MPI RUNTIMES AT JSC, NOW AND IN THE FUTURE

Which, why and how do they compare in our systems?

08.07.2018 I MUG'18, COLUMBUS (OH) I DAMIAN ALVAREZ

MPI RUNTIMES AT JSC

Outline

- FZJ' mission
- JSC's role
- JSC's vision for Exascale-era computing
- JSC's systems
- MPI runtimes at JSC
- MPI performance at JSC systems
- MVAPICH at JSC

MPI RUNTIMES AT JSC

FZJ's mission

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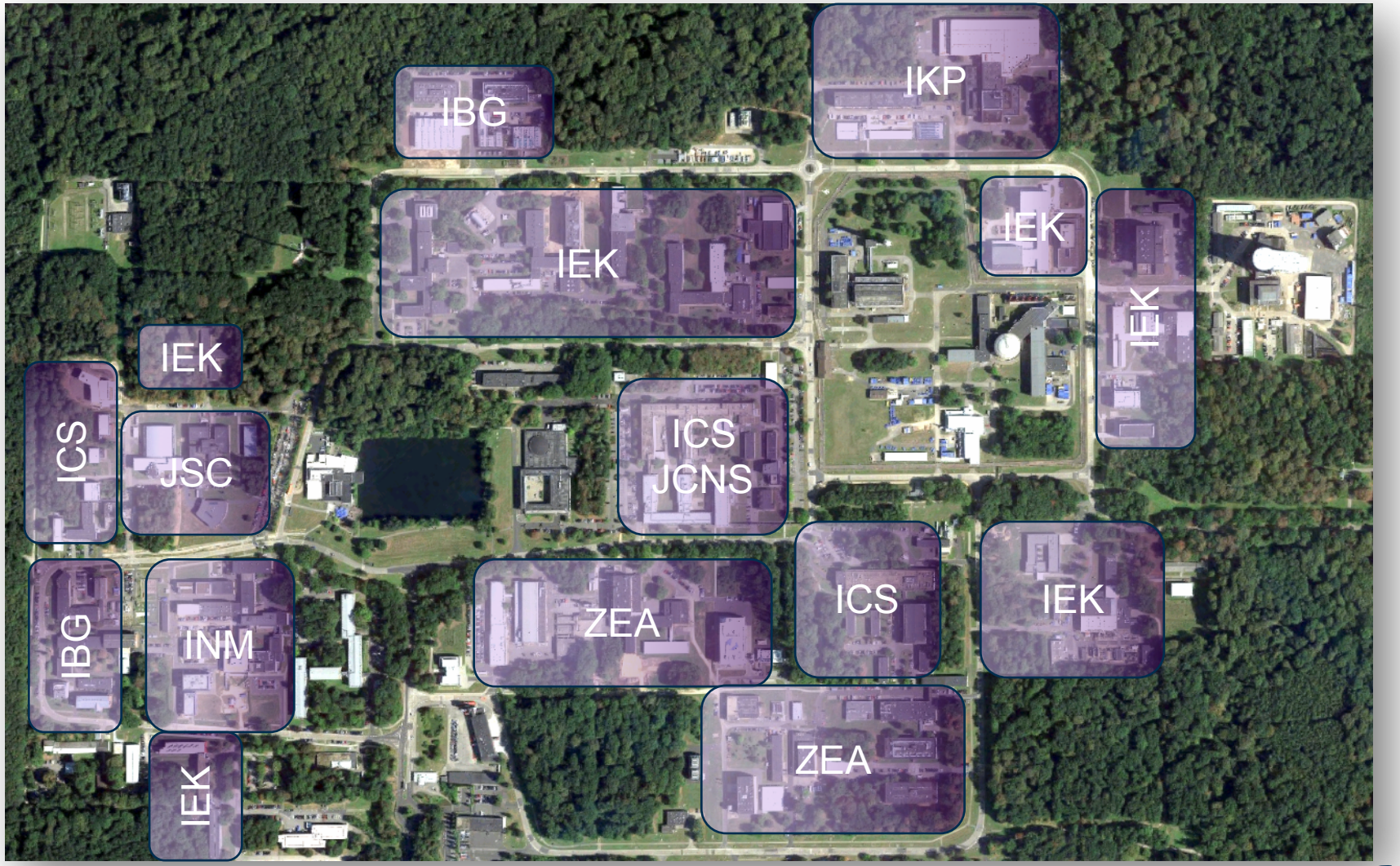
MPI RUNTIMES AT JSC

FZJ's mission



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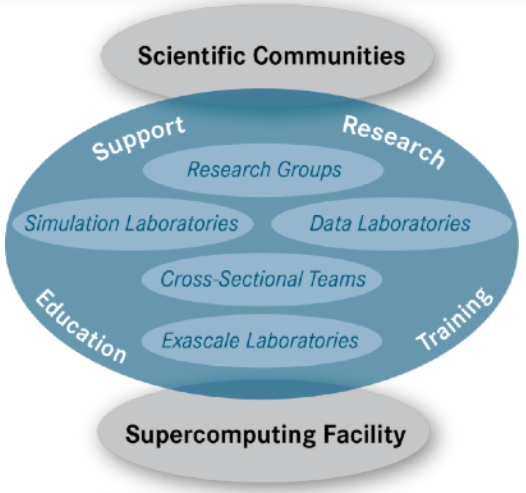
MPI RUNTIMES AT JSC

JSC's role

- **Supercomputer operation for:**
  - Centre – FZJ
  - Region – RWTH Aachen University
  - Germany – Gauss Centre for Supercomputing
    John von Neumann Institute for Computing
  - Europe – PRACE, EU projects
- **Application support**
  - Unique support & research environment at JSC
  - Peer review support and coordination
- **R&D work**
  - Methods and algorithms, computational science, performance analysis and tools
  - Scientific Big Data Analytics with HPC
  - Computer architectures, Co-Design
    Exascale Labs together with IBM, Intel, NVIDIA
- **Education and training**



DEEP

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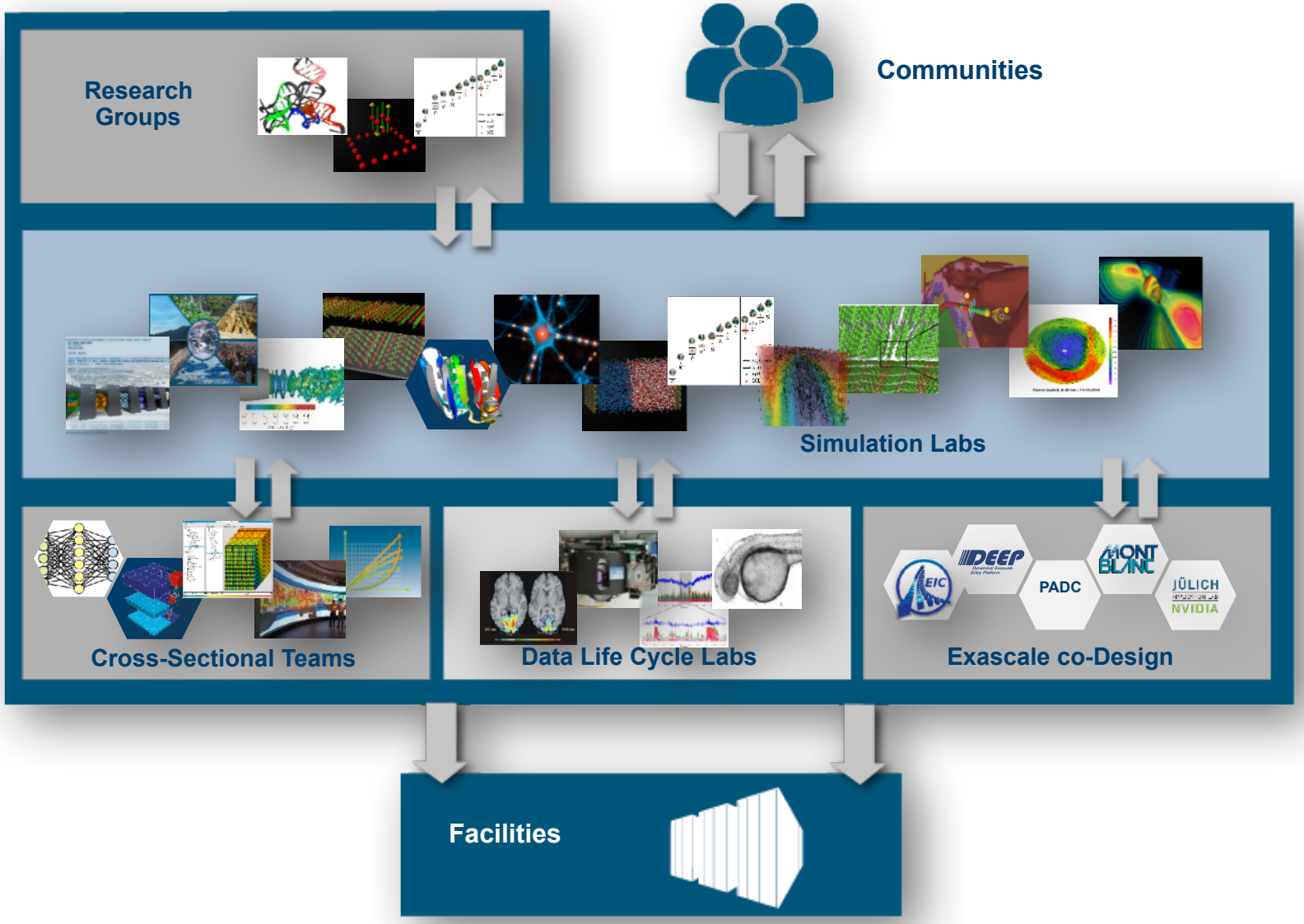
MPI RUNTIMES AT JSC

JSC's role



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MPI RUNTIMES AT JSC

JSC's role

Dominant Sites

#	Site	Country	Norm-HPL
1	LLNL	USA	1,466
2	LANL	USA	810
3	ORNL	USA	737
4	SNL	USA	652
5	NSCC Guangzhou	China	449
6	RIKEN AICS	Japan	354
7	**NASA/Ames**	**USA**	**352**
8	**FZ Jülich**	**Germany**	**333**
9	JAMSTEC	Japan	325
10	**NERSC**	**USA**	**303**
11	**ANL**	**USA**	**298**

Steady Sites

Never #1

TOP500

Source: Jack Dongarra, 30 Years of Supercomputing: History of TOP500, February 2018

MPI RUNTIMES AT JSC

JSC's role

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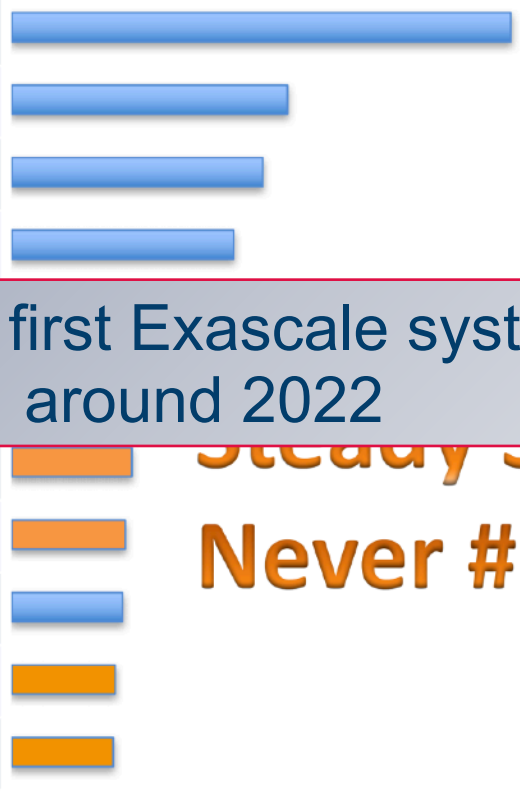


JSC will host the first Exascale system in the EU around 2022

Steady Sites

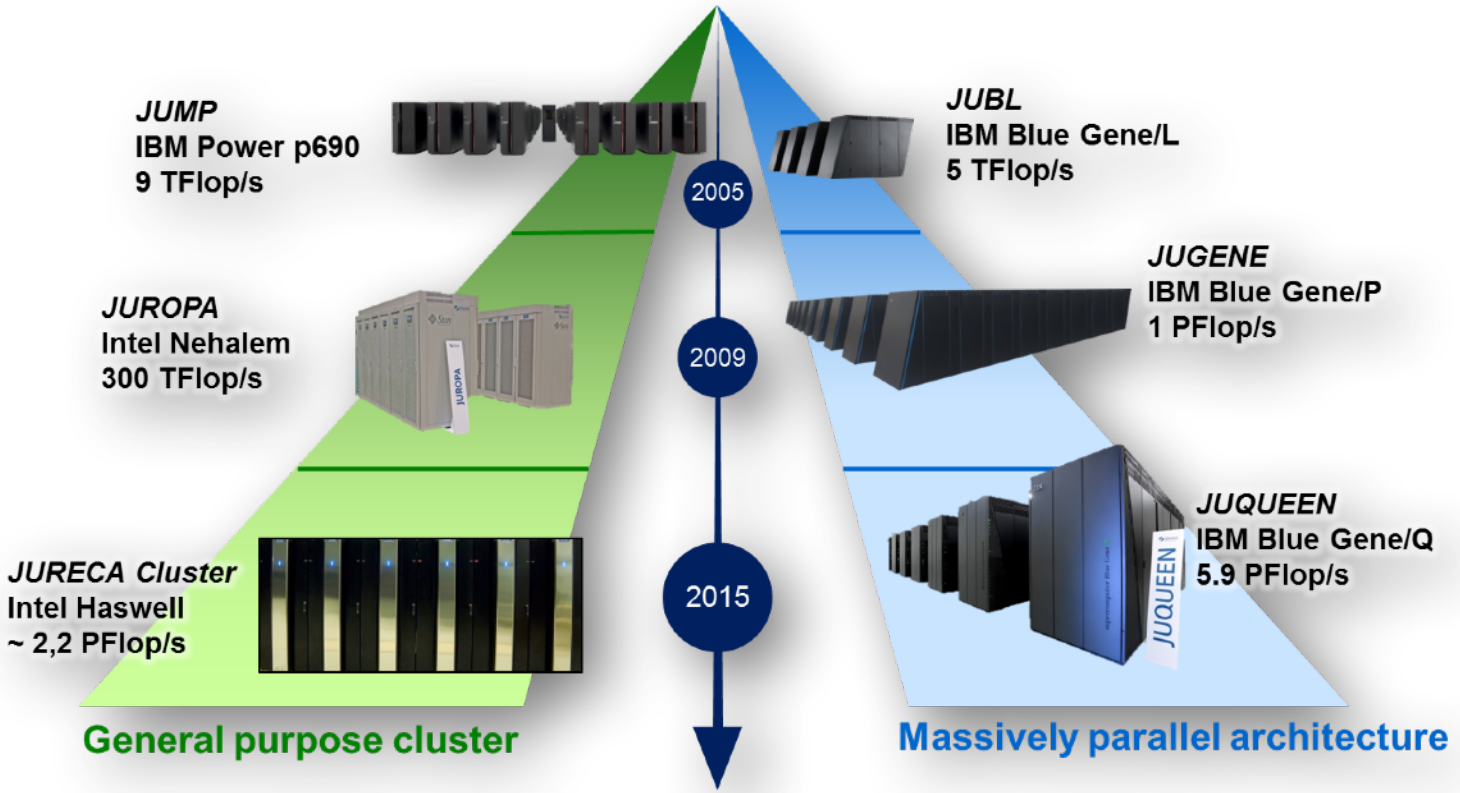
Never #1

TOP500

Source: Jack Dongarra, 30 Years of Supercomputing: History of TOP500, February 2018

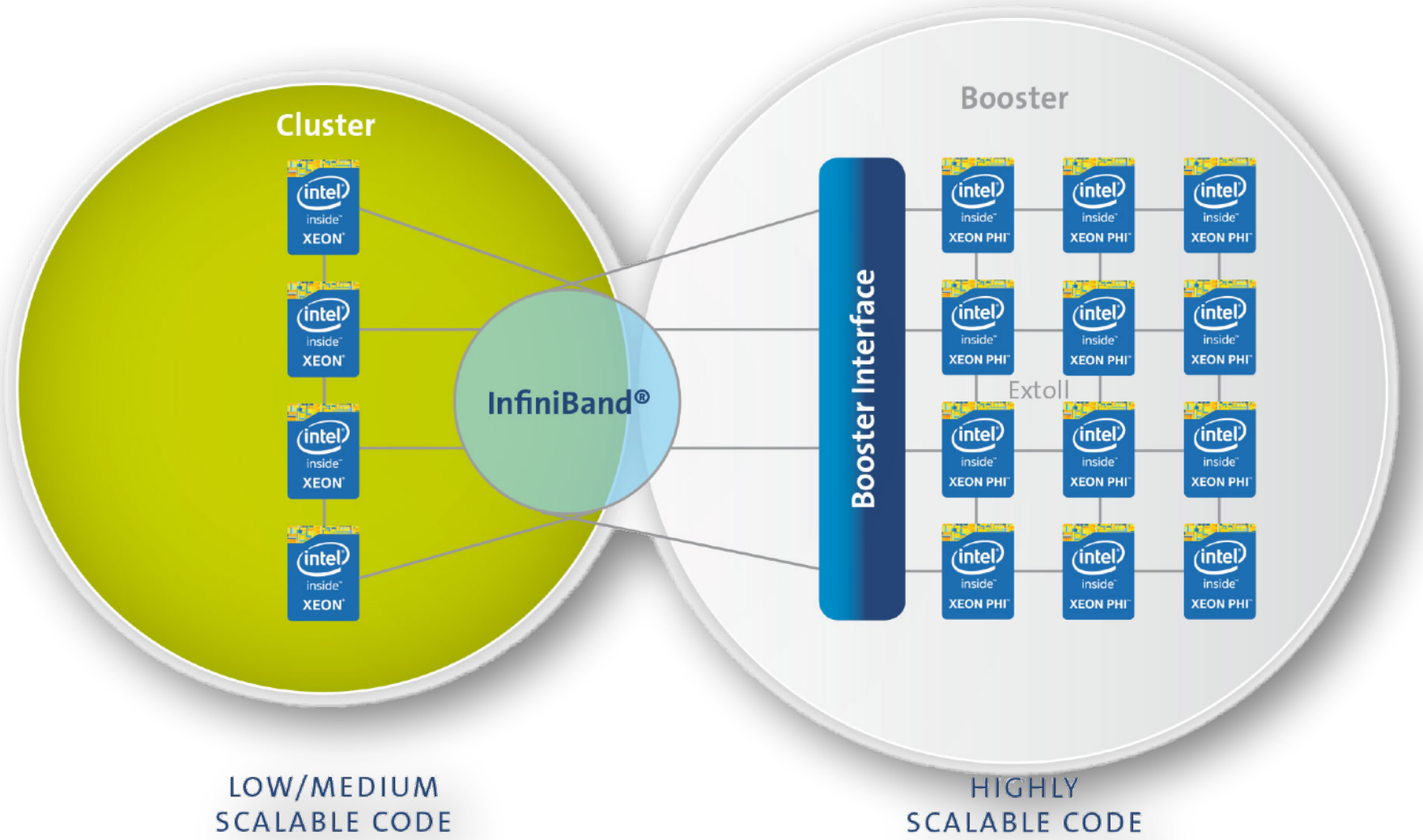
MPI RUNTIMES AT JSC

JSC's vision



MPI RUNTIMES AT JSC

JSC's vision



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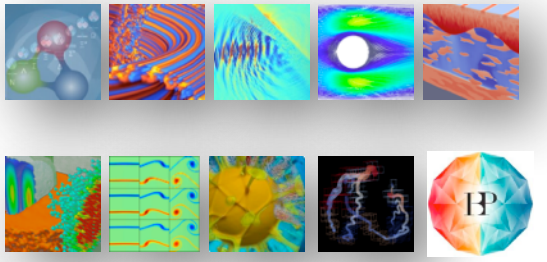
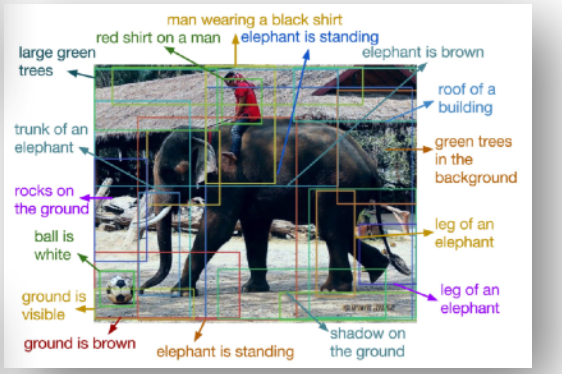
MPI RUNTIMES AT JSC

JSC's vision

Extreme Scale Computing



Big Data Analytics

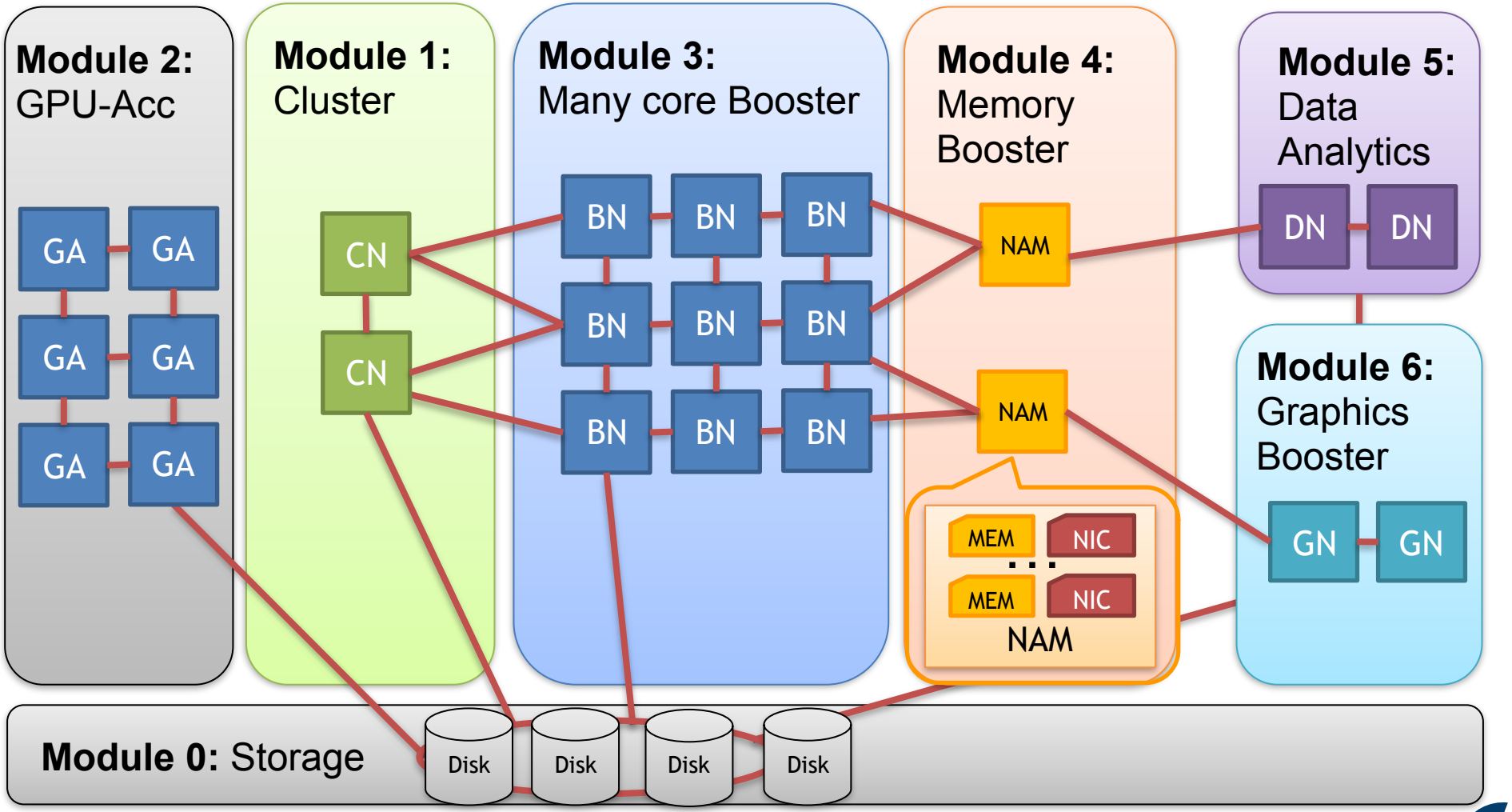


Deep Learning

Interactivity

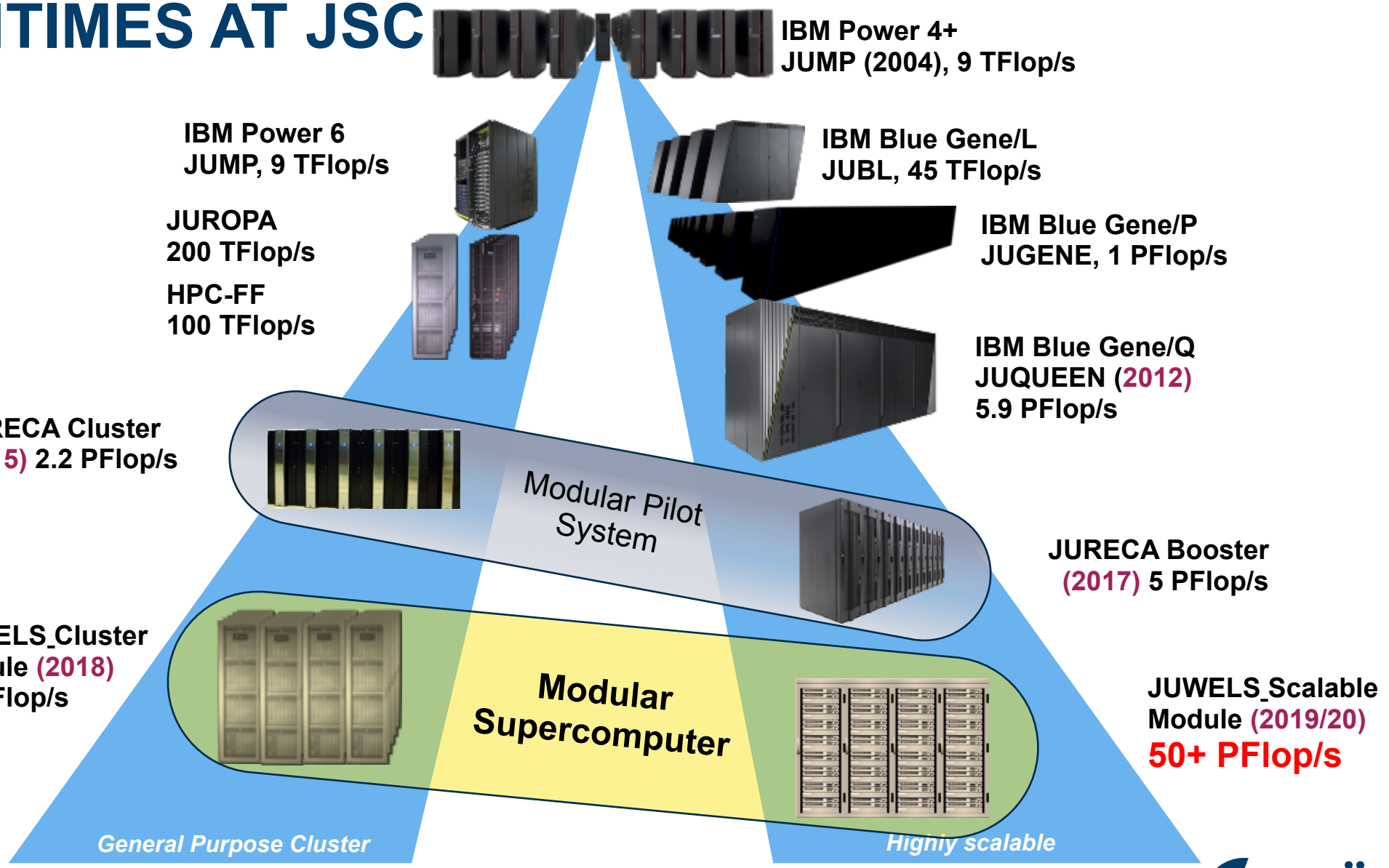
MPI RUNTIMES AT JSC

JSC's vision



MPI RUNTIMES AT JSC

JSC's vision



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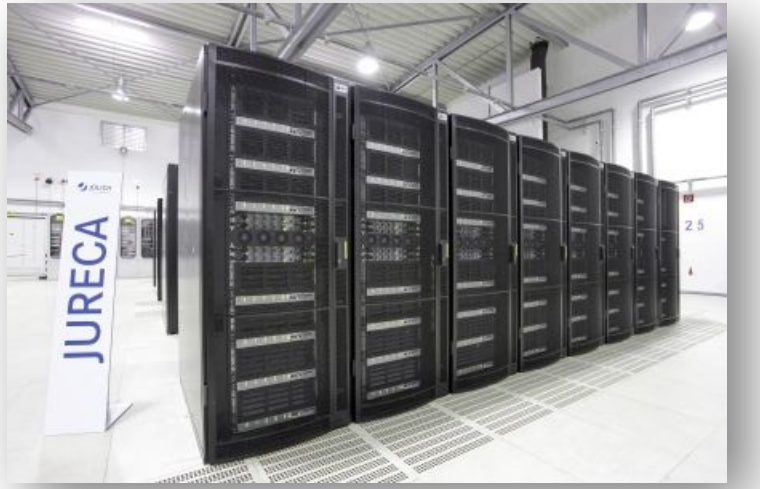
MPI RUNTIMES AT JSC

JSC's systems

JURECA

- Dual-socket Intel Haswell (E5-2680 v3)
  - 12× cores/socket
  - 2.5 GHz
  - ≥ 128 GB main memory
- 1,884 compute nodes (45,216 cores)
  - 75 nodes: 2× K80 NVIDIA GPUs
  - 12 nodes: 2 × K40 NVIDIA GPUs
    512 GB main memory
- Peak performance: **2.2 Petaflop/s** (1.7 w/o GPUs)
- Mellanox InfiniBand EDR
- Connected to the GPFS file system on JUST
  - ~15 PByte online disk and
  - 100 PByte offline tape capacity

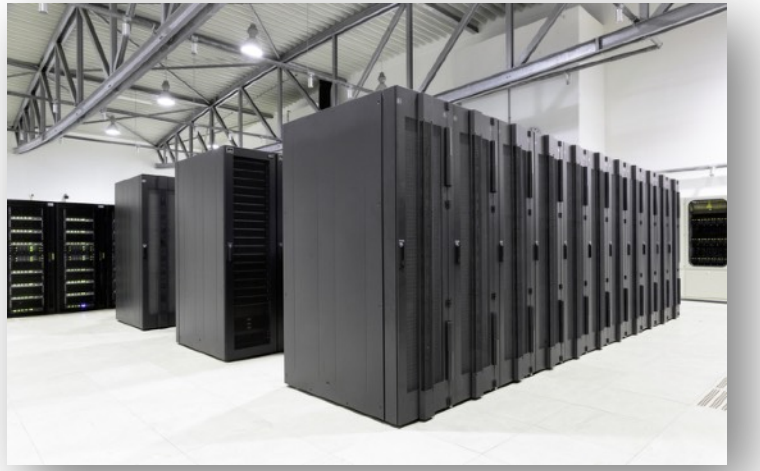


MPI RUNTIMES AT JSC

JSC's systems

JURECA Booster

- Intel Knights Landing (7250-F)
  - 68× cores
  - 1.4 GHz
  - 16 + 64 GB main memory
- 1,640 compute nodes (111,520 cores)
- Peak performance: **~5 Petaflop/s**
- Intel OmniPath
- Connected to GPFS



+JURECA

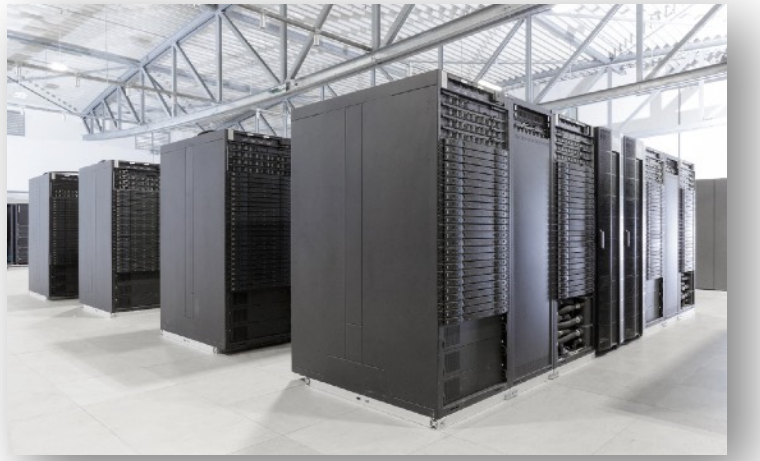
June 2018:
#14 in Europe
#38 worldwide
#66 in Green500

MPI RUNTIMES AT JSC

JSC's systems

JUWELS

- Dual-socket Intel Skylake (Xeon Platinum 8168)
  - 24× cores/socket
  - 2.7 GHz
  - ≥ 96 GB main memory
- 2,559 compute nodes (122,448 cores)
  - 48 nodes: 4× V100 NVIDIA GPUs, 192 GB main memory
  - 4 nodes: 1× P100 NVIDIA GPUs, 768 GB main memory
- Peak performance: **12 Petaflop/s** (10.4 w/o GPUs)
- Mellanox InfiniBand EDR
- Connected to the GPFS file system on JUST

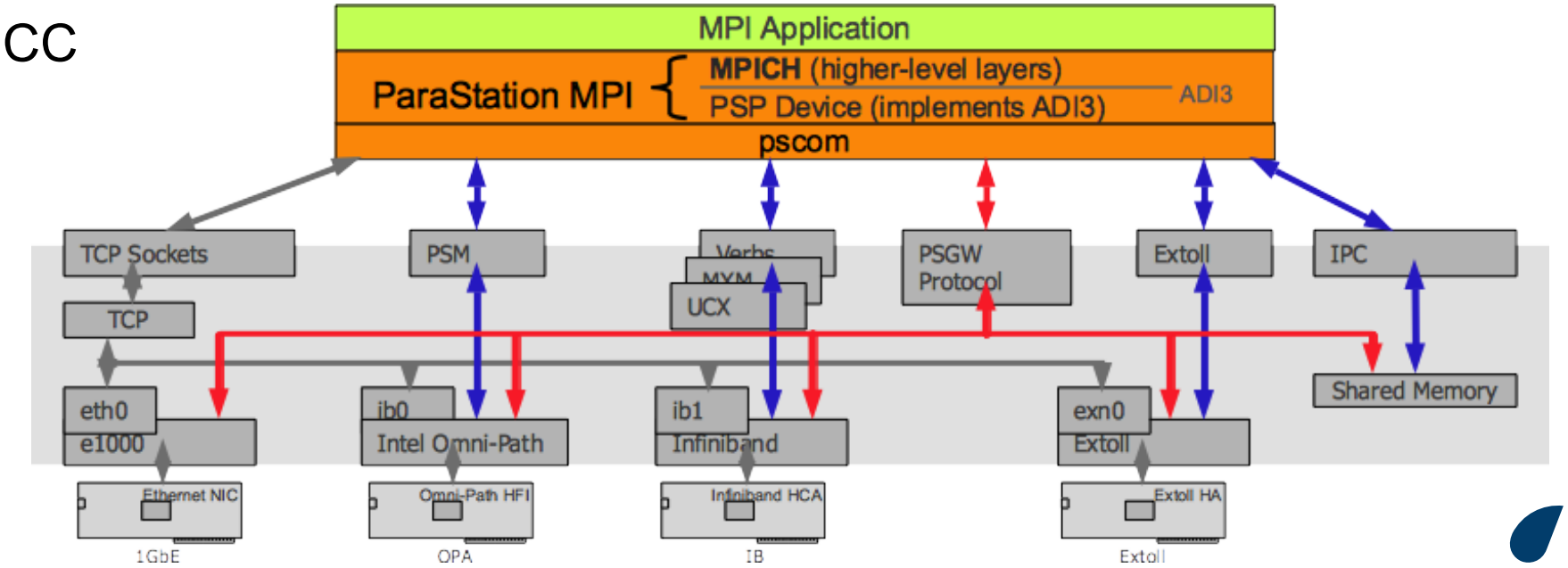


June 2018:
#7 in Europe
#23 worldwide
#29 in Green500

MPI RUNTIMES AT JSC

MPI runtimes

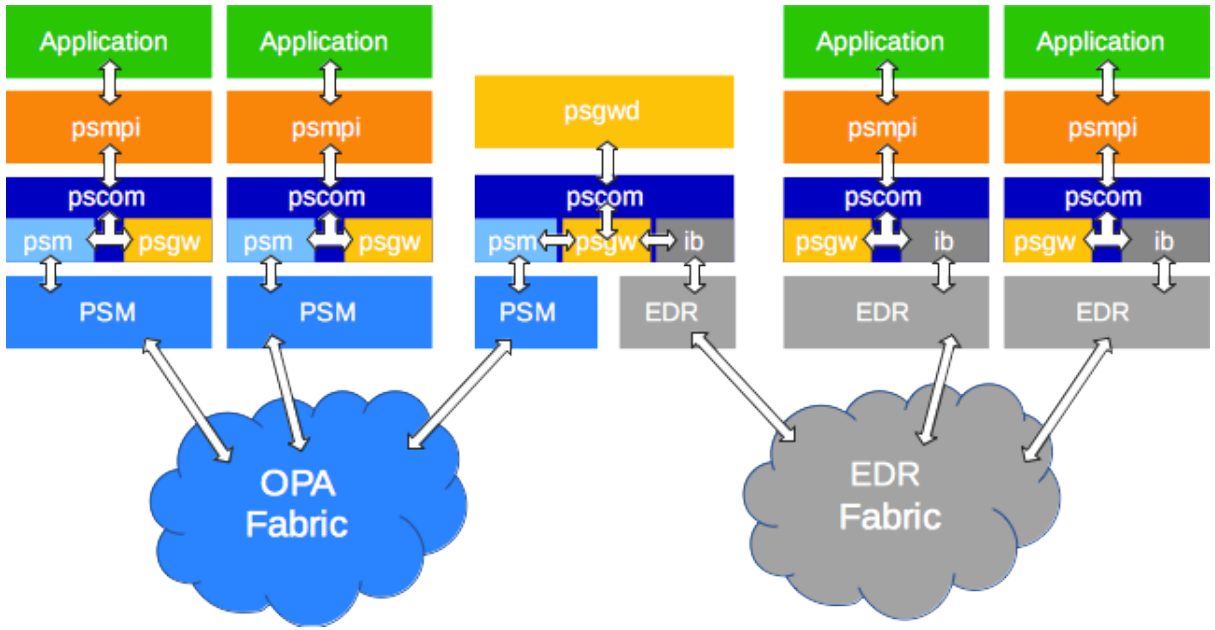
- ParaStationMPI
  - Preferred MPI runtime
  - Developed in a consortium including JSC, ParTec, KIT and University of Wüppertal
  - Based on MPICH
  - Intel + GCC



MPI RUNTIMES AT JSC

MPI runtimes

- ParaStationMPI
  - For the JURECA Cluster-Booster System, the ParaStation MPI Gateway Protocol bridges between Mellanox EDR and Intel Omni-Path
  - In general, the ParaStation MPI Gateway Protocol can connect any two low-level networks supported by *pscom*.
  - Implemented using the *psgw* plugin to pscom, working together with instances of the *psgwd*, the ParaStation MPI Gateway daemon.



MPI RUNTIMES AT JSC

MPI runtimes

- IntelMPI
  - As back up of ParaStationMPI
  - Software stack mirrored between these 2 MPI runtimes
  - Intel compiler

- MVAPICH2-GDR
  - Purely for GPU nodes (but can run in normal nodes)
  - PGI + GCC (and Intel in the past)

MPI RUNTIMES AT JSC

MPI performance

- Microbenchmarks: Intel MPI Benchmarks
  - PingPong
  - Broadcast, gather, scatter and allgather
- ParaStationMPI, Intel MPI 2018.2, Intel MPI 2019 beta, MVAPICH2 and OpenMPI
- JURECA, Booster and JUWELS
- 1 MPI process per node. Average times. No cache disabling.

MPI RUNTIMES AT JSC

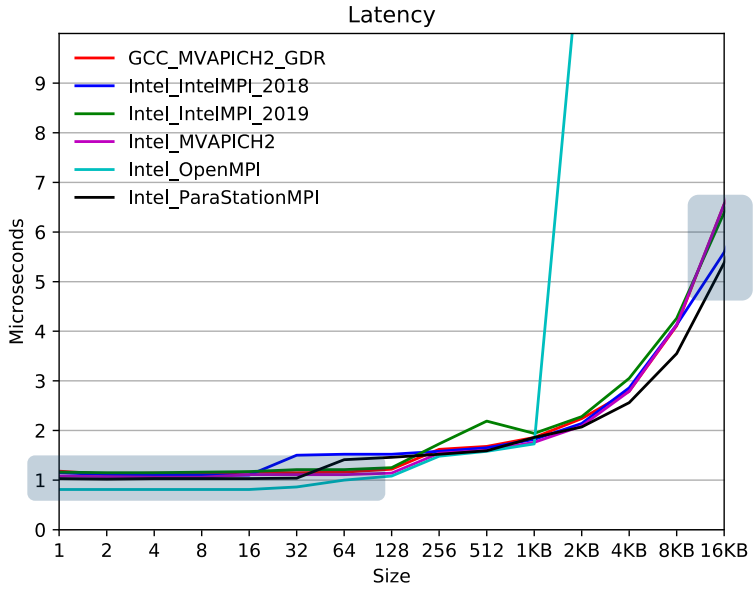
MPI performance

	Jureca	Booster	Juwels
ParaStationMPI	Verbs	PSM2	UCX
Intel 2018	Default (DAPL+Verbs)	Default (PSM2)	Default (DAPL+Verbs)
Intel 2019	Default (libfabric+Verbs)	Default (libfabric+PSM2)	Default (libfabric+verbs)
MVAPICH2-GDR	Verbs	-	-
MVAPICH2	Verbs	PSM2	Verbs
OpenMPI	Default (UCX, Verbs and libfabric+Verbs enabled)	-	-

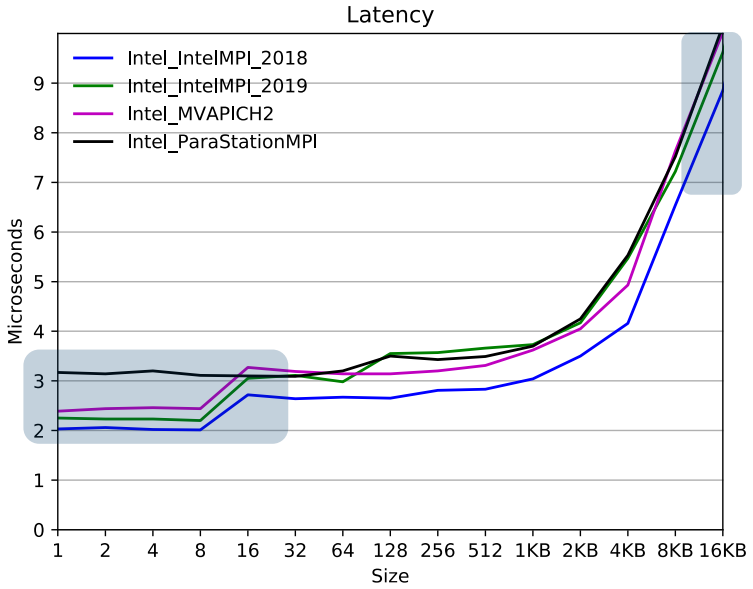
MPI RUNTIMES AT JSC

MPI performance (PingPong)

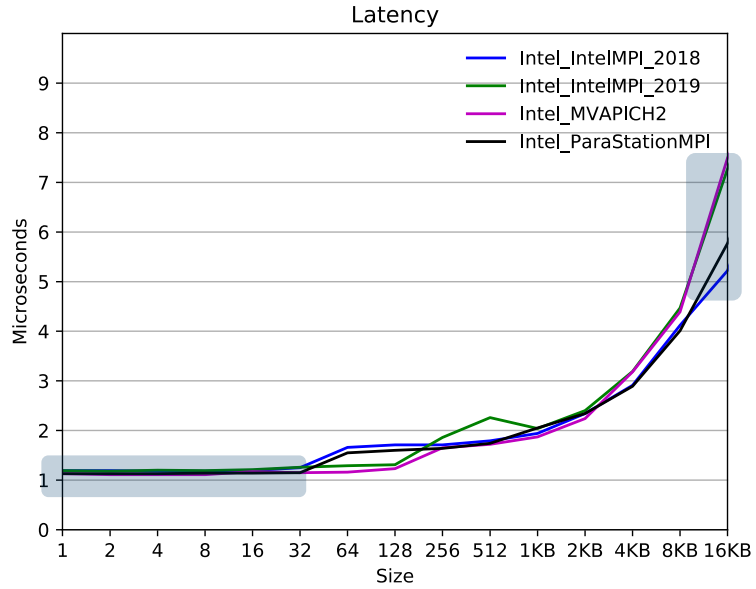
Jureca



Booster



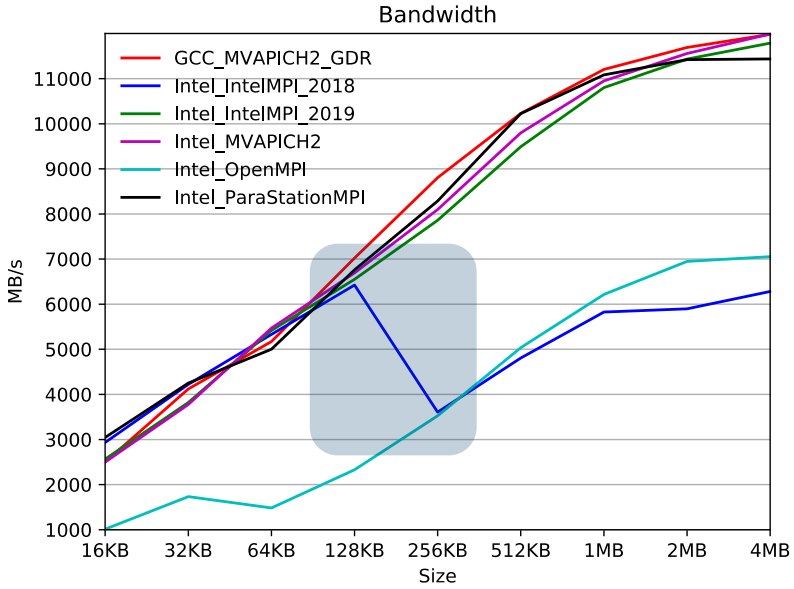
Juwels



MPI RUNTIMES AT JSC

MPI performance (PingPong)

Jureca



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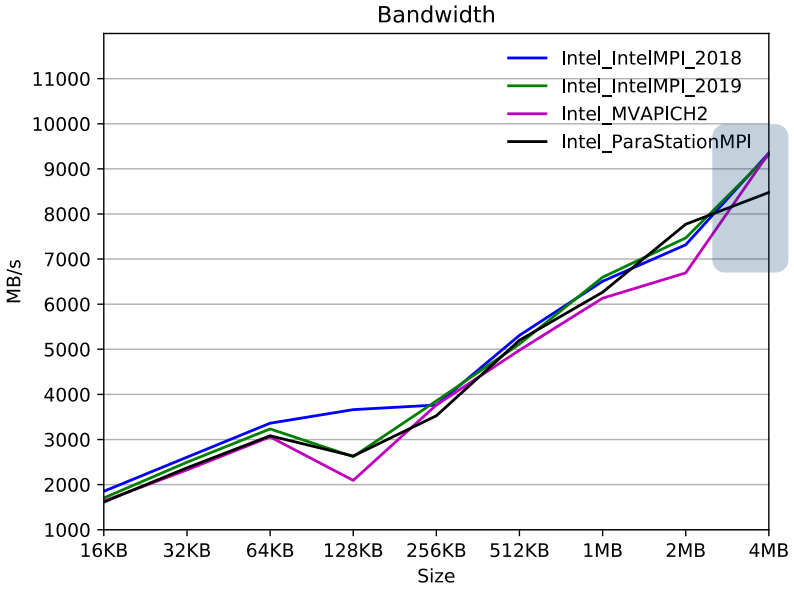
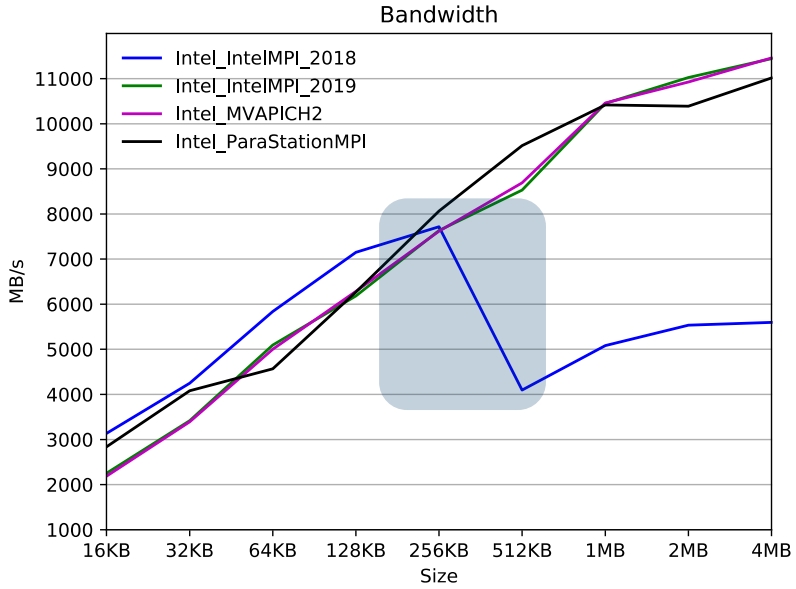


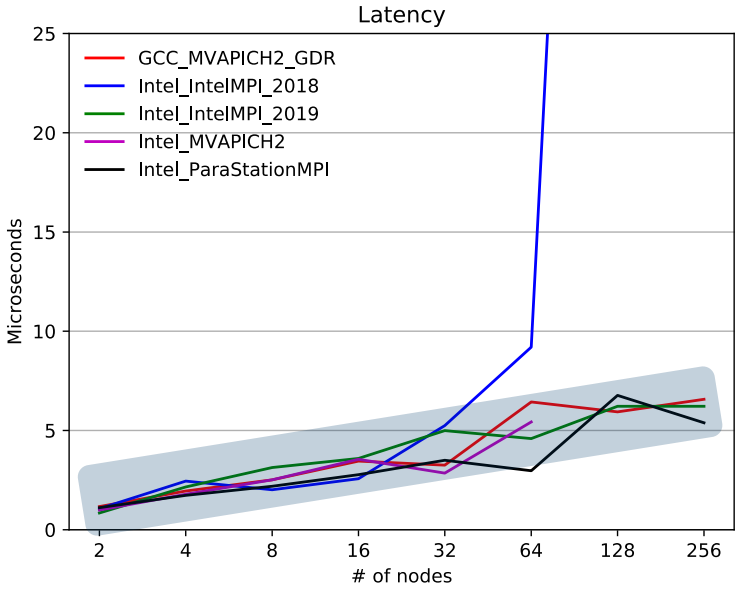
Juwels



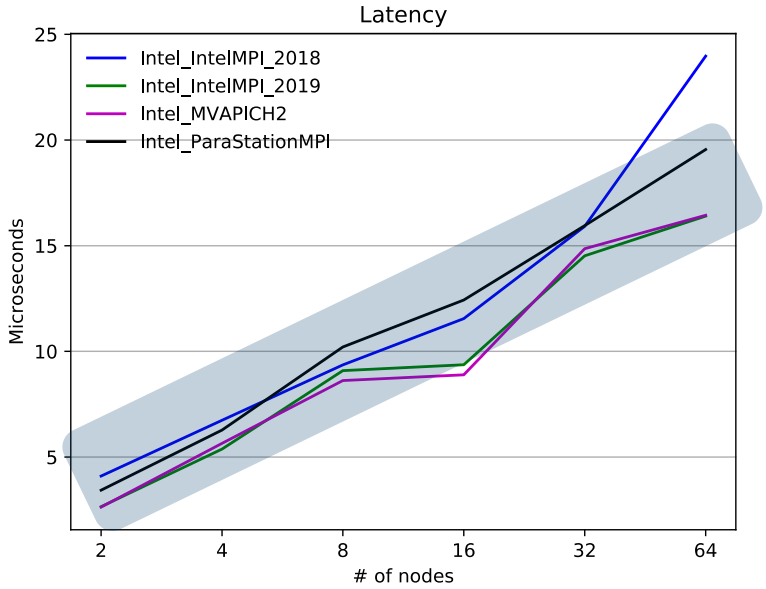
MPI RUNTIMES AT JSC

MPI performance (Broadcast, msg size 1 byte)

Jureca



Booster



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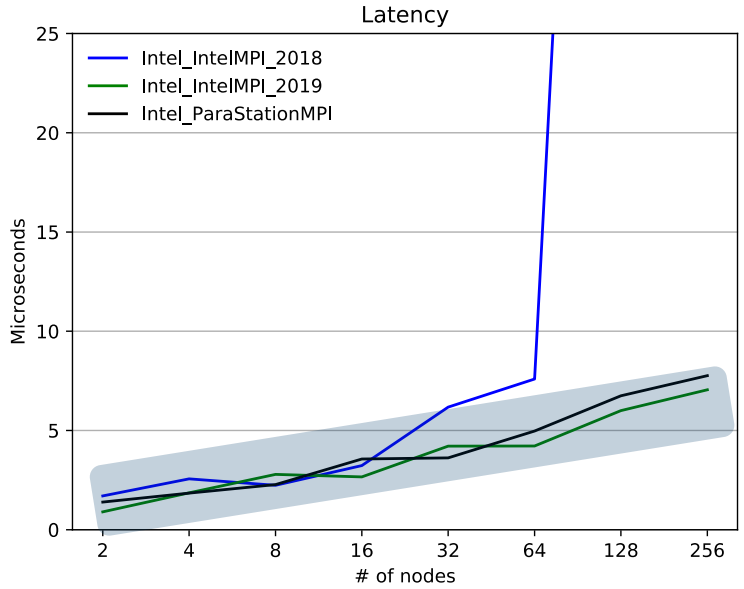

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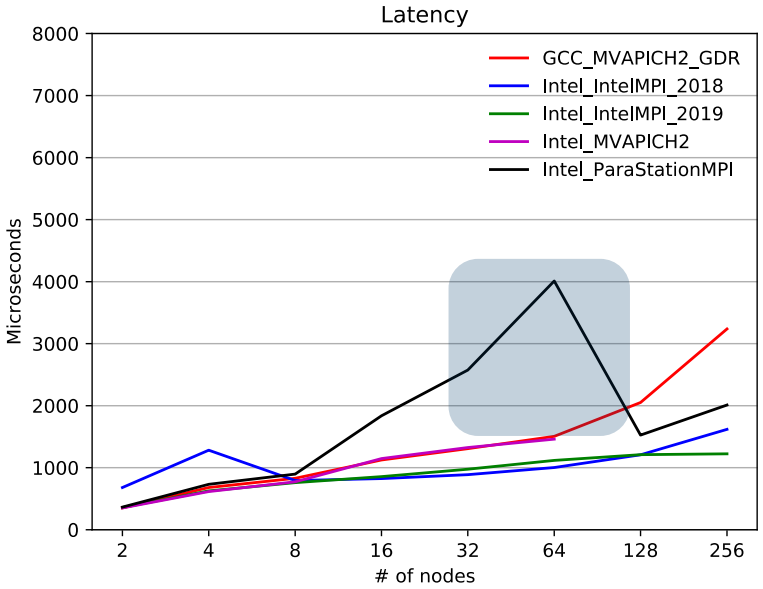
MPI RUNTIMES AT JSC

MPI performance (Broadcast, msg size 4MB)

Jureca



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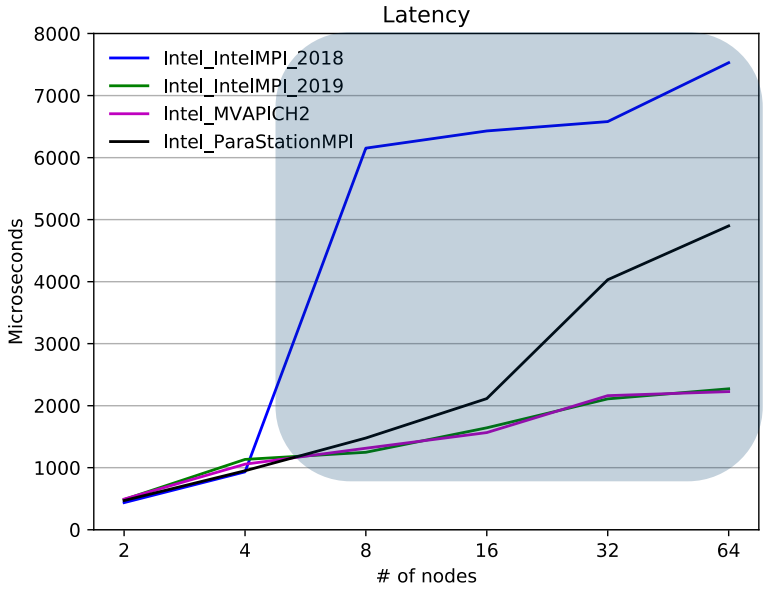
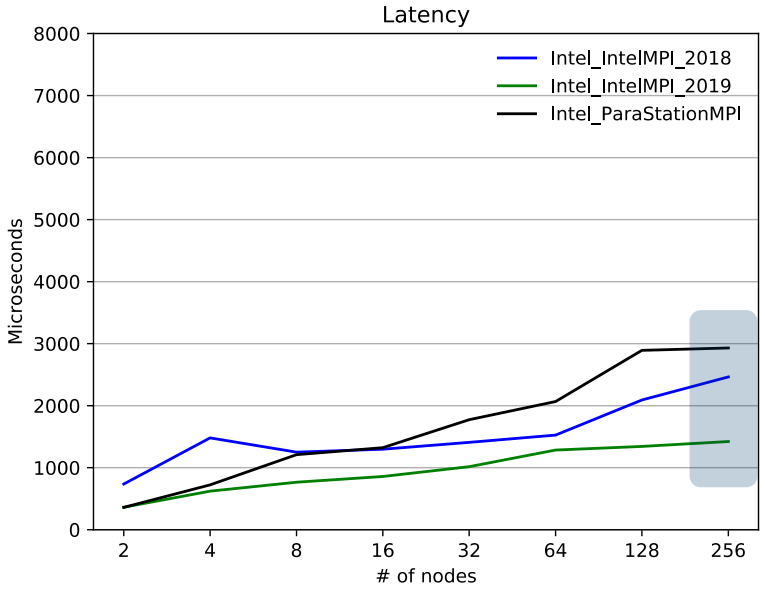


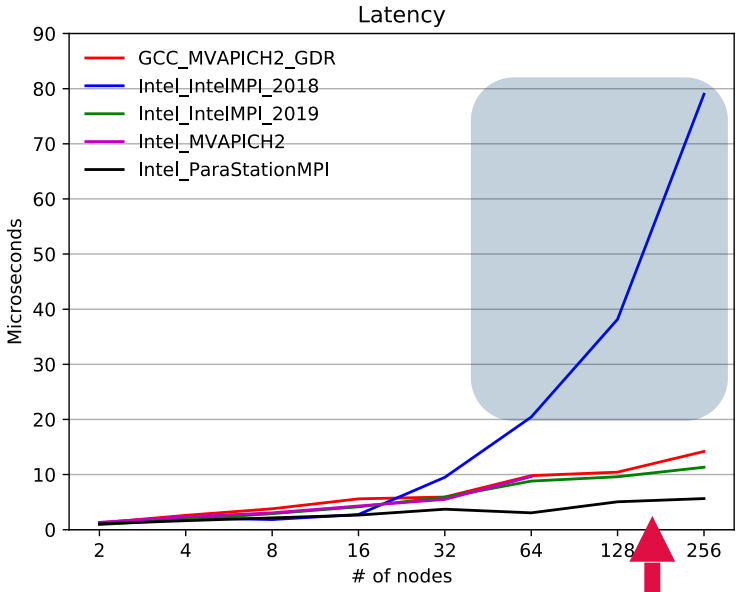
Juwels



MPI RUNTIMES AT JSC

MPI performance (Scatter, msg size 1 byte)

Jureca



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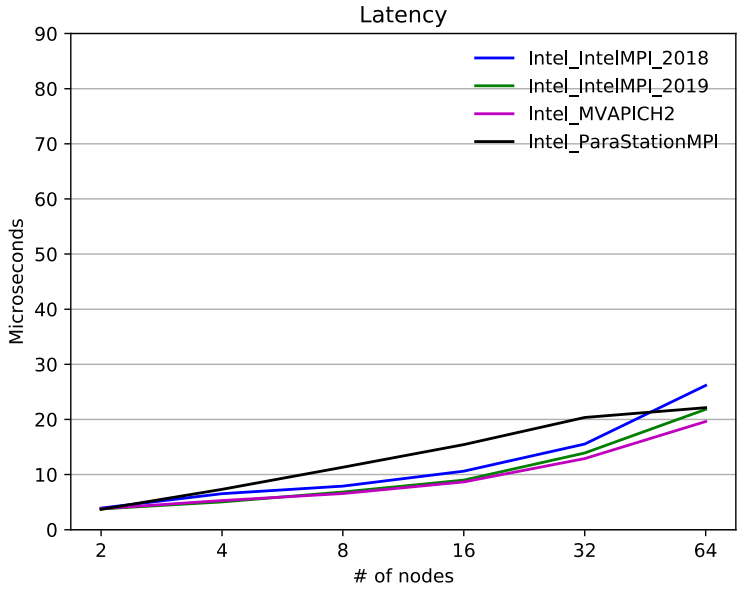

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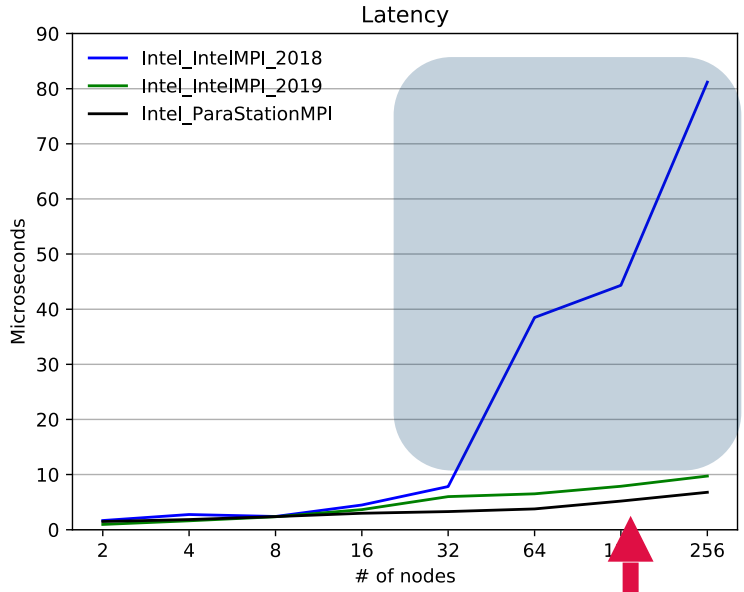
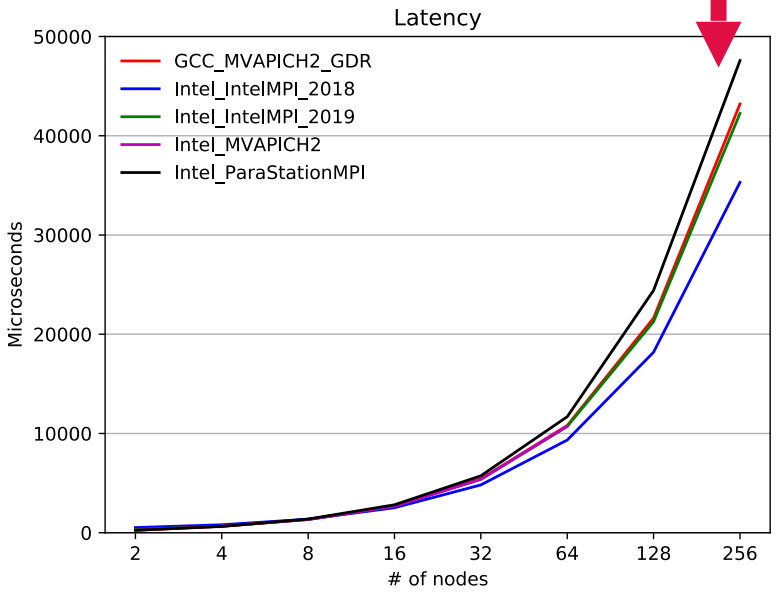


MPI RUNTIMES AT JSC

MPI performance (Scatter, msg size 2MB)

Jureca



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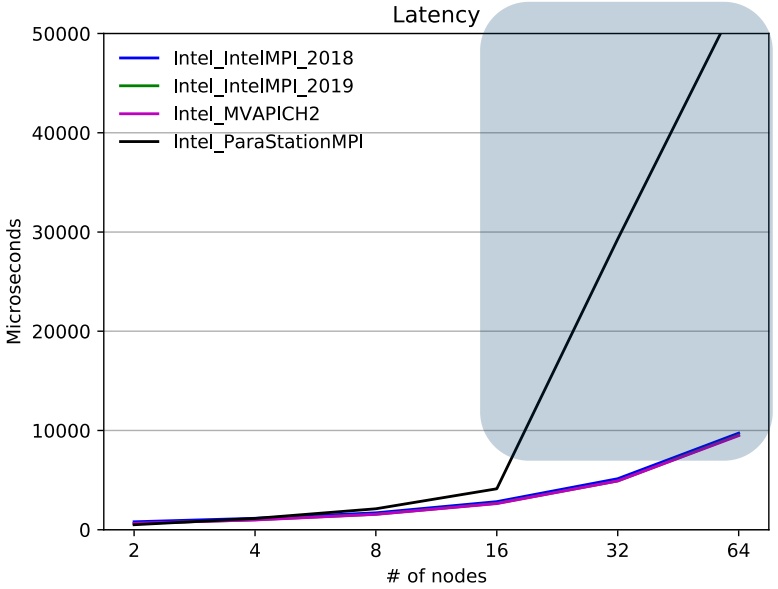

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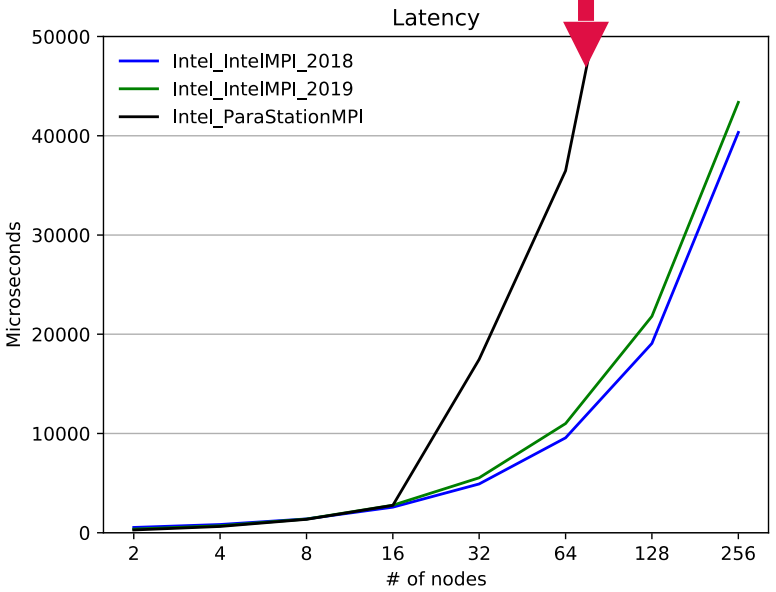
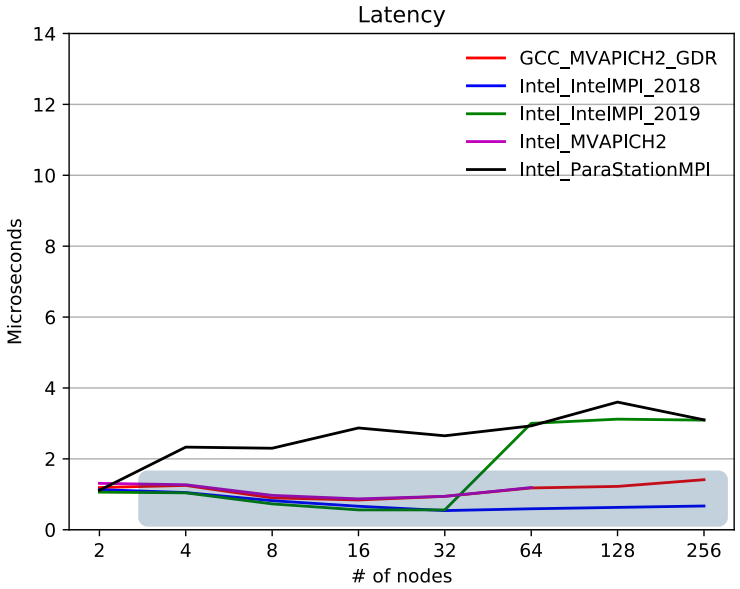


MPI RUNTIMES AT JSC

MPI performance (Gather, msg size 1 byte)

Jureca



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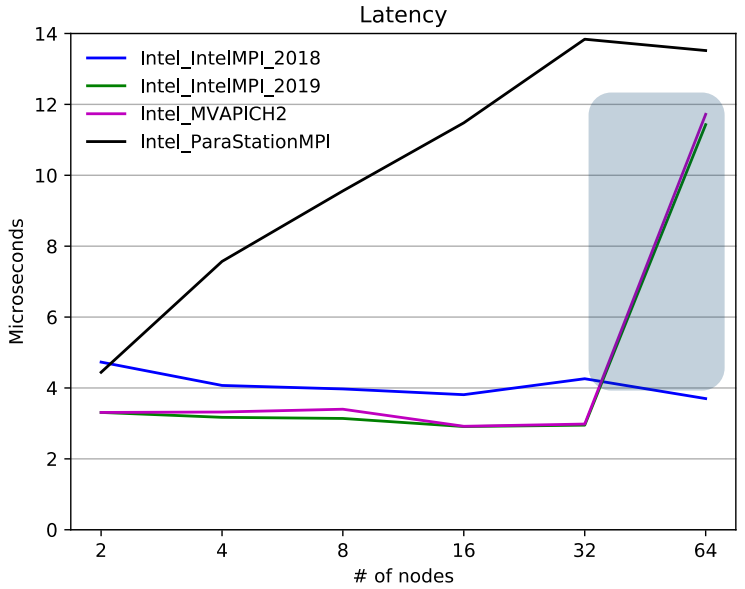

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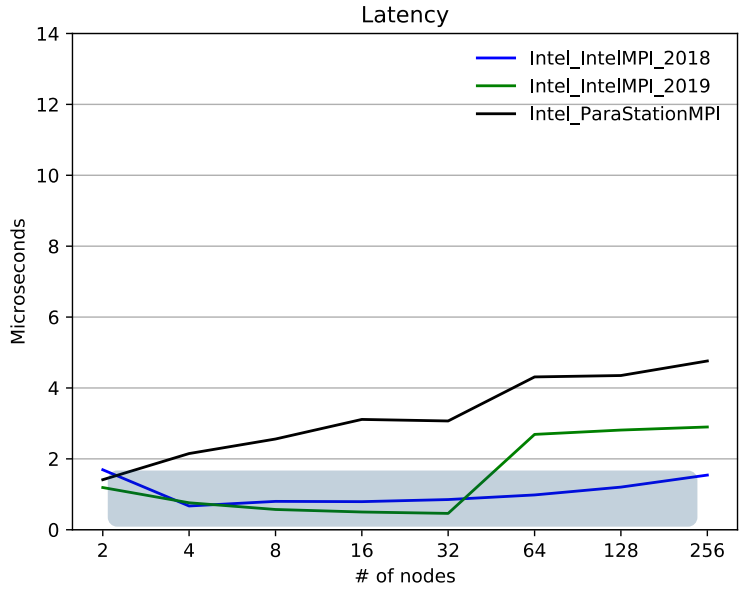
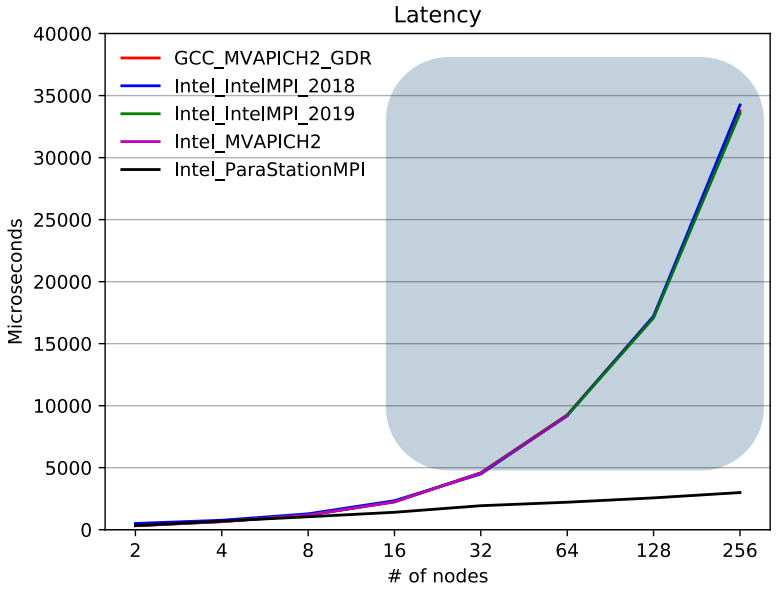


MPI RUNTIMES AT JSC

MPI performance (Gather, msg size 2MB)

Jureca



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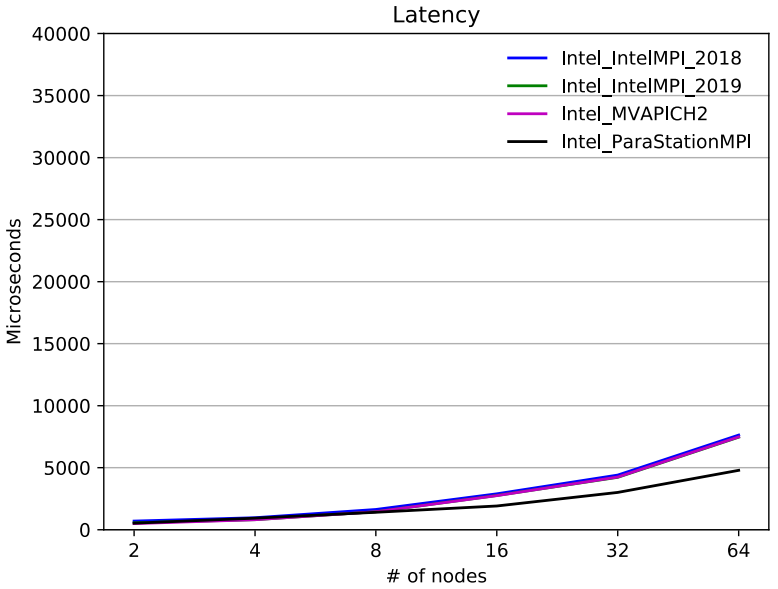

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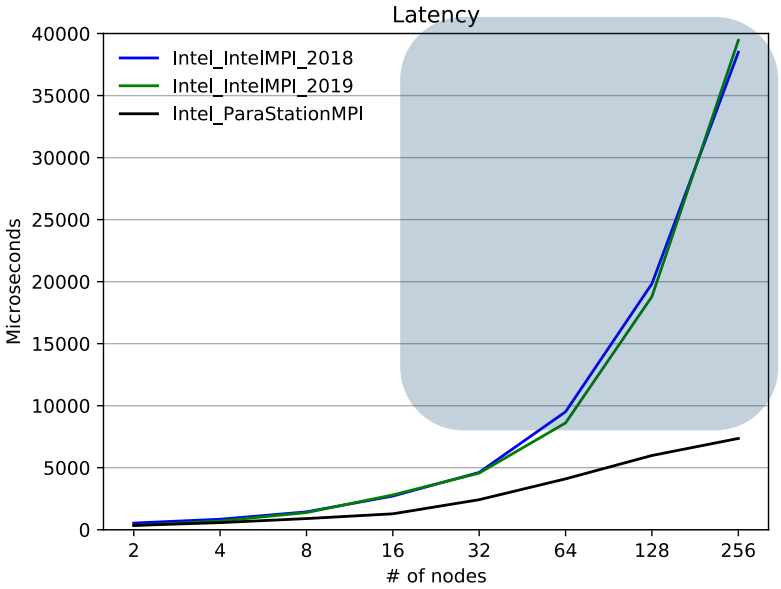


MPI RUNTIMES AT JSC

MPI performance

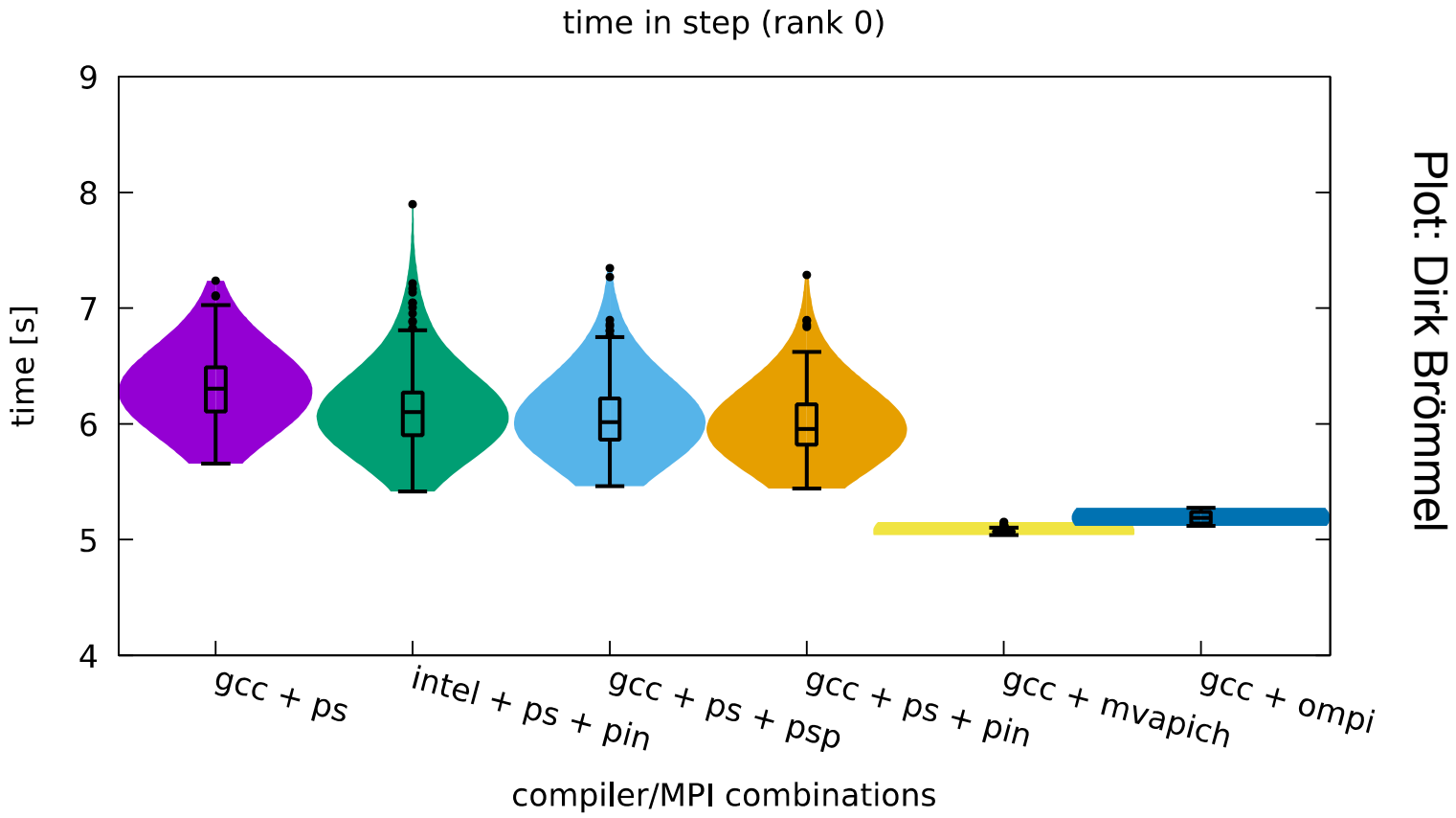
PEPC performance

- N-Body code
- Asynchronous communication based in a communicating thread spawned using pthreads
- 2 algorithms tested
  - Single particle processing with pthreads
  - Tile processing using OpenMP tasks
- Experiments in JURECA using 16 nodes, 4 MPI ranks per node and 12 computing threads per MPI rank (SMT enabled)
- Violin plots show average time per timestep and its distribution

MPI RUNTIMES AT JSC

MPI performance

- PEPC performance with single particle processing



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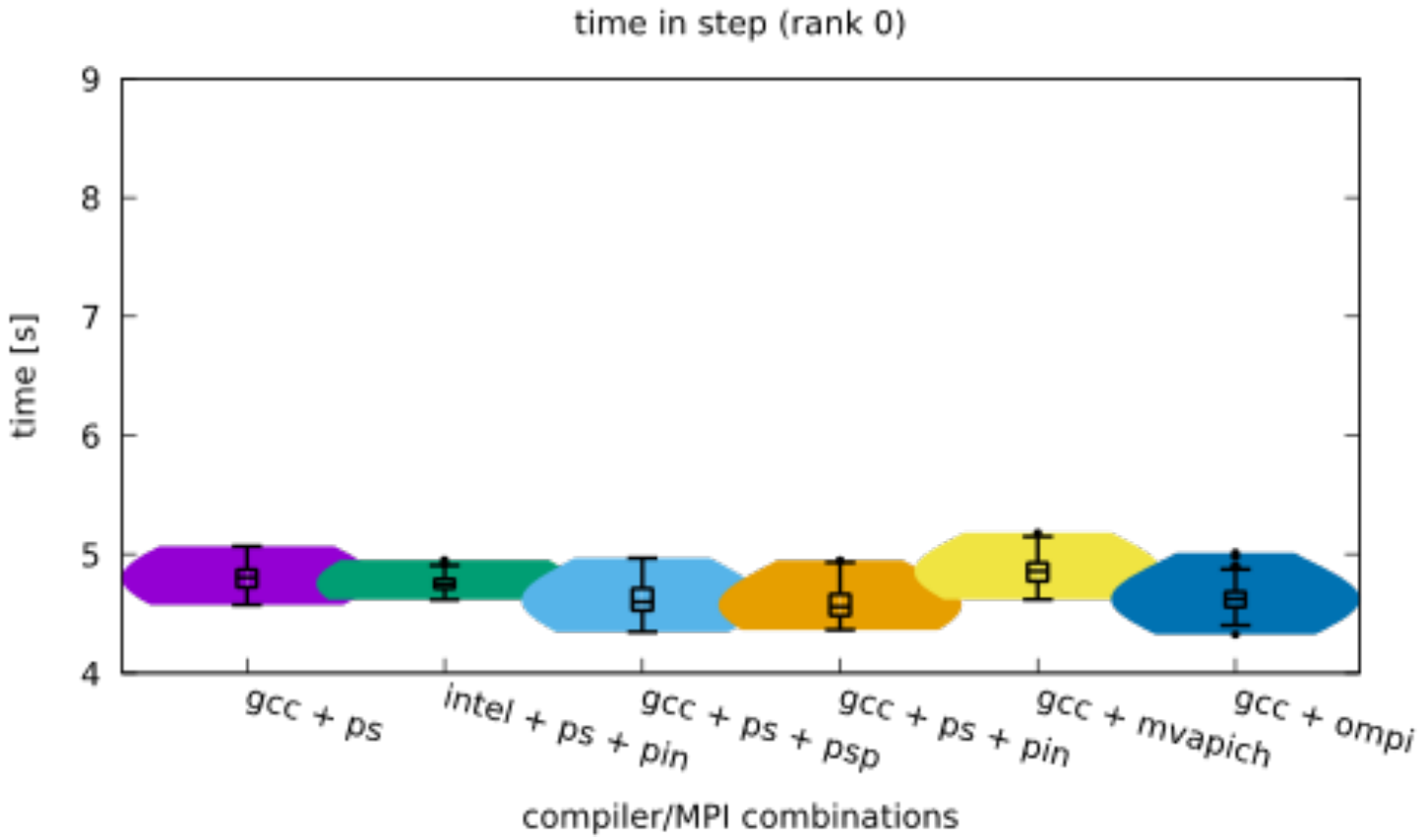
MPI RUNTIMES AT JSC

MPI performance

- PEPC performance with tile processing



Plot: Dirk Brömmel

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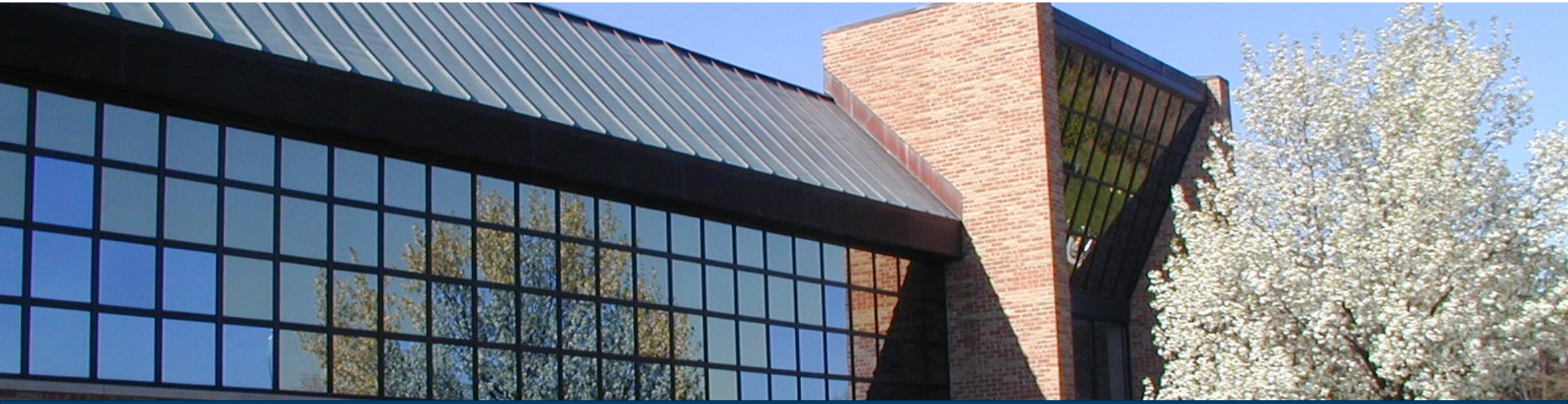
MPI RUNTIMES AT JSC

MVAPICH at JSC

- Generally it's been a positive experience. But (as the guy in charge of installing all software in our systems)….
- The fact that MVAPICH2-GDR is a binary only package poses some annoyances
  - Need to ask the MVAPICH2 team for binaries for particular compiler versions
  - No icc/icpc/ifort version
  - Patching of compiler wrappers (xFLAGS used during compilation leak into them)
- The Deep Learning community is pushing for OpenMPI as CUDA-Aware MPI of choice in our systems



THANK YOU!