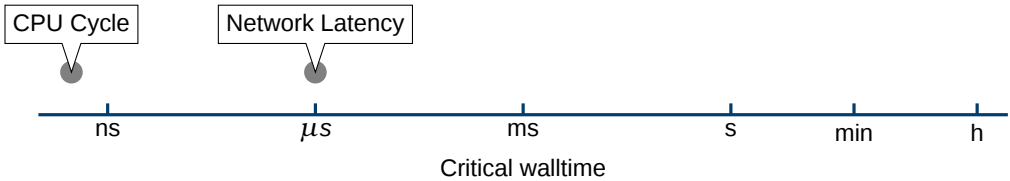
Adding Inter-node Communication to a C++ Tasking Framework

April 15, 2019 | M. Innerberger, L. Morgenstern, A. Beckmann, I. Kabadshow | Juelich Supercomputing Centre

HPC ≠ HPC


CPU Cycle
Network Latency
ns
μs
ms
s
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Critical walltime

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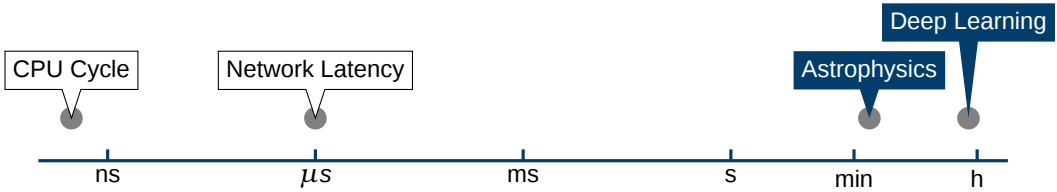
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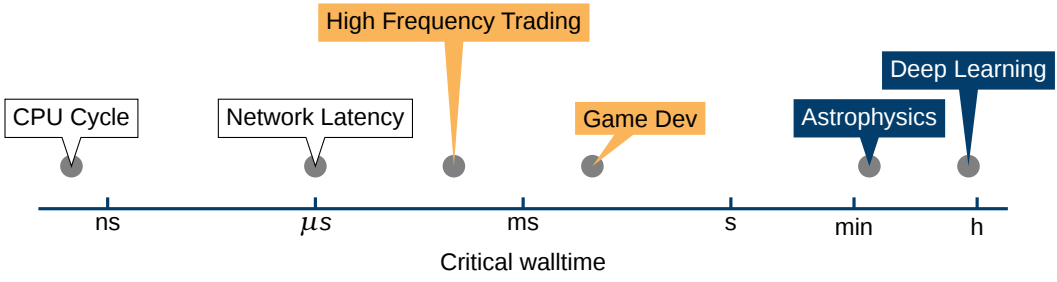
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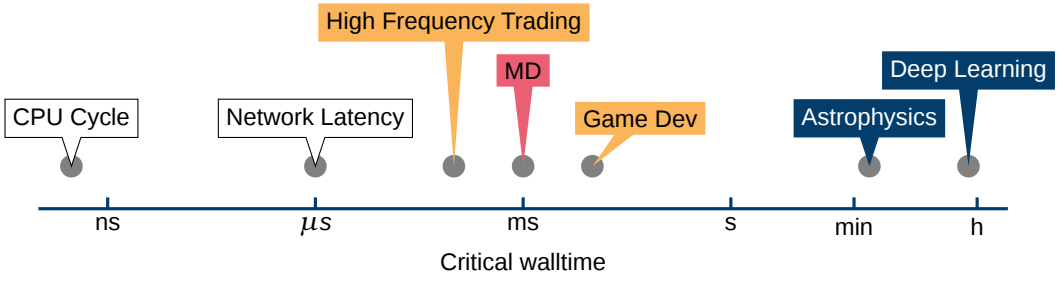
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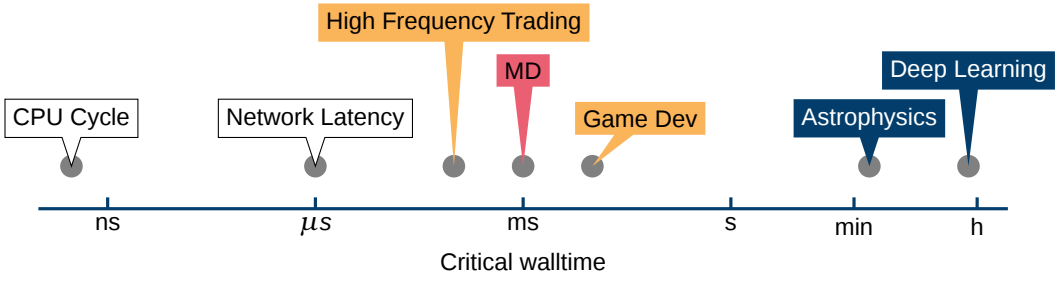


Requirements for MD

- Strong scalability
- Performance portability

Our Motivation

Solving Coulomb problem for Molecular Dynamics

Task: Compute all pairwise interactions of N particles

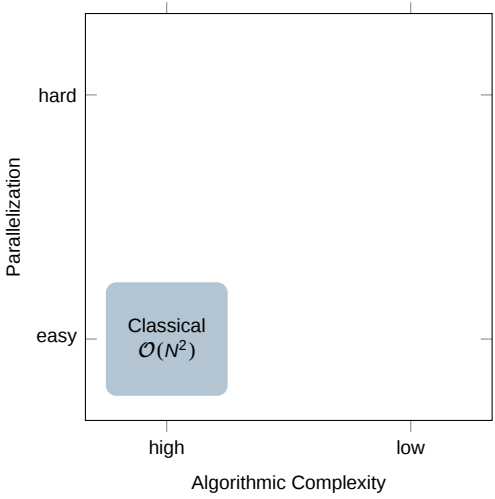
N-body problem: $\mathcal{O}(N^2) \rightarrow \mathcal{O}(N)$ with FMM

Why is that an issue?

- MD targets $< 1ms$ runtime per time step
- MD runs millions or billions of time steps
- not compute-bound, but synchronization bound
- no libraries (like BLAS) to do the heavy lifting

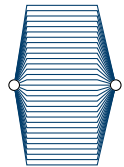
We might have to look under the hood ... and get our hands dirty.

Parallelization Potential



Classical Approach

- Lots of independent parallelism



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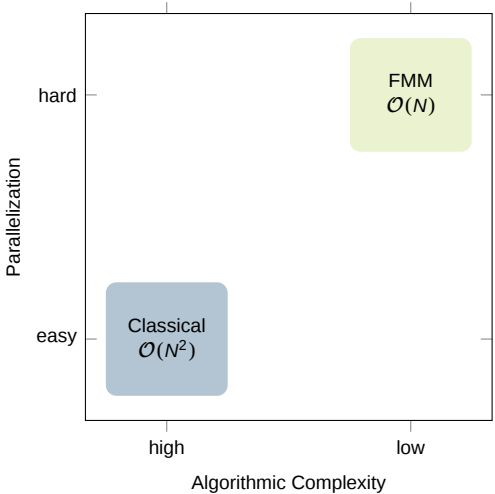
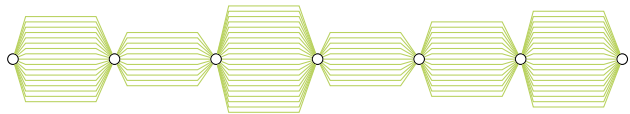


Fast Multipole Method (FMM)

- Many dependent phases
- Varying amount of parallelism



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Coarse-Grained Parallelization

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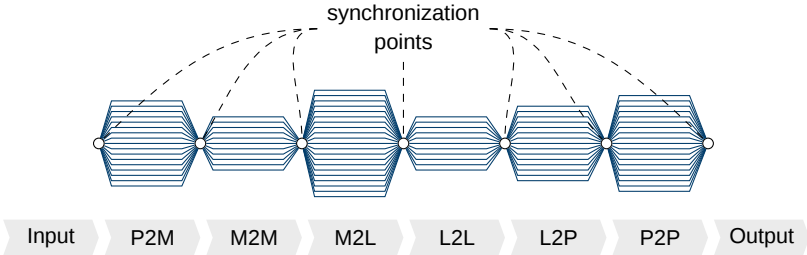

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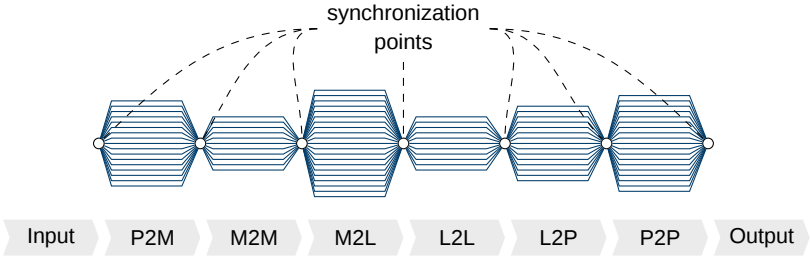

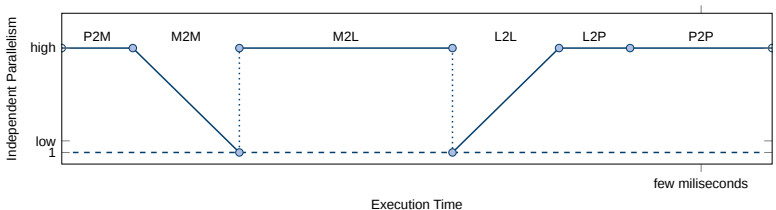

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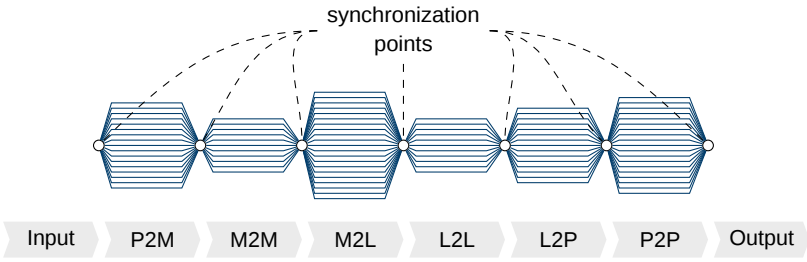
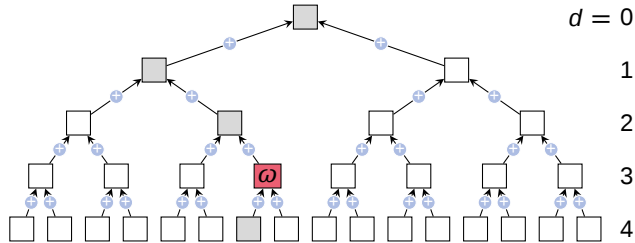


- Different amount of available loop-level parallelism within each phase
- Some phases contain sub-dependencies
- Synchronizations might be problematic

FMM Algorithmic Flow

Multipole to multipole (M2M), shifting multipoles upwards



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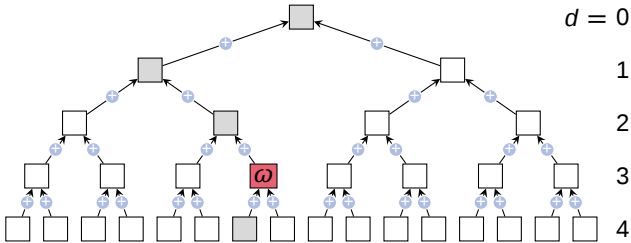
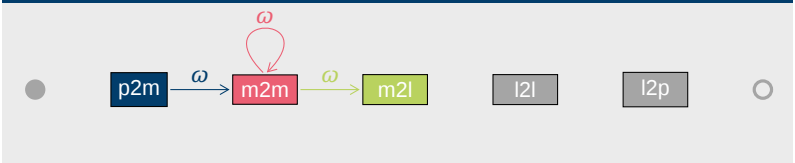
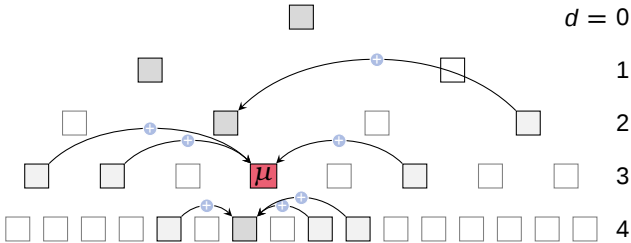


Dataflow – Fine-grained Dependencies



FMM Algorithmic Flow

Multipole to local (M2L), translate remote multipoles into local taylor moments



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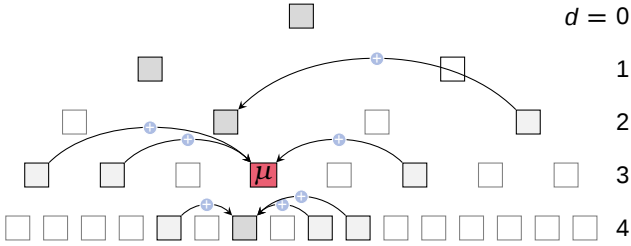

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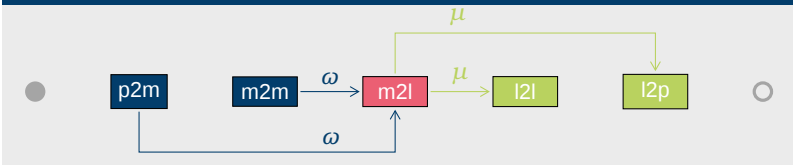

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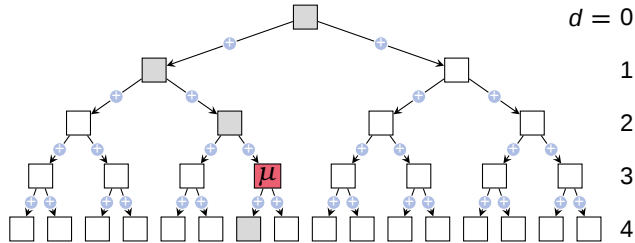
Local to local (L2L), shifting Taylor moments downwards



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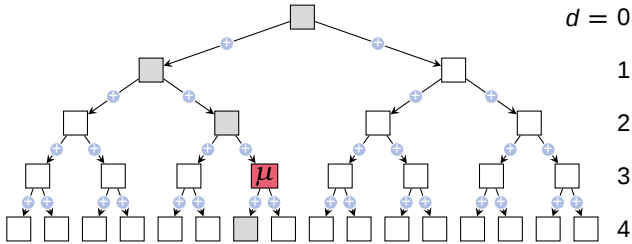

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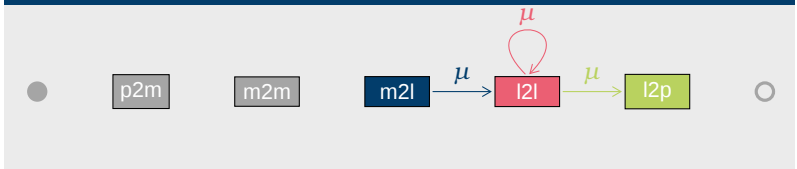
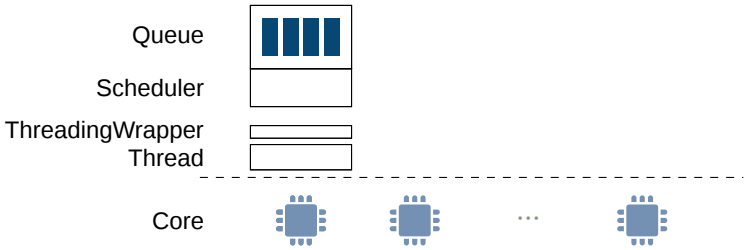


CPU Tasking Framework



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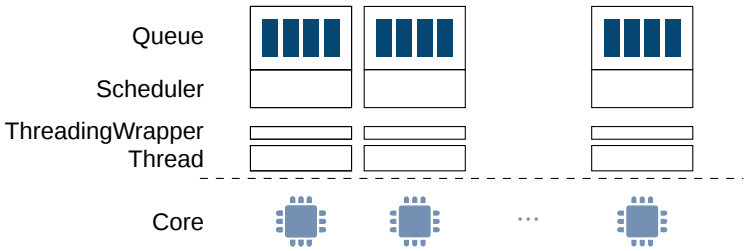

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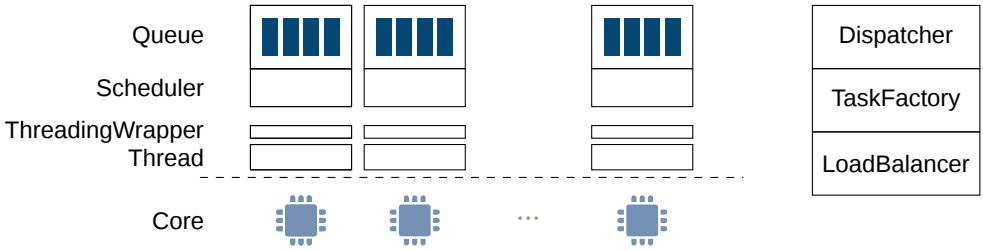

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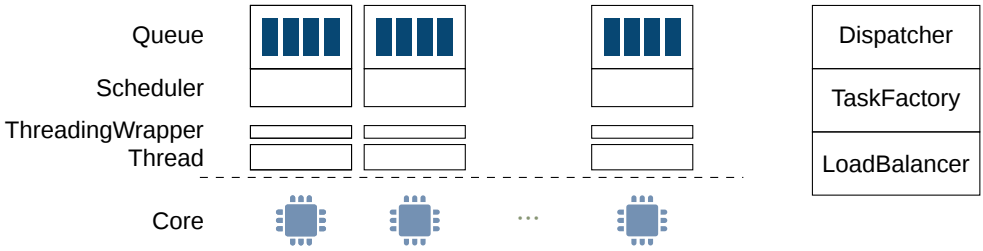
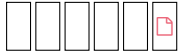


CPU Tasking Framework

Task life-cycle per thread



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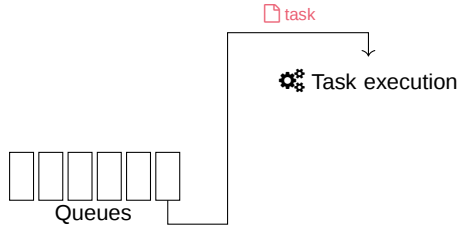

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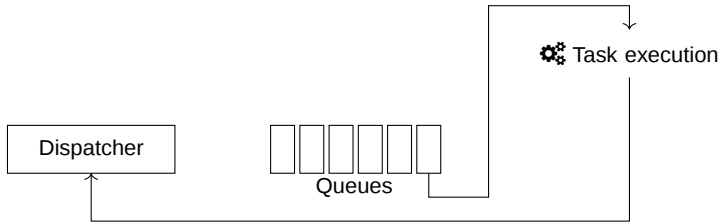

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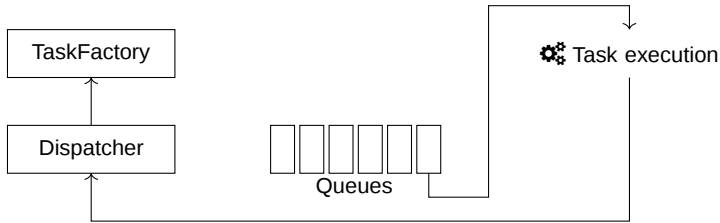

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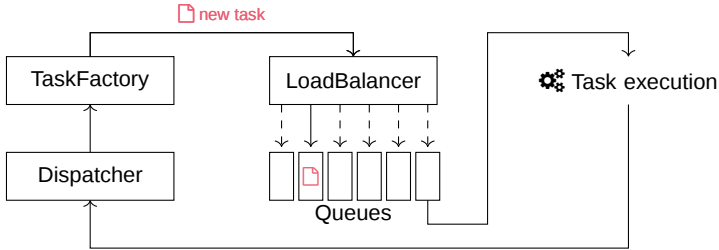
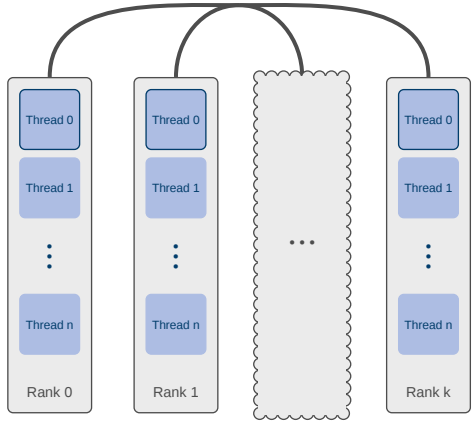


- Tasks can be prioritized by task type
- Only ready-to-execute tasks are stored in queue
- Workstealing from other threads is possible

Part I: Inter-node Parallelization

Adding Inter-node Communication via MPI



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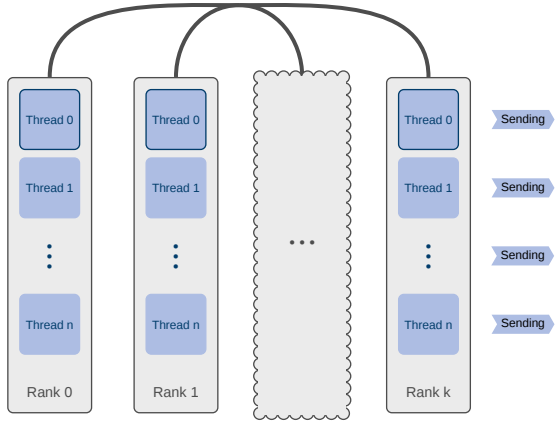

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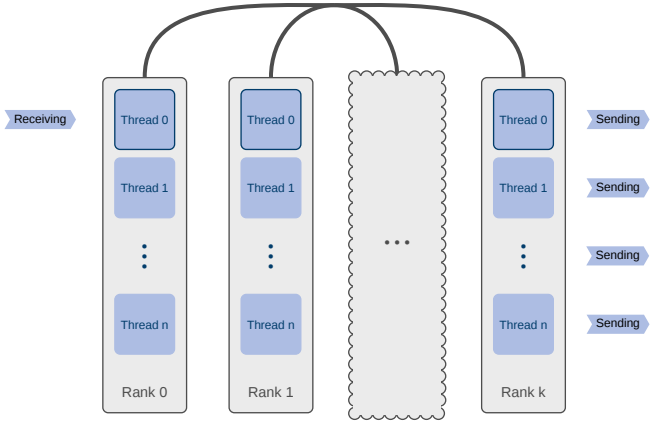

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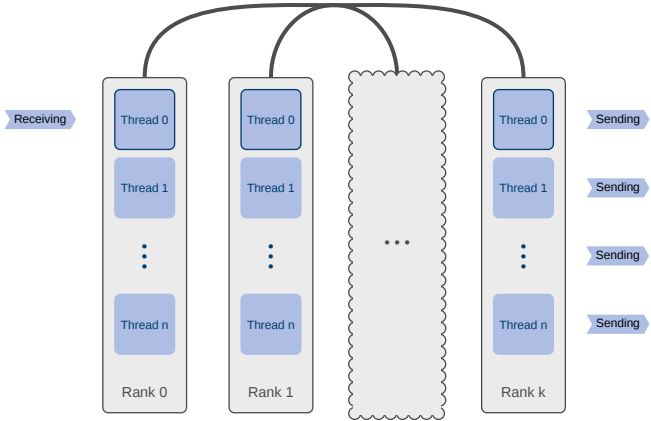

Rationale: writing to data structure should not be concurrent ⟶ avoid critical sections

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- Only necessary local moments are computed during M2L
- Computation of forces also restricted (L2P and P2P)

Part II: Implementation

General Remarks

- Tasking engine for shared memory already existing

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- Currently, `std::threads` is used for intra node parallelization

MPI Details

Code

```
while (notFinished()){
  executeTask();
  Status = Communicator.Iprobe();
  if (Status.MessageNeeded()){
    Communicator.Irecv(); }
  else {
    Communicator.Discard(); }
  /*do something else */
  Communicator.Wait();
  /*use received data */
}
```

MPI Calls

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MPI Calls

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- Call Irecv for messages in any case
- If message not needed, write data to dummy buffer
- Call Wait before using data

Distinguishing Incoming Messages

```
MPI_I[send|recv](buf,
                 count,
                 datatype,
                 [dest|source],
                 tag,
                 comm,
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It’s in the Tag

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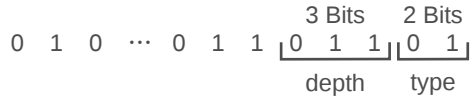

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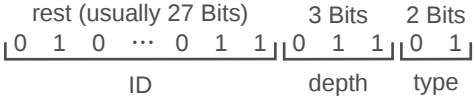

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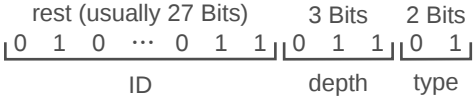

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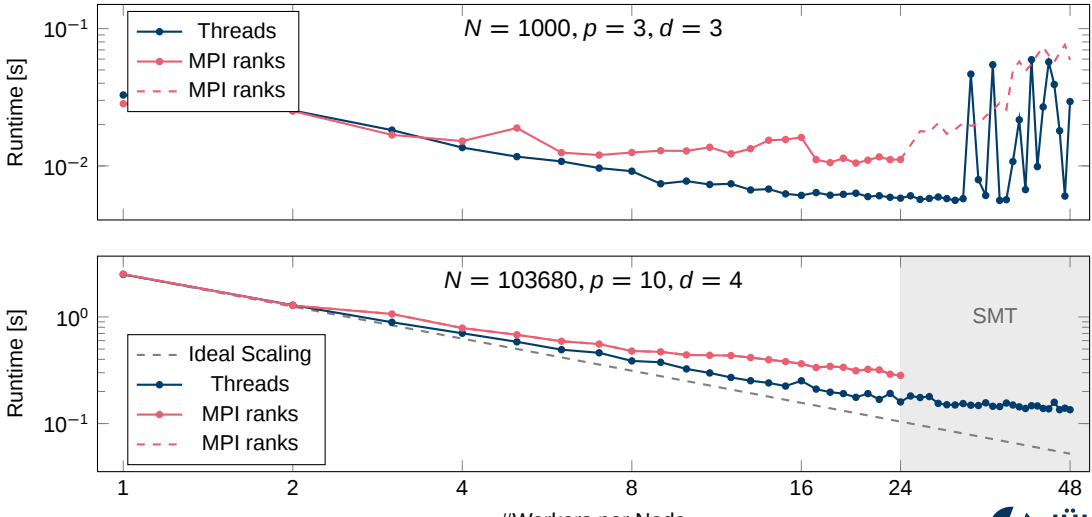
- Information can be encoded in this tag
- Type of sent data (multipole, local moment, particle)
- Level of the corresponding box ($2^{d \cdot \text{level}}$ boxes)
- ID of box on this level
- This essentially mimics a matching probe / receive operation

Part III: Results and Outlook

Results from JURECA



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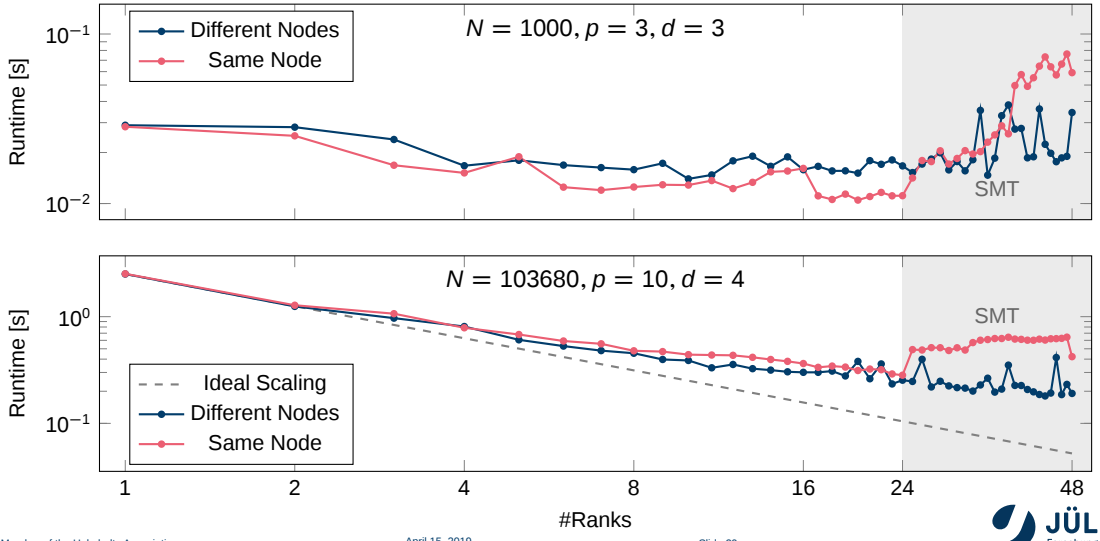

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Adding Inter-node Communication to a C++ Tasking Framework

April 15, 2019 | M. Innerberger, L. Morgenstern, A. Beckmann, I. Kabadshow | Juelich Supercomputing Centre