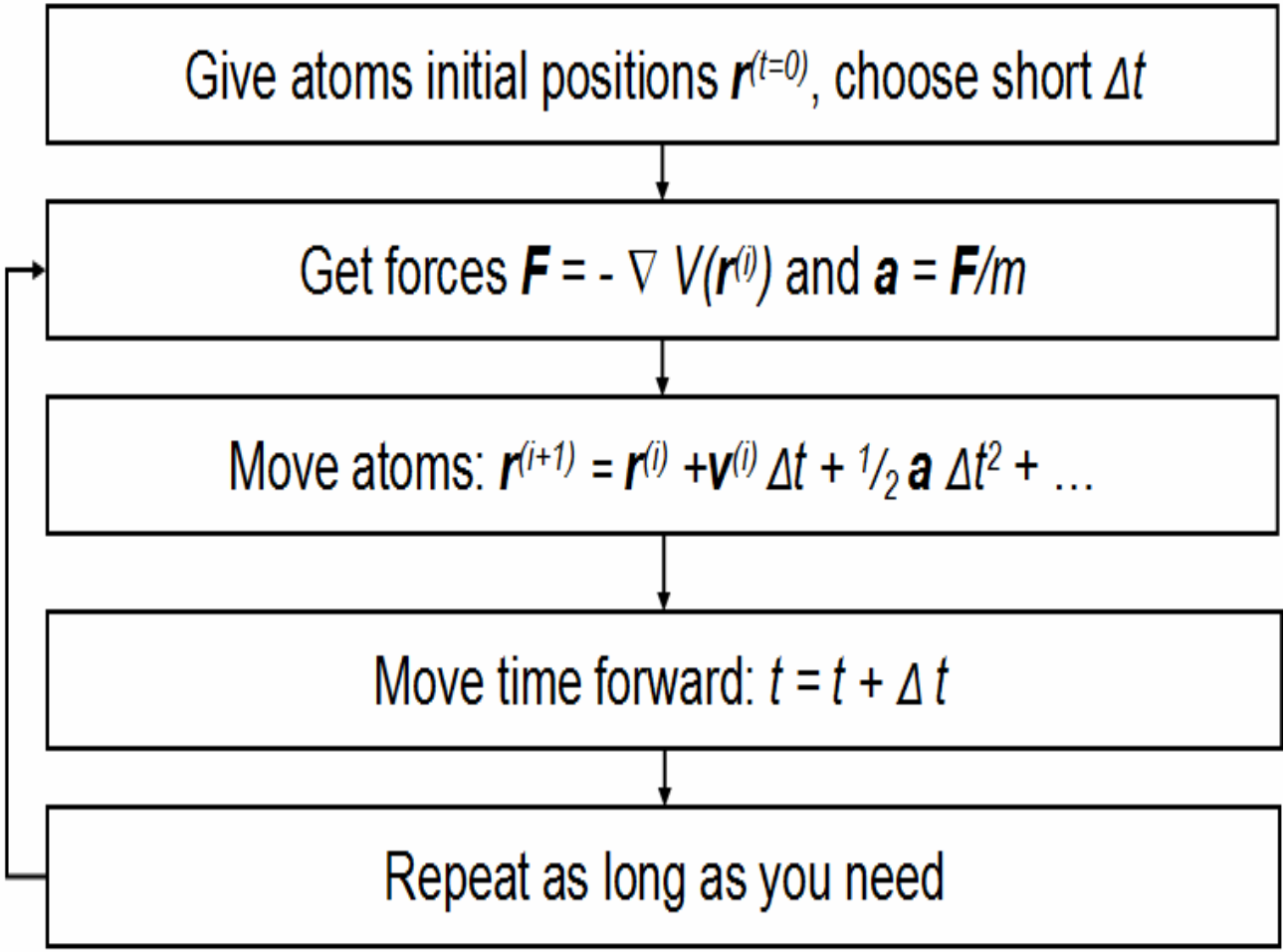
Molecular Dynamics - Gromacs

JURECA BOOSTER-CLUSTER / P. Petkov, S. Markov & V. Pavlov

Molecular dynamics

- Molecular Dynamics (MD) - solving Newtonian equations (F=m*a) of motion of atomic system to calculate its time evolution
- Forces are calculated from classical approximation of interatomic potential function called Force Field (FF). In general FF:
- Bonded terms (bonds, angles, dihedrals, …) – Real Space (Particle) Node – PP node
- Long-range interactions, Electrostatic and Van der Waals terms - Particle Mesh Ewald Algorithm (PME Node)



JURECA

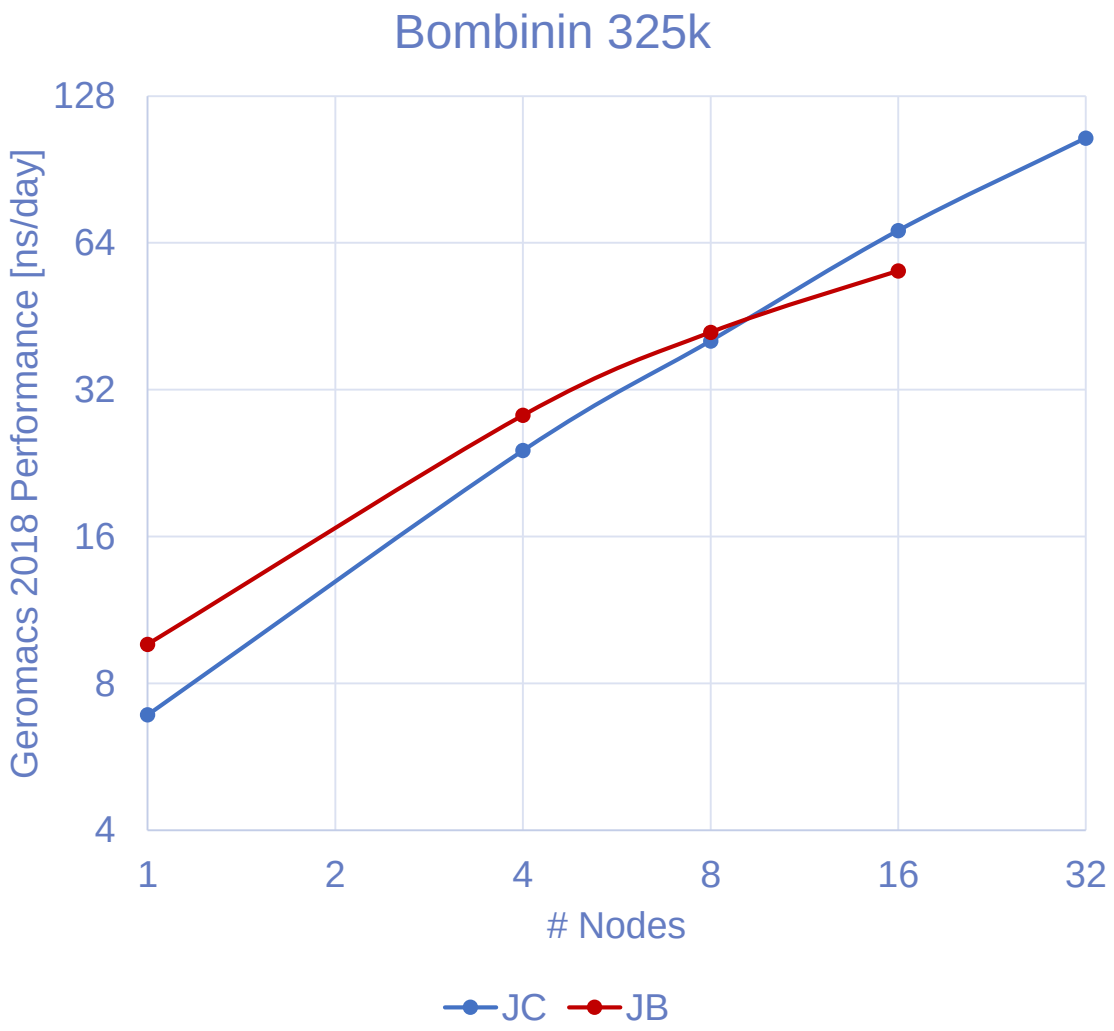
JURECA Cluster

- 1882 compute nodes based on dual-Socket Intel Xeon Haswell - 2680v3, 24 cores, 2.5 GHz
- Mellanox InfiniBand EDR100 Gb/s network !
- Full fat-tree topology
- 2.2 PF/s
- Standard configuration: 128 GB main memory
  - 128 nodes with 256 GB
  - 64 nodes with 512 GB
- 75 nodes with 2× Nvidia K80 GPUs

JURECA Booster

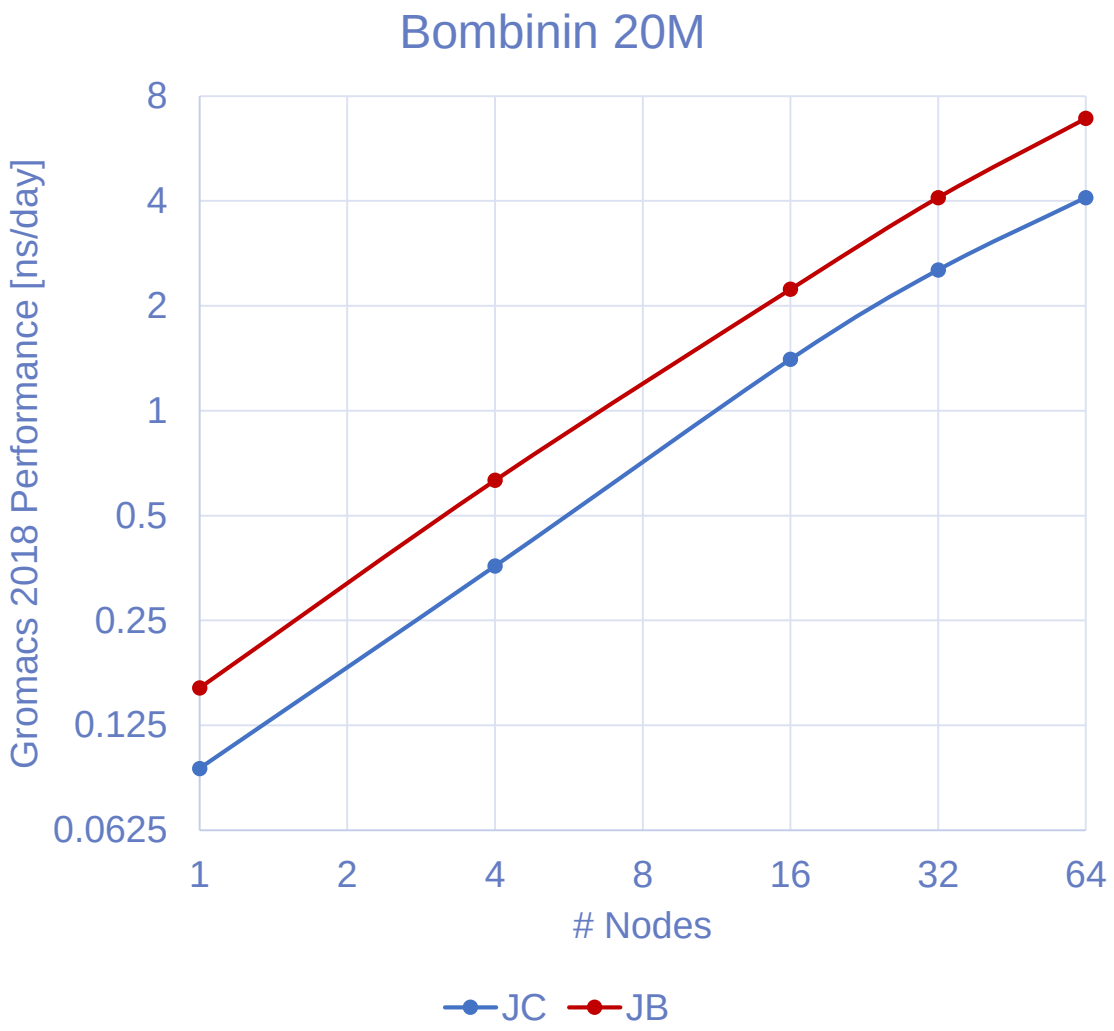
- 1640 compute nodes based on Intel Xeon Phi 7250-F - 7250-F, 68 cores, 1.7 GHz, **quad** mode, 96 GB main memory, + 16 GB MCDRAM, Currently: **hybrid50** mode
- Intel Omni-Path Architecture 100 Gb/s network !
- Full fat-tree topology
- 5 PF/s

Performance test – Bombinin 325k atoms Rc=1.2nm



- JURECA (JC):
  - 24 MPIs per Node
  - 2 OpenMP Threads per MPI
  - NPME ~0.125*(Total #MPIs)
- JURECA BOOSTER (JB):
  - 64 MPIs per Node
  - 2 OpenMP Threads per MPI
  - NPME ~(0.3 – 0.4)*(Total #MPIs)

Performance test – Bombinin 20M atoms Rc=1.2nm



- JURECA (JC):
  - 24 MPIs per Node
  - 2 OpenMP Threads per MPI
  - NPME ~0.25*(Total #MPIs)
- JURECA BOOSTER (JB):
  - 64 MPIs per Node
  - 2 OpenMP Threads per MPI
  - NPME ~(0.3 – 0.4)*(Total #MPIs)

JURECA Cluster+Booster architecture

Cluster

1884 nodes
Mellanox EDR IB
1.8 + 0.4 PF/s

Bridging: 20 Tb/s

Booster

1640 nodes
Xeon Phi 7250-F
Intel OPA
5 PF/s peak

198 MPI bridge nodes

Routing: 1.4 Tb/s

IP routing: 2 Tb/s

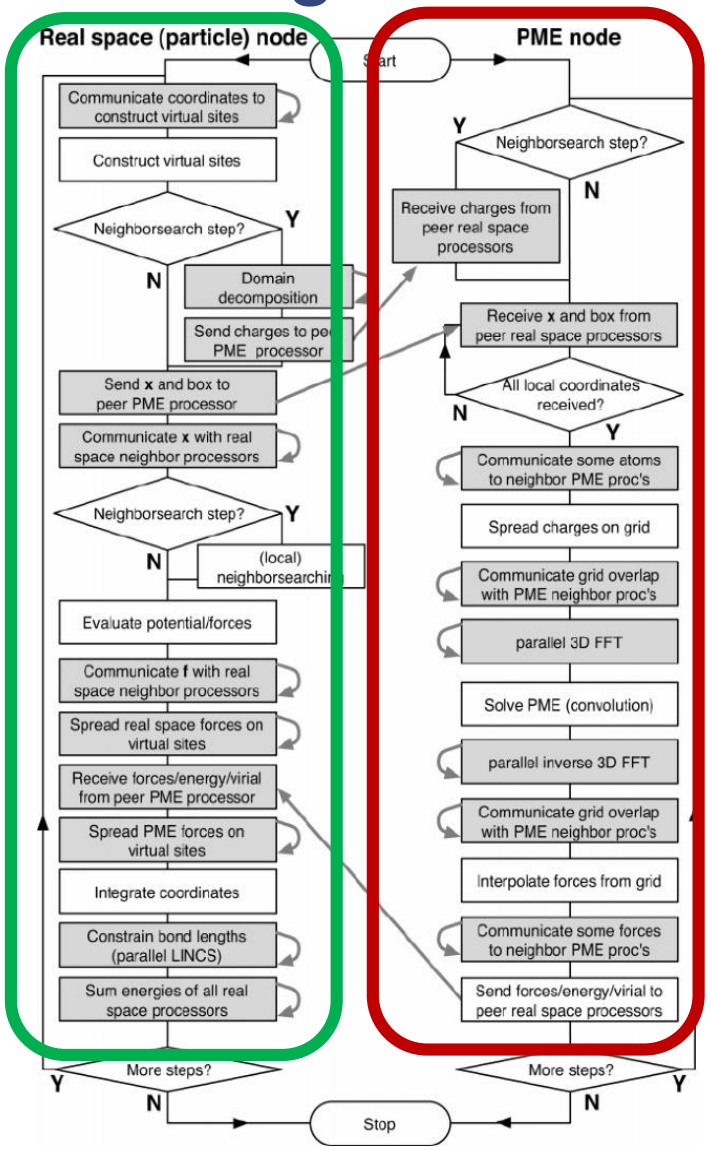
JUST Storage cluster

JURECA Cluster-Booster communication

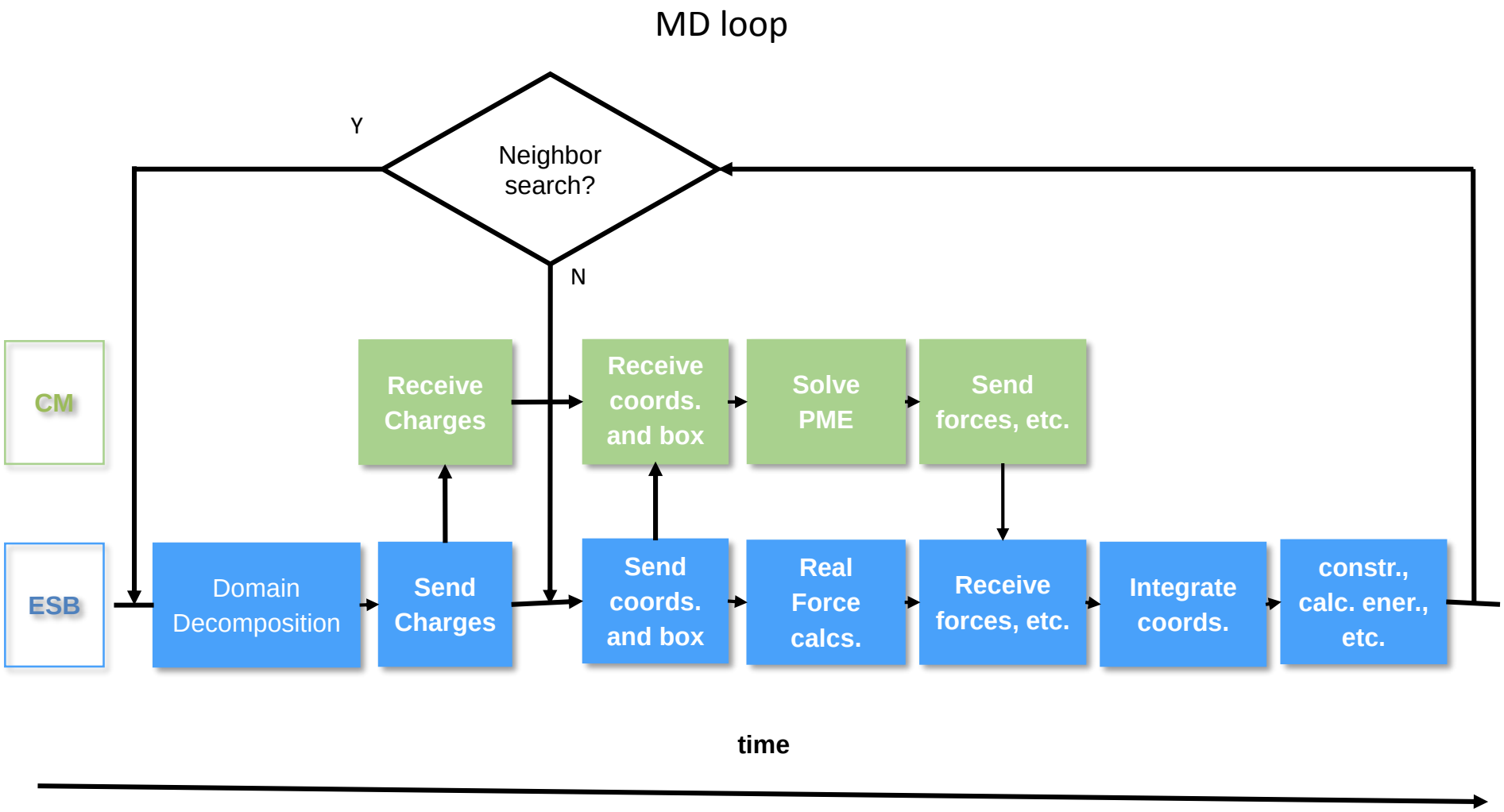
- **Hardware**
  - 198 bridge nodes: each node with 1× EDR InfiniBand HCA and 1× Omni-Path Architecture HFI
    - *Ca. 20 TB/s line-speed bridging capabilities*
- **Software**
  - Slurm 17.11 + ParaStation Modulo: psslurm plugin
    - *Unique feature: Support for heterogeneous jobs with common* ***MPI_COMM_WORLD***
    - *Note: Official Slurm support for heterogeneous MPI jobs started in version 18.08*
  - ParaStation Modulo: Gateway (GW) protocol
    - *ParaStation psgwd gateway daemons launched on bridge nodes*
    - *GW protocol integrated in ParaStation pscom layer ⇨ Transparent for MPI application using ParaStation MPI (except routing choices)*

Gromacs Flow Chart and Application partitioning

- In GROMACS one can divide MPI ranks into two groups one for real-space calculations (PP nodes) and the rest dedicated to PME calculations (PME nodes).
- At the beginning of the time step, each PP node **sends coordinates and charges** to its corresponding PME node and ones the **PME calculations are done** each PME node **sends the resulting forces back** to the corresponding PP node.
- Meanwhile, **all collective communications** go **only between PME nodes** and **only between PP nodes** which **overlaps FFT communications (exchanged between PME nodes only) with real-space calculations.**



Application mapping

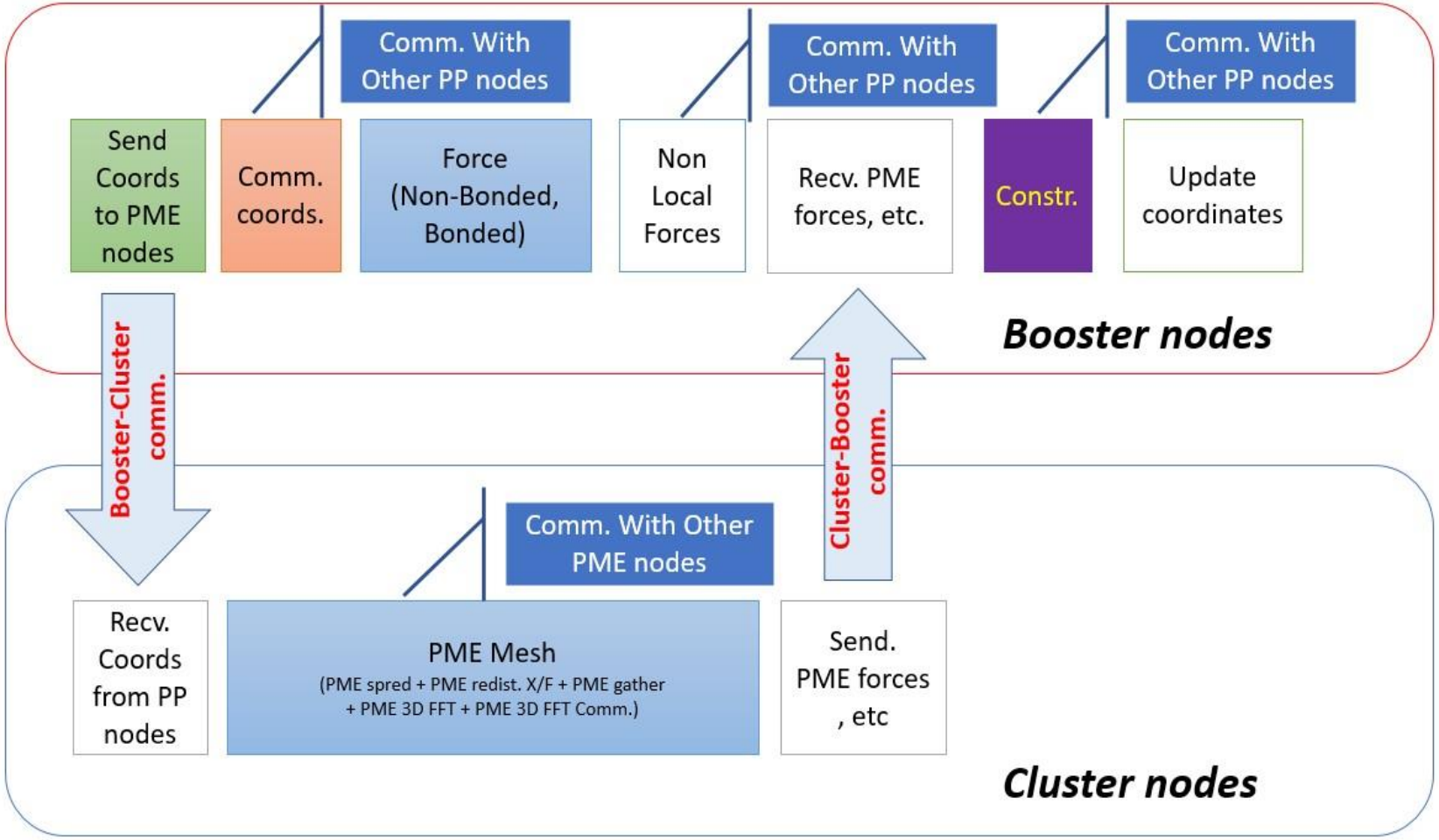


Gromacs performance counters

Gromacs performance counters description (herein we will mention only a subset of them, mainly those used in the analysis due to their non-negligible influence on the performance scalability judgement):

- PP MPI processes
  - Send X to PME – time spent by PP ranks for sending atoms' coordinates to PME ranks
  - Comm. coord. – time spent to exchange atoms' data used for calculations wih other domains
  - Force – pair interactions force calculations
  - Wait + Comm. F (named "non-local forces" in the next slide) – time needed to communicate forces contributions calculated on other domains
  - Update (named "Update coordinates" in the next slide) – set new coordinates and velocities at the end of the timestep calculations
  - Constraints – in the particular case, calculations and communication time need for keeping bonds length fixed and water molecule rigid.
- PME PMI processes
  - PME mesh – the time needed for PME forces calculations
  - PME redist. X/F – redistribute atoms parameters and coordinates before each FFT calculation
  - PME spread and PME gather – spreading and gathering the data across PME ranks
  - PME 3D-FFT and PME 3D-FFT Comm. – time spent in FFT itself and needed communications, respectively.

Gromacs performance counters (II)

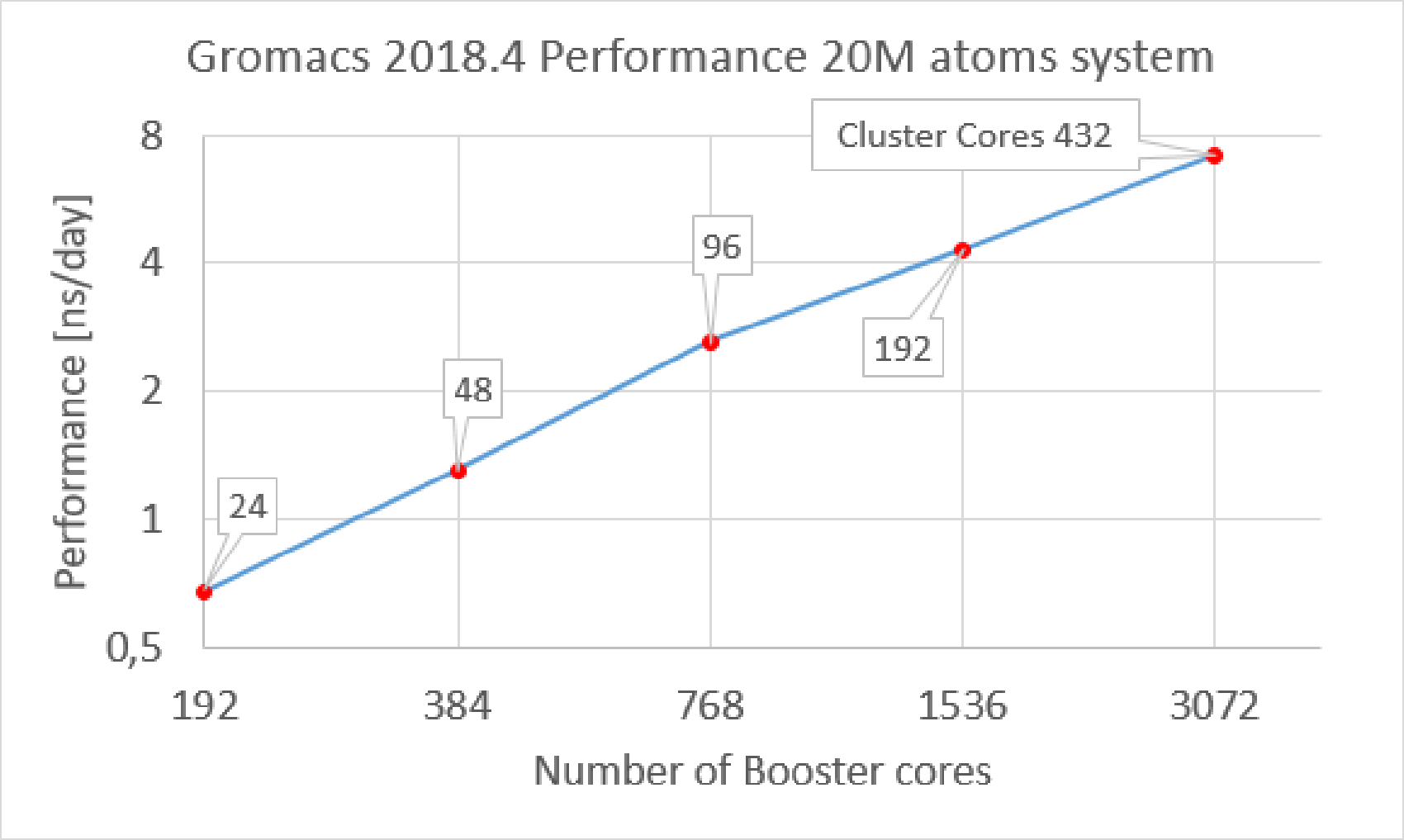


Test simulations

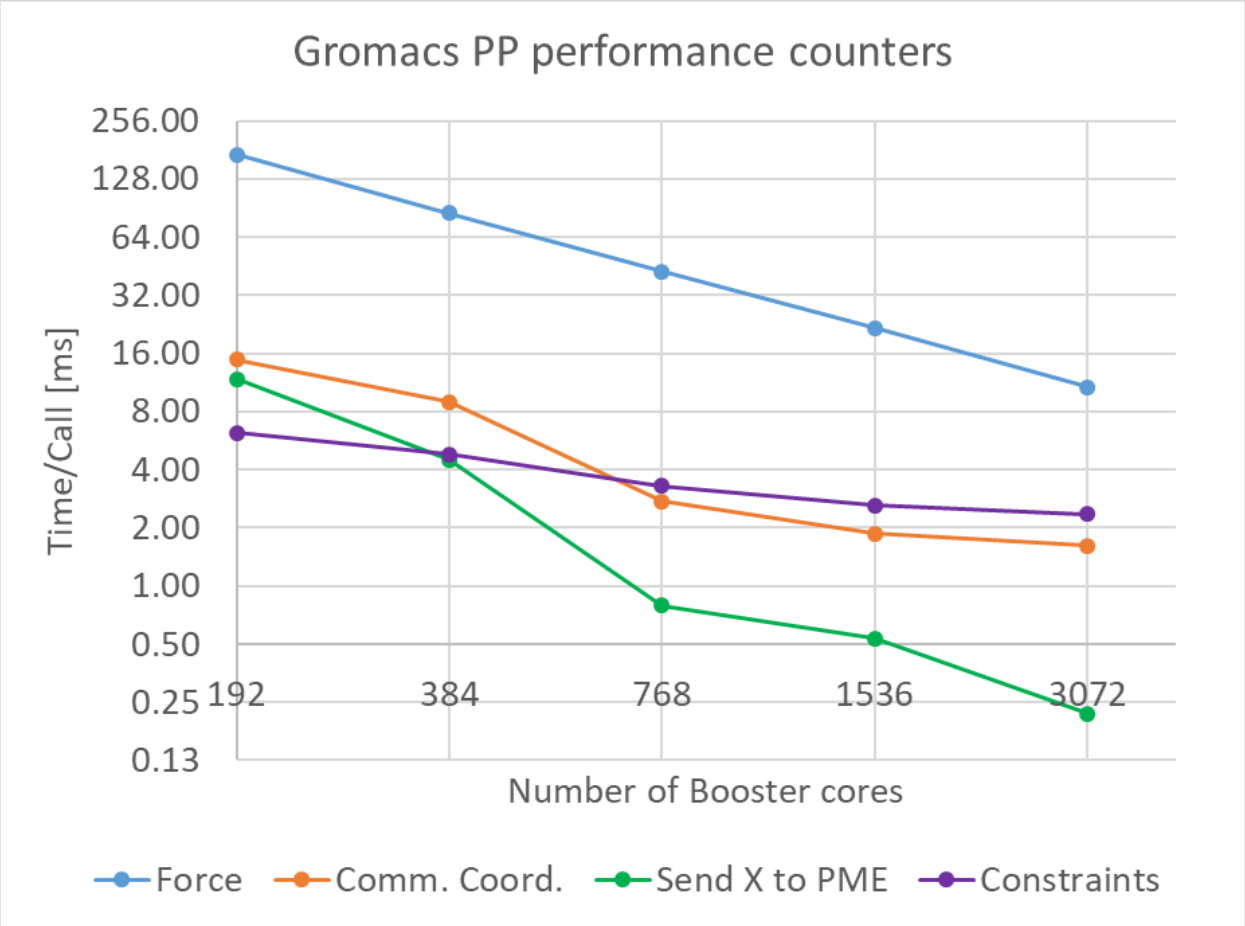
BOOSTER NODES	TOTAL NUMBER OF BOOSTER CORES	BOOSTER MPIS / THREADS PER MPI	CLUSTER NODES	TOTAL NUMBER OF CLUSTER CORES	CLUSTER MPIS / THREADS PER MPI	NUMBER OF GATEWAYS
3	192	192/2	1	24	24/2	8
6	384	384/2	2	48	48/2	8
12	768	768/2	4	96	96/2	32
24	1536	1536/2	8	192	192/2	64
48	3072	3072/2	18	432	432/2	128

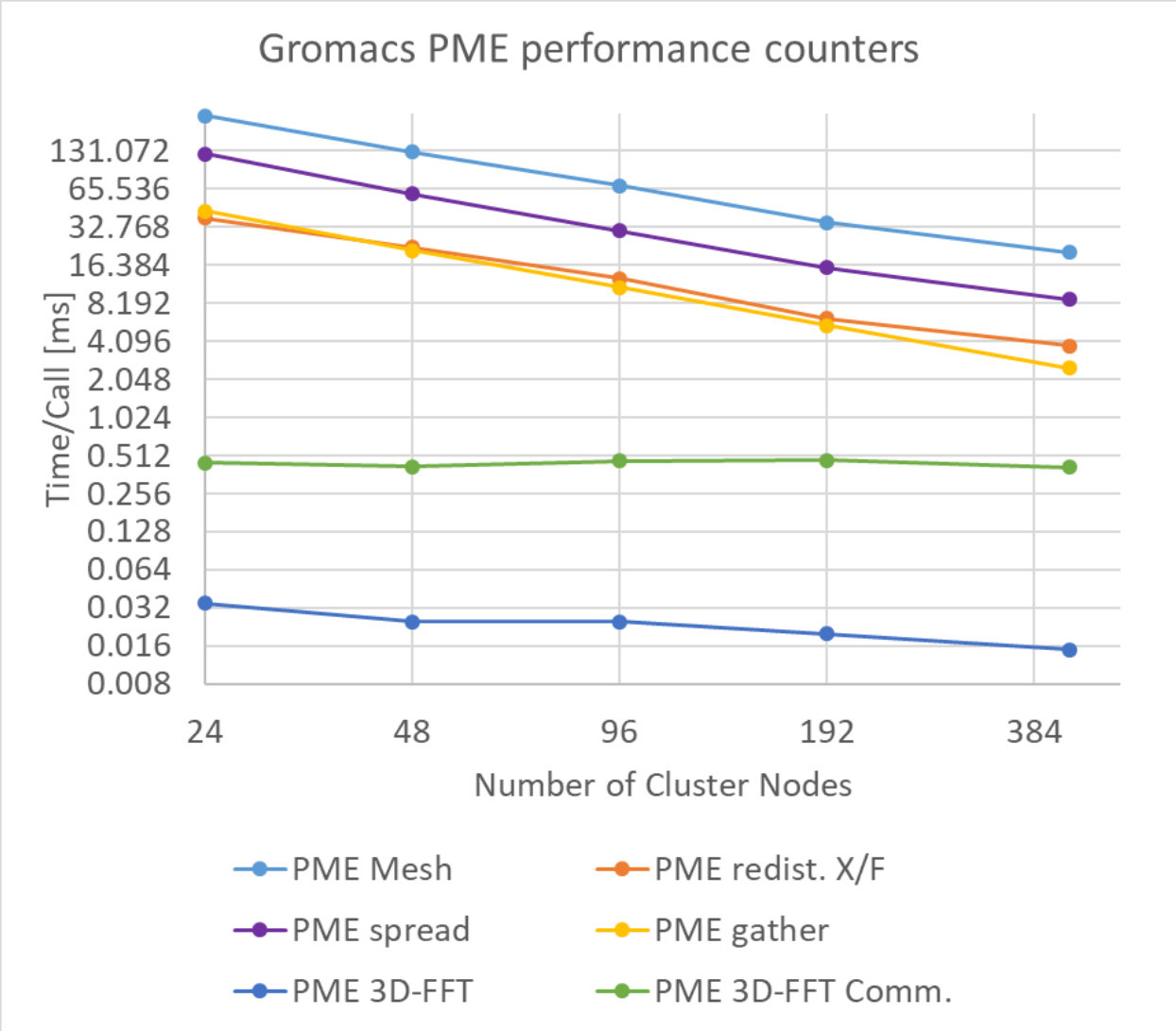
N.B.: The job parameters like PP/PME MPI ranks ratio and number of gateways were optimized for maximal performance for given number of BOOSTER nodes.

Performance scalability results – 20M atoms MD simulation

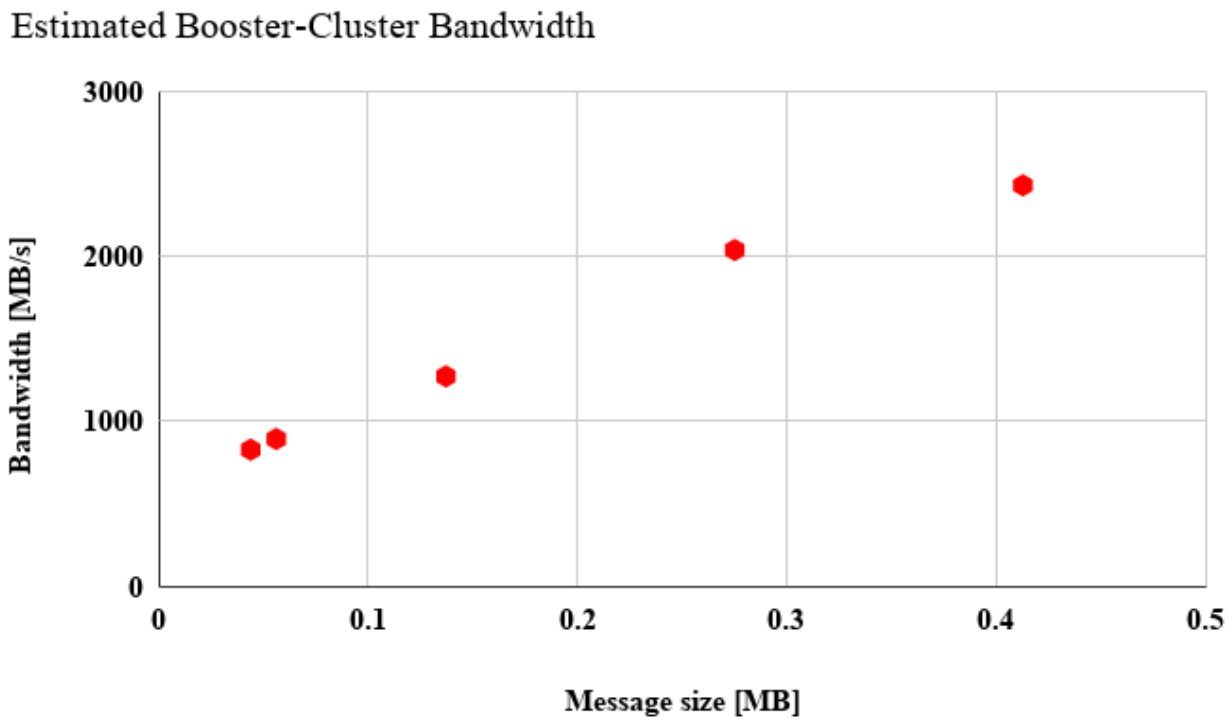


Gromacs performance counters analysis





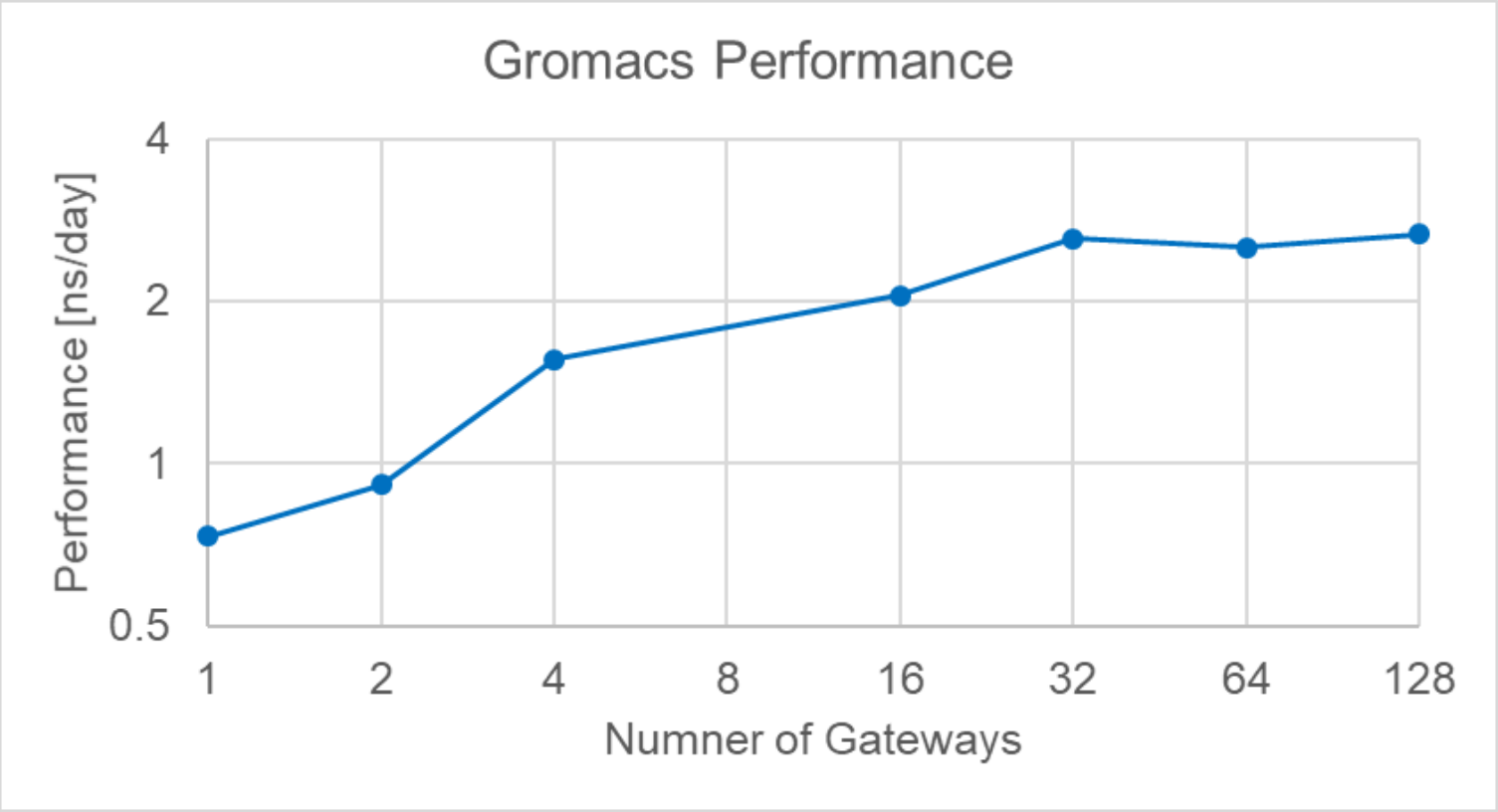
Estimated Cluster-Booster bandwidth



- Test simulations with 2.2 M and 20 M atoms on a various number of Booster and Cluster nodes keeping nPP/nPME ration about 3 to have the same domain decomposition as in performance scalability test, but the different length of the messages.
- The number of gateways used was always 8.

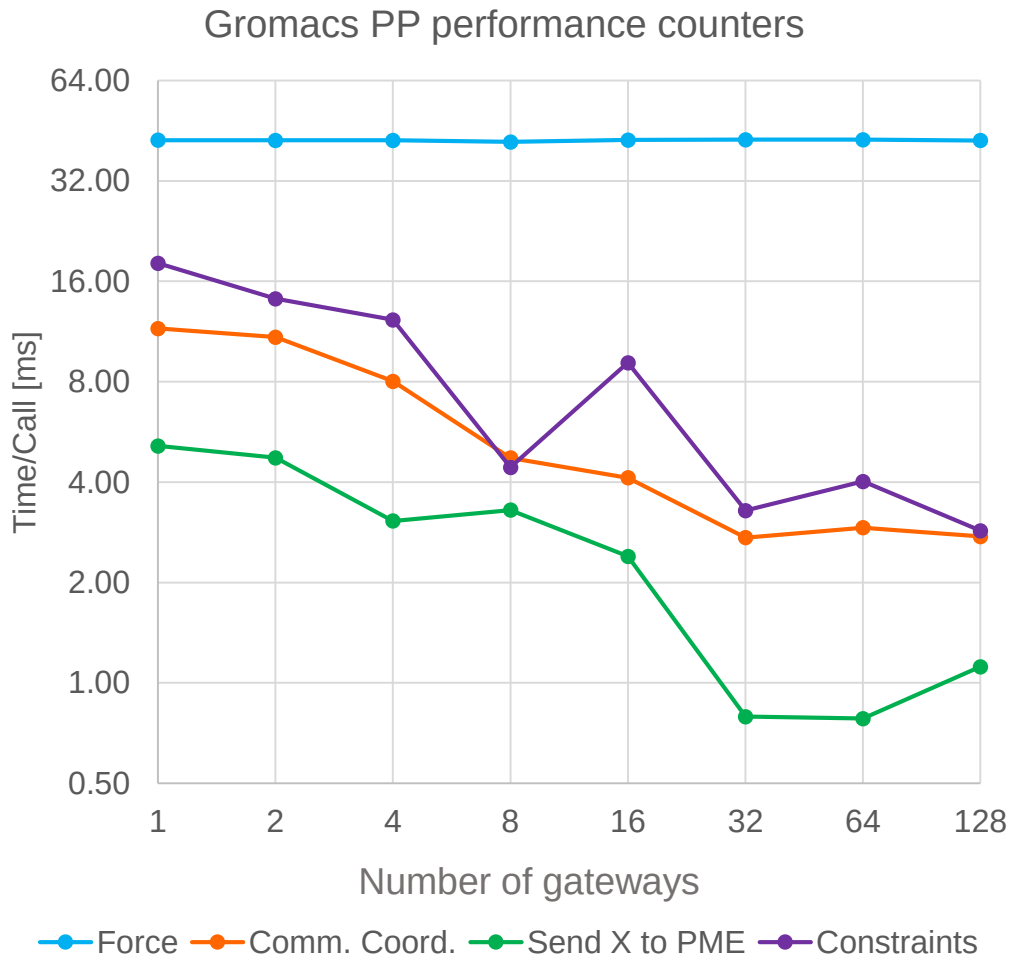
in a very good agreement with the result from the synthetic tests reported in https://bscw.zam.kfa-juelich.de/bscw/bscw.cgi/2712620

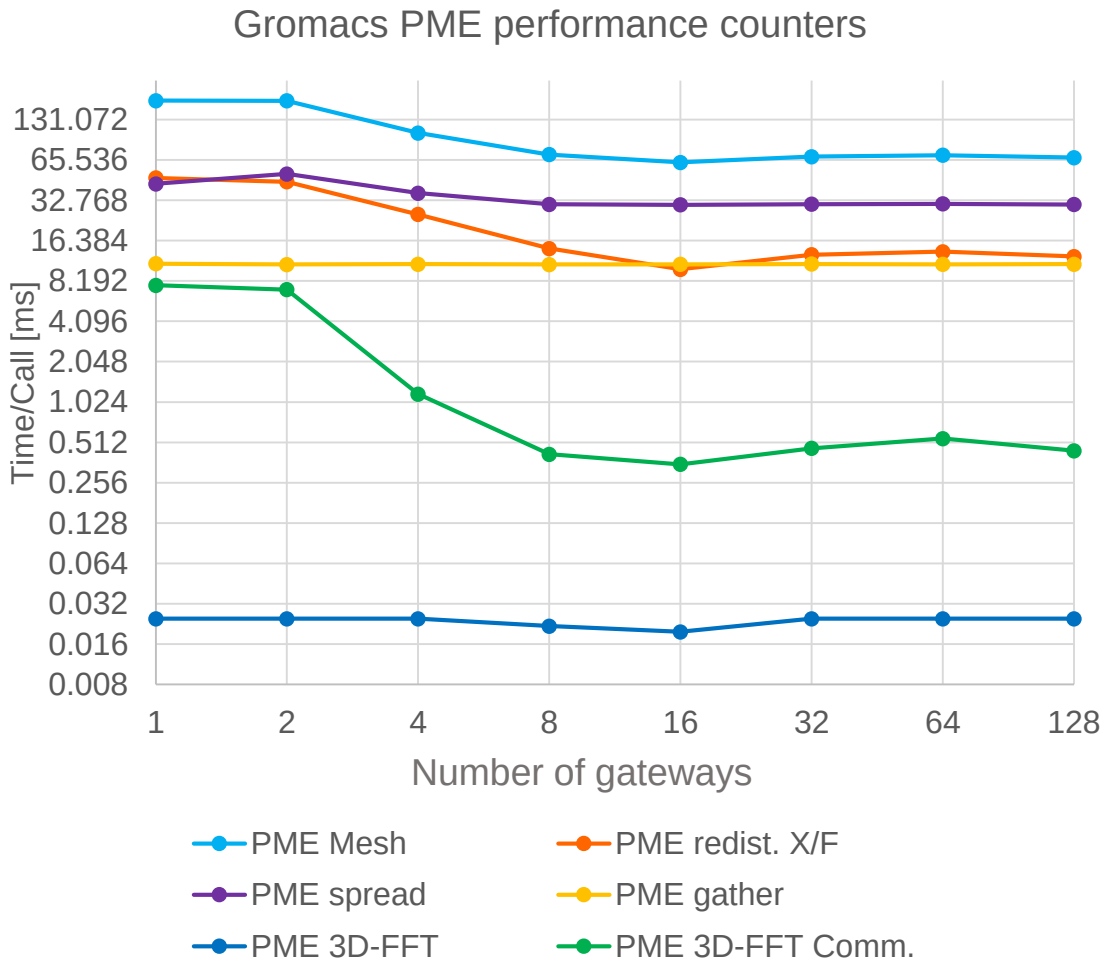
Performance vs. Number of Gateways



- 12 Booster nodes and 4 Cluster nodes with a different number of gateways

Gromacs performance counters vs. number of gateways





Conclusions

- The simulations showed good enough performance scalability and proper utilizations of the computational resources due to a good module interconnecting system.
- inter-modular influence on intra-modular communications bandwidth?
- In general our results show that JURECA system could be used for large-scale MD simulations with Gromacs in Cluster-Booster configuration.

Acknowledgements

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