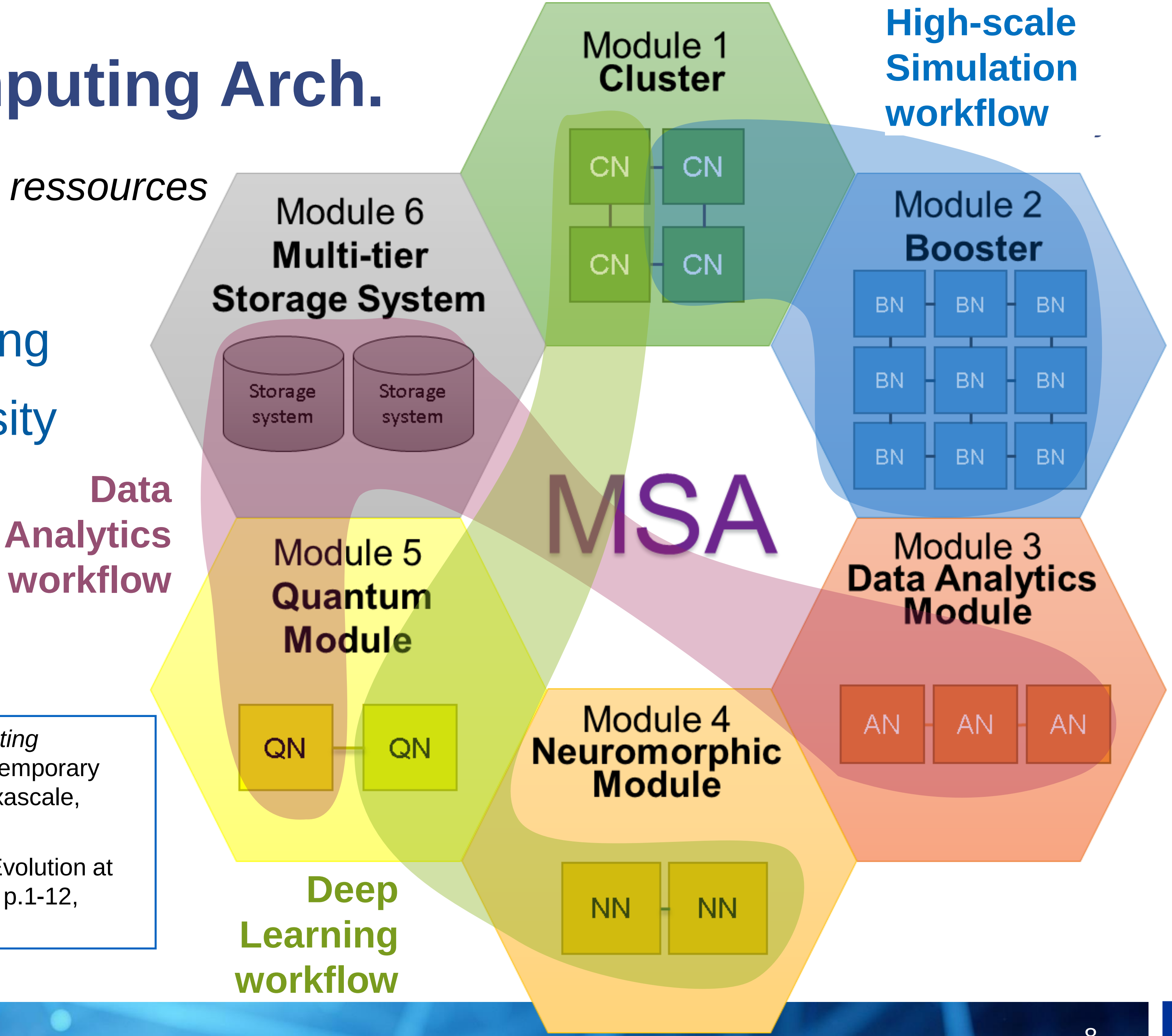
Highly heterogeneous node

CPU accel-1
accel-2 accel-3
DDR NVM HBM

Modular Supercomputing Arch.

Composability of heterogeneous ressources

- Effective resource-sharing
- Match application diversity



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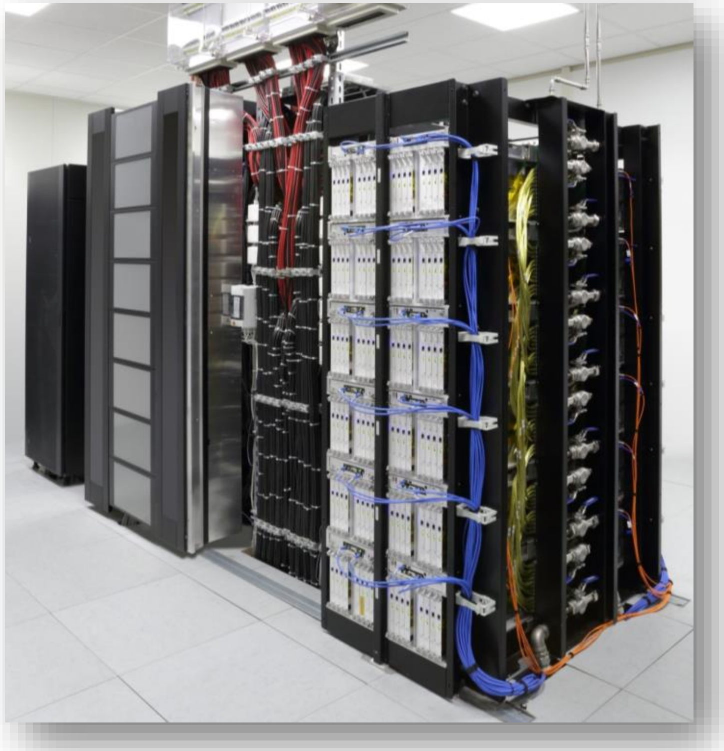
The hardware Prototypes

2015



2016

2020

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

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

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

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)

Heterogeneity from user’s PoV

- **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 part2 ./second
```

- **Full support for job packs in ParaStation psslurm**, with **unique features** for modular jobs:
  - Support for heterogeneous jobs with common MPI_COMM_WORLD, or with separated / interconnected MPI_COMM_WORLDS
  - 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*
- **ParaStation has further features that make is MSA-ware**
  - E.g. hierarchical collective operations

Source: Thomas Moschny

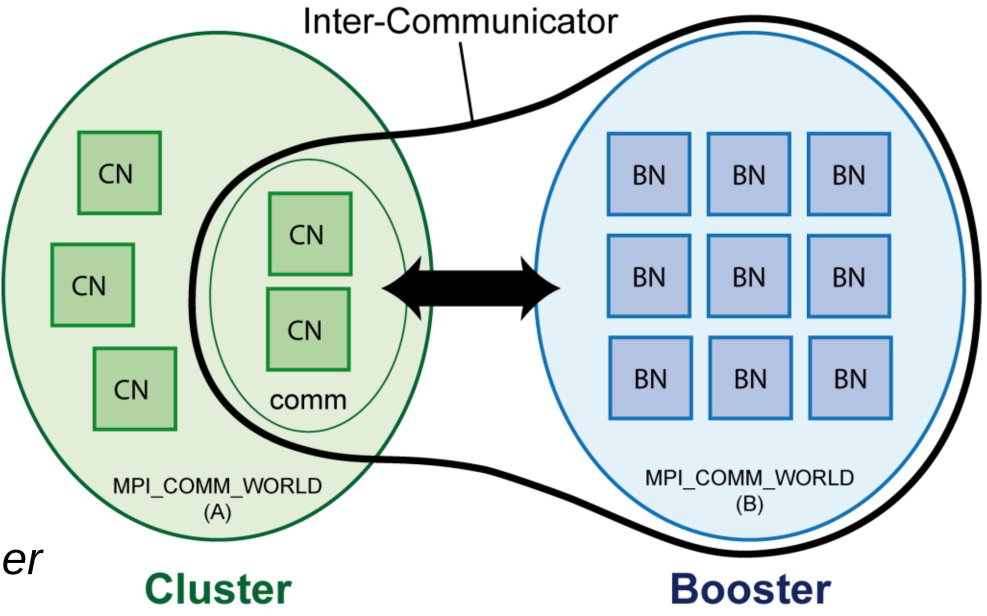
ParaStation Global MPI for MSA

- 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()`

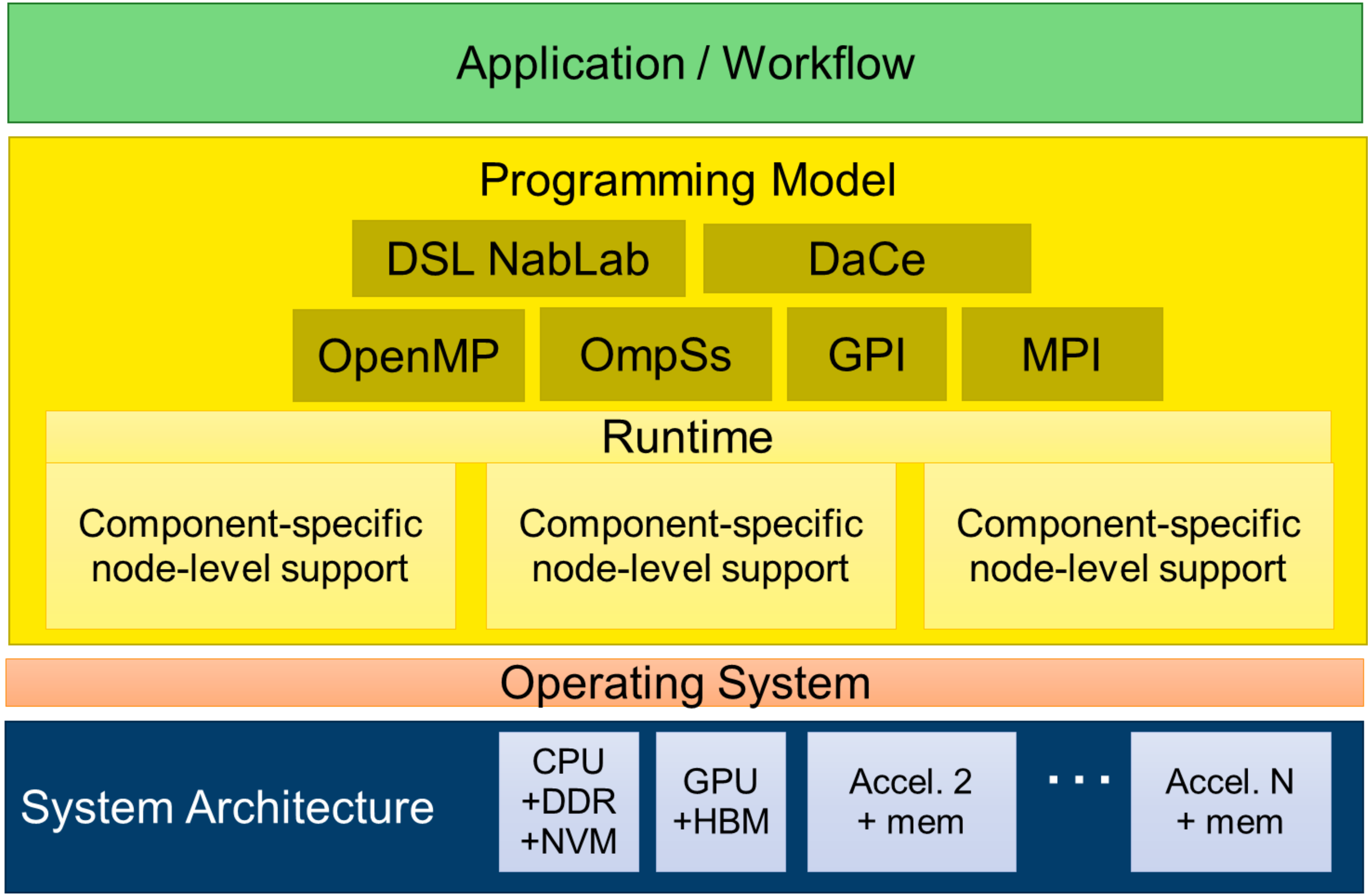
- Or have one single common `MPI_COMM_WORLD` and split it into subcommunicators via `MPI_Comm_Split()`



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

DEEP-SEA: Extending the software stack

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



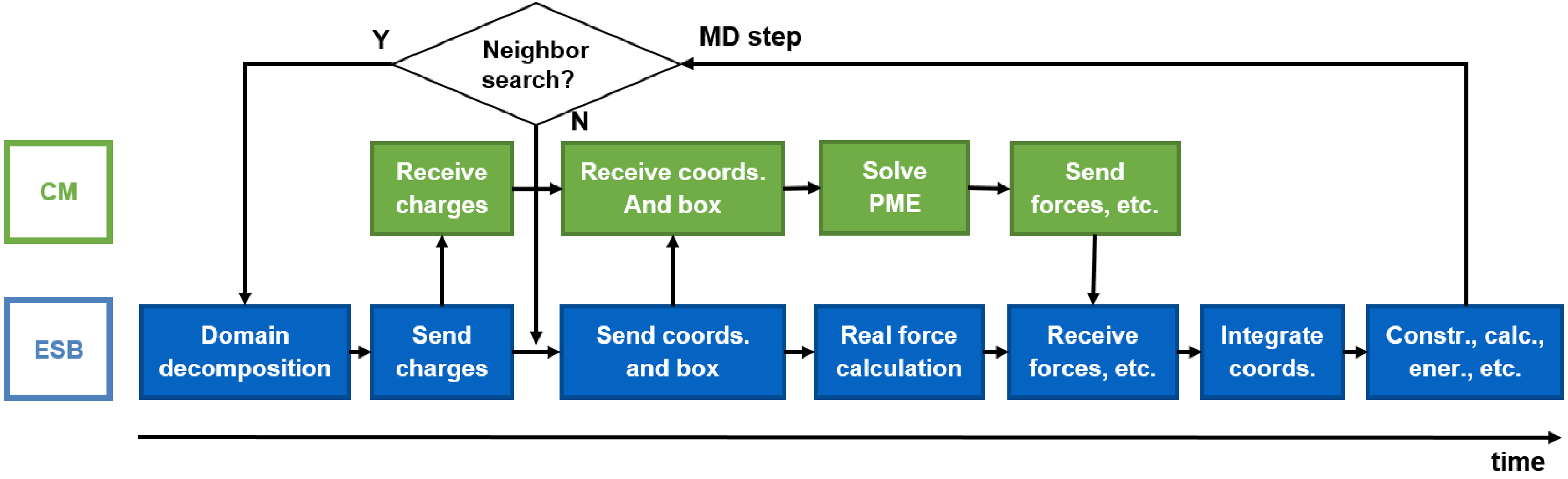
Co-design Applications

Feed user requirements in SW development, evaluate the SW-packets

- Application areas
  - Space Weather: xPic, AIDApy
  - Weather Forecast: IFS
  - Seismic imaging: RTM, BSIT
  - Molecular dynamics: GROMACS
  - Computational fluid dynamics: Nek5000
  - Neutron Monte Carlo transport for nuclear energy: PATMOS
  - Earth System Modelling: TSMP
- Additionally: low-level and synthetic benchmarks
- User support
- Early access program

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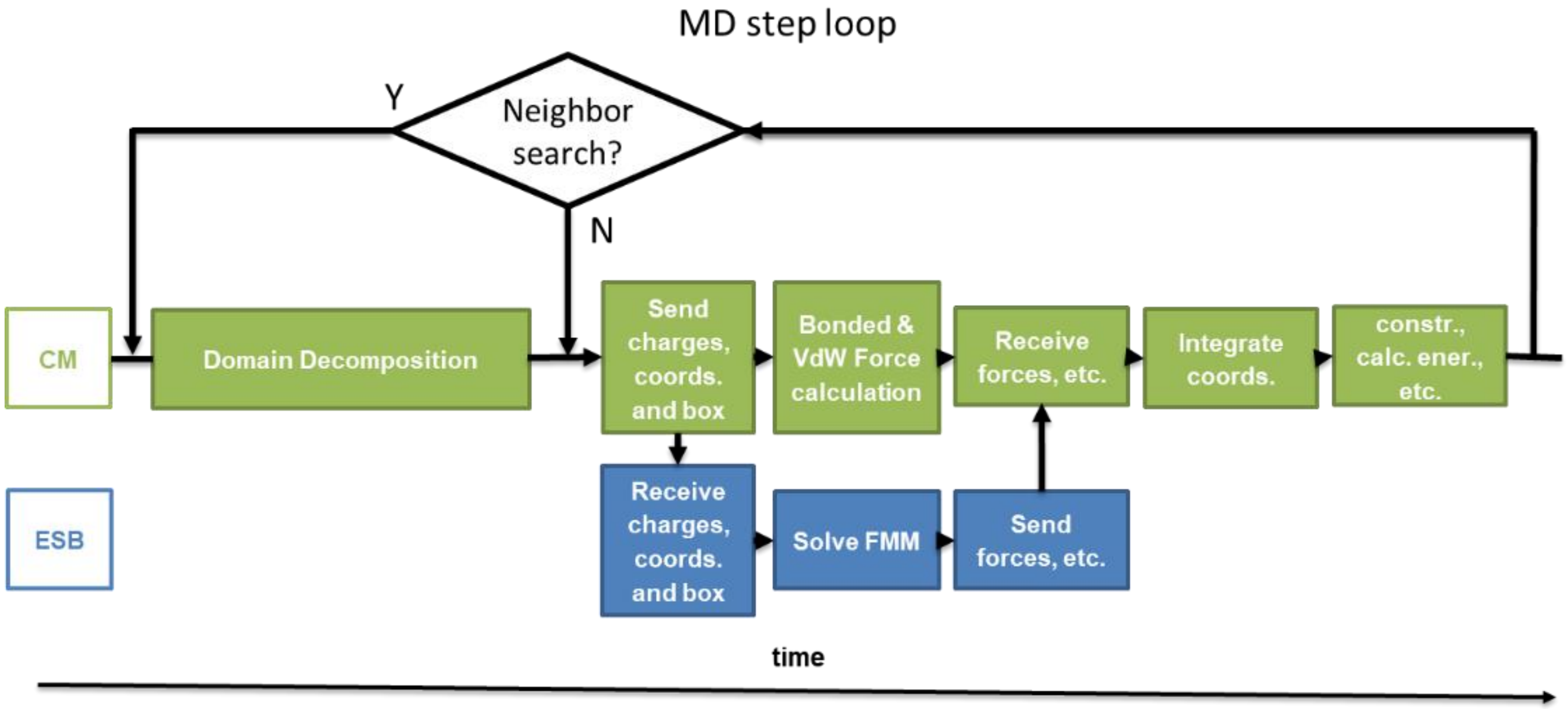
  - Very large volume (>10^6 nm^3): Replace PME with FMM (Fast Multipole Method) running on ESB



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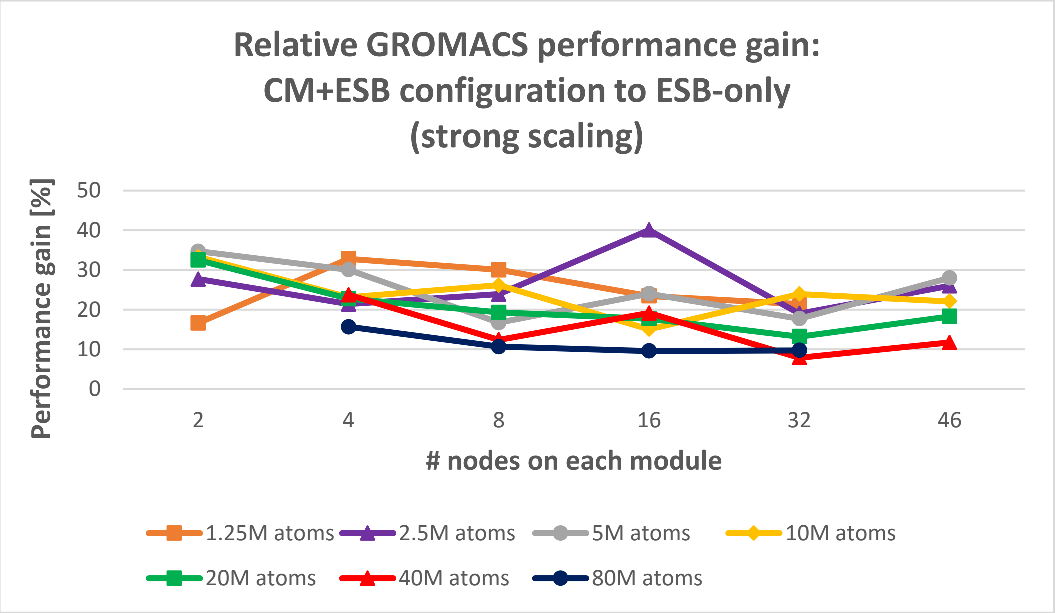
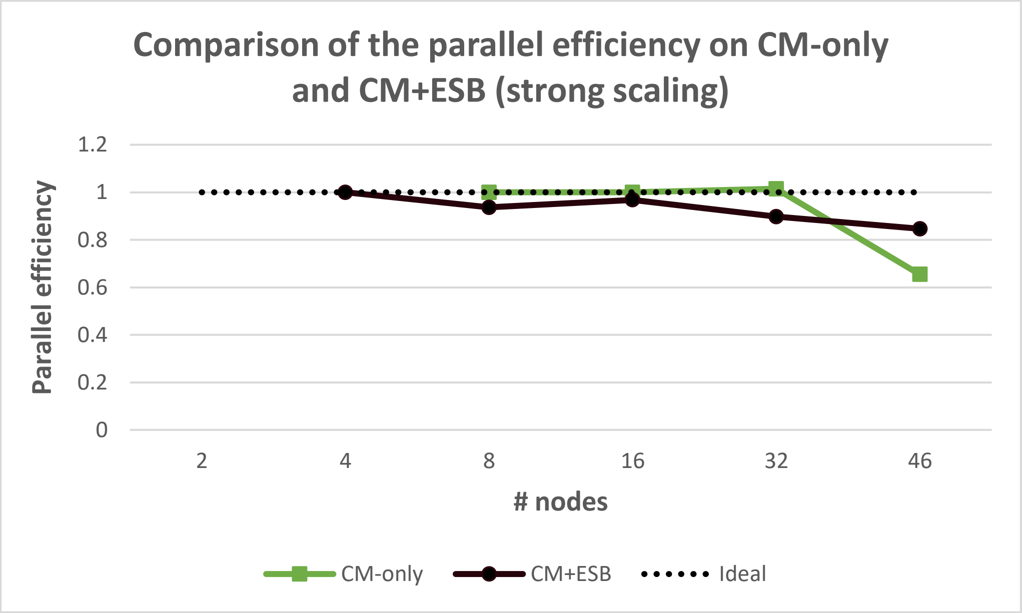
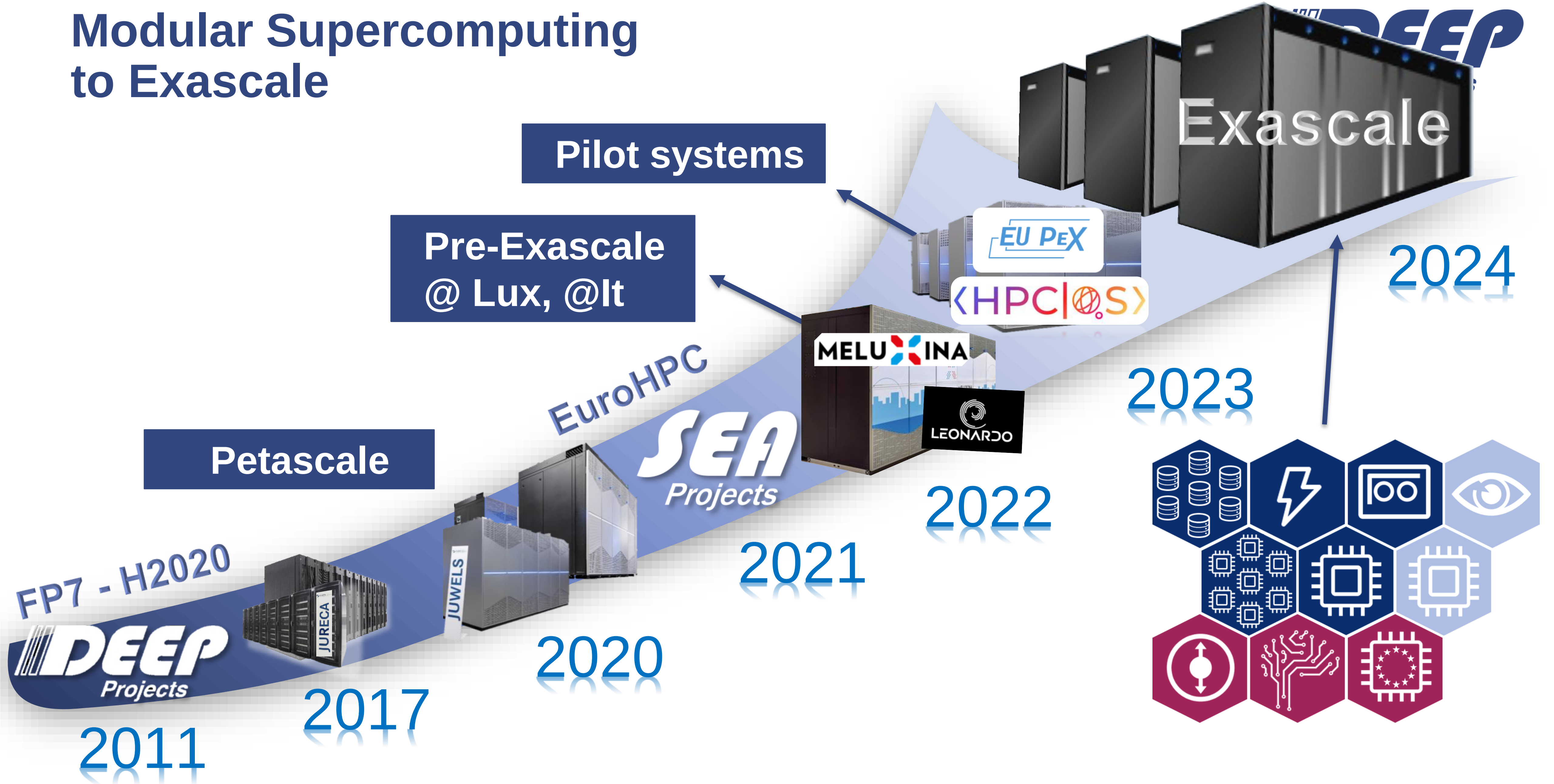




Conclusions

- **The Modular Supercomputing Architecture (MSA)**
  - Orchestrates heterogeneity at system level
  - 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



Petascale

Pre-Exascale @ Lux, @It

Pilot systems

Exascale

FP7 - H2020

EuroHPC

2011

2017

2020

2021

2022

2023

2024

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DEEP Projects

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