How to do nothing in less time

GROMEX Minisymposium

26. January, 2016 | D. Haensel, A. Beckmann, I. Kabadshow | Jülich Supercomputing Centre

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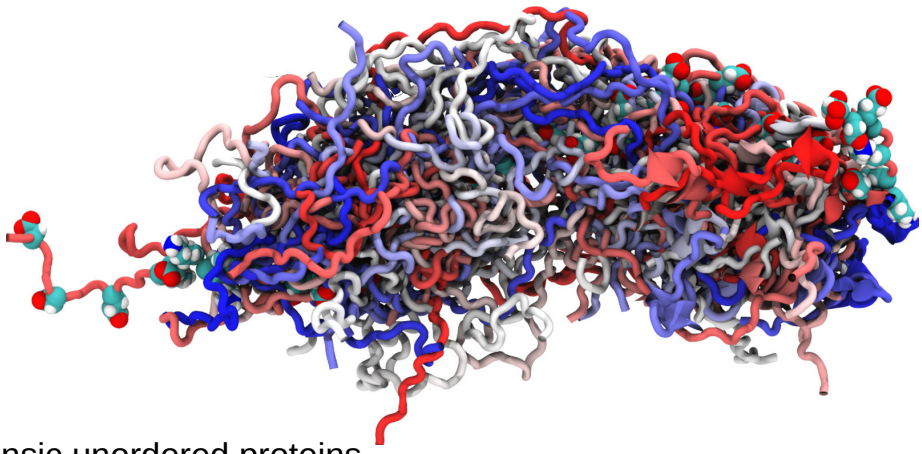
Motivation

Coulomb problem: $1/r$ potential and the extension to λ-dynamics

Task: Compute all pairwise interactions of N particles

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



- Intrinsic unordered proteins
  (courtesy of Th. Ullmann - MPI BPC Göttingen)

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Computing a single force classically

$$\mathbf{F}(\mathbf{r}_i) = q_i \sum_{j=1}^{N} \frac{q_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} \mathbf{r}_{ij} \qquad (i \neq j)$$

Computing a single force via expansion

$$\mathbf{F}(\mathbf{a}_i) \approx \sum_{l=0}^{p} \sum_{m=-l}^{l} \nabla \omega_{lm}^{A}(\mathbf{a}_i) \mu_{lm}^{\bar{A}}(\cdots)$$

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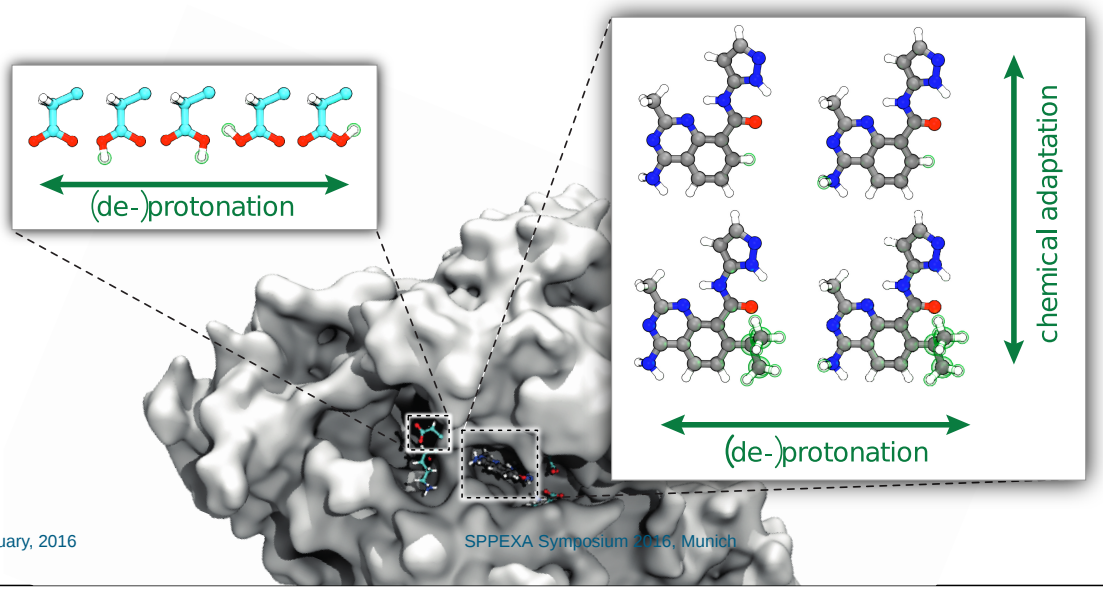
SPPEXA Project: GROMEX

Calculating electrostatic long-range interactions with λ-dynamics

GROMACS MD code

Used on different and heterogeneous hardware



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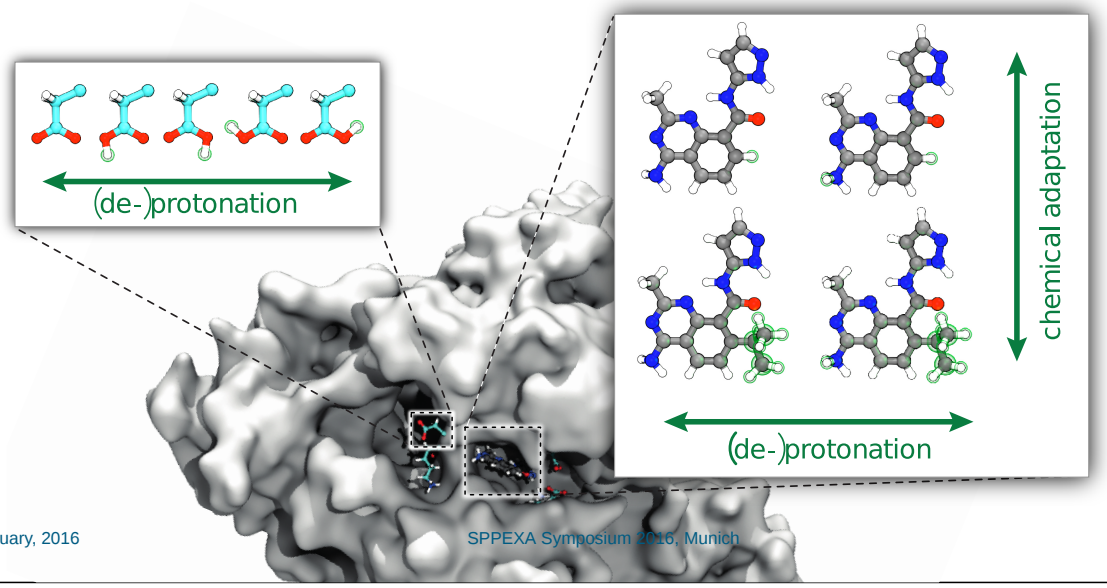
SPPEXA Project: GROMEX

Calculating electrostatic long-range interactions with λ-dynamics

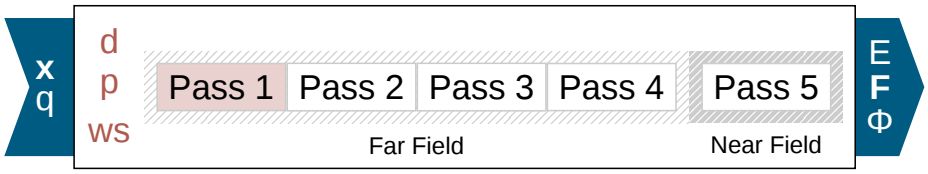
Goal: Strong scaling

Automatic parallel run-time minimization

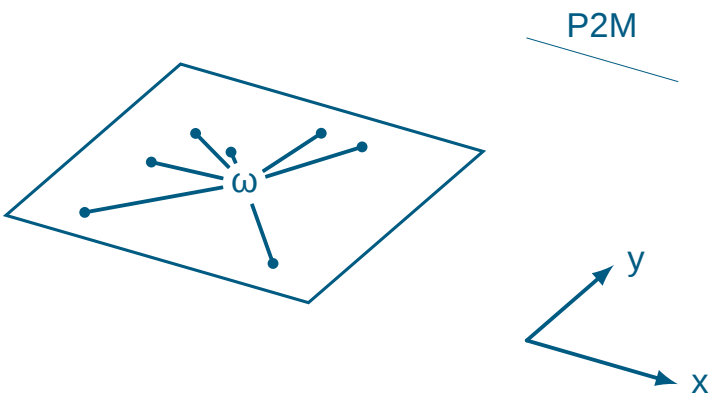


The Fast Multipole Method in a Nutshell

Workflow



Pass 1: Particle-to-Multipole $\mathcal{O}(Np^2)$



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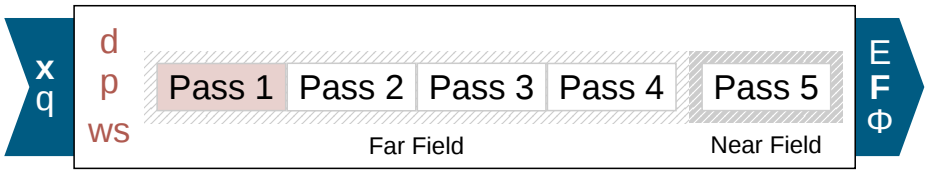
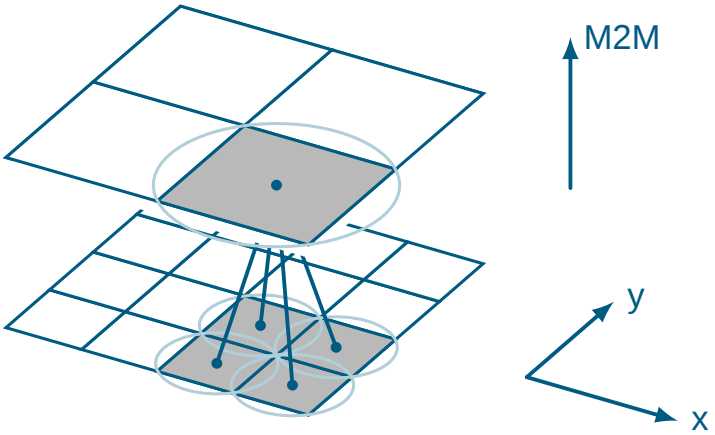


Pass 1: Multipole-to-Multipole $\mathcal{O}(p^3)$ || $\mathcal{O}(p^4)$



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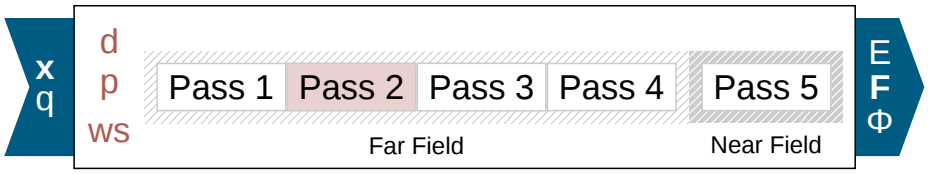
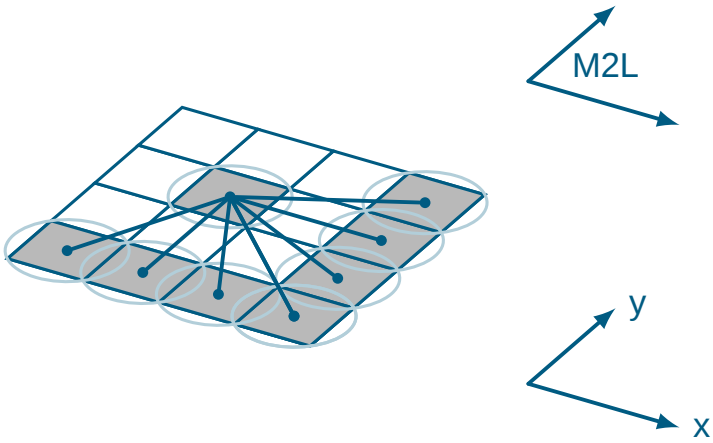


Pass 2: Multipole-to-Local $\mathcal{O}(p^3)$ || $\mathcal{O}(p^4)$



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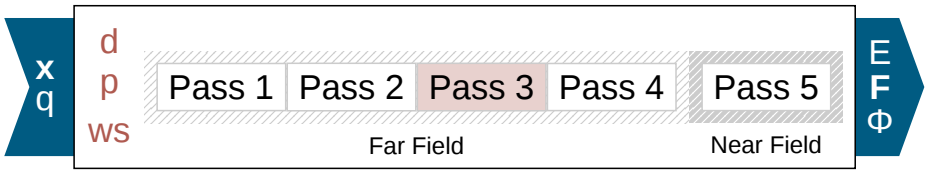
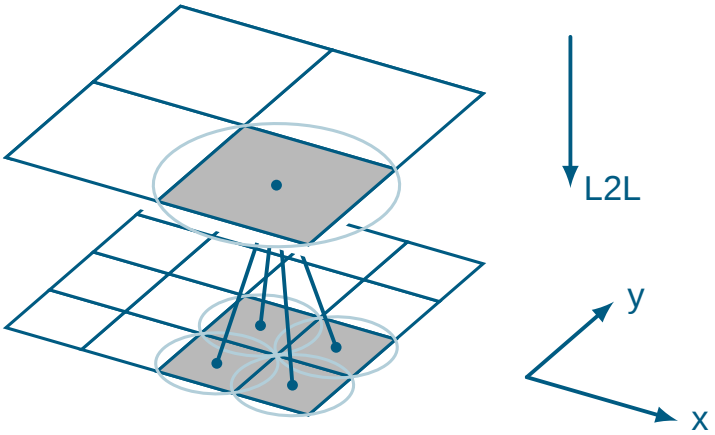


Pass 3: Local-to-Local $\mathcal{O}(p^3)$ || $\mathcal{O}(p^4)$



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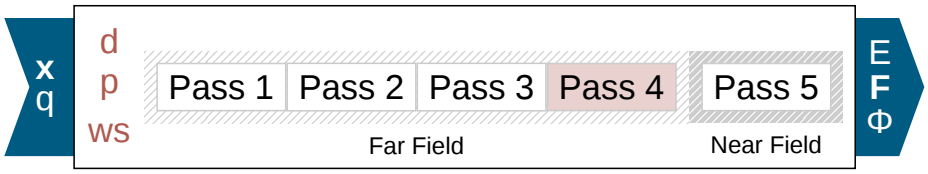
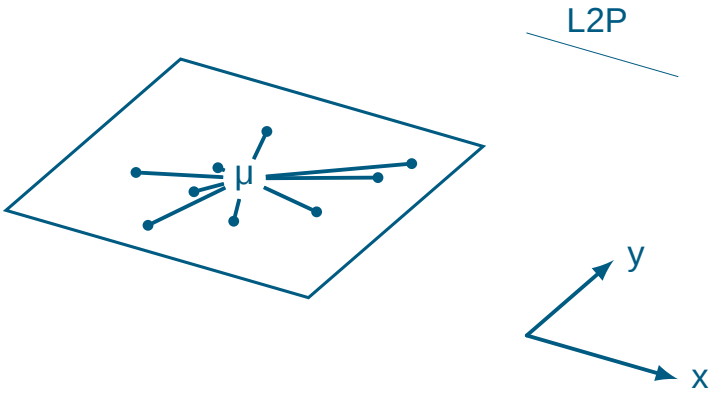
The Fast Multipole Method in a Nutshell

Workflow



Pass 4: Local-to-Particle $\mathcal{O}(Np^2)$



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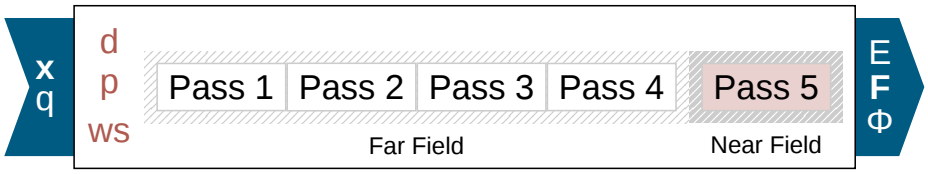
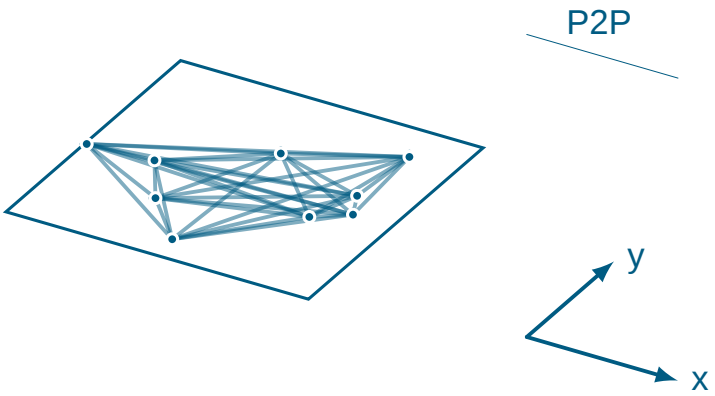


Pass 5: Particle-to-Particle $\mathcal{O}(M^2)$



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Code Optimization Directions

Intranode

- Vectorization
- GPU Support
- Threading

Internode

- Overlapping Computation/Computation
- Communication-Avoiding Algorithms

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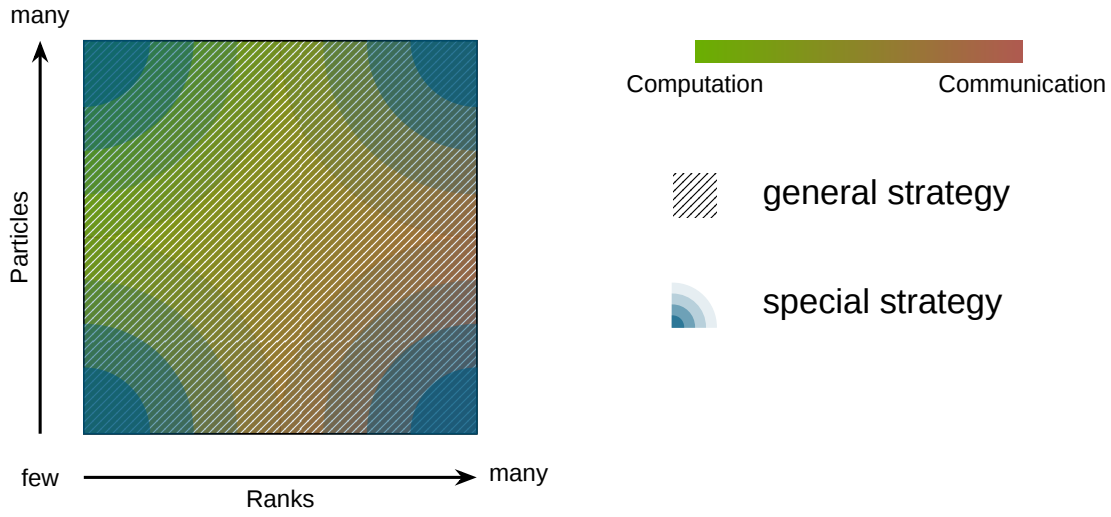
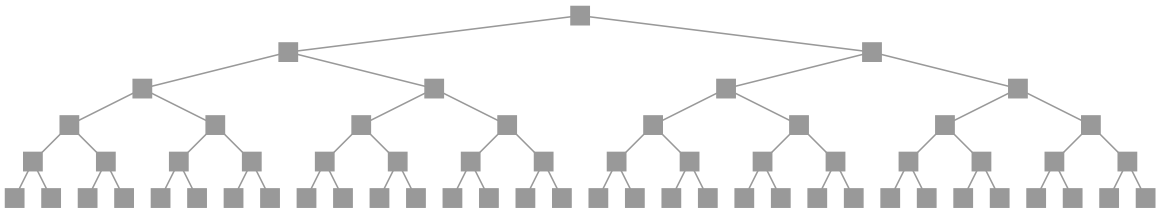
Parallelization Strategies

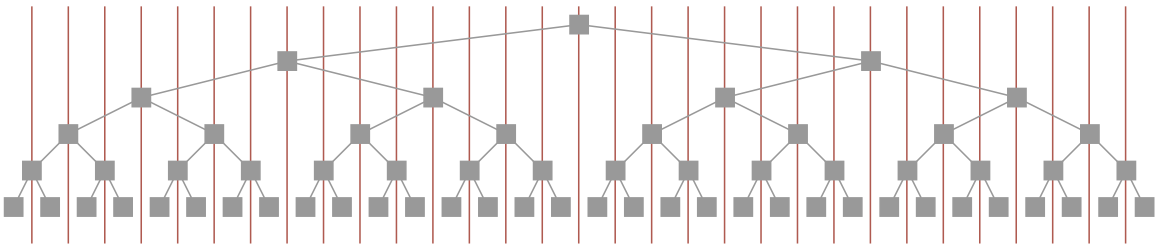


Octree Workload Distribution



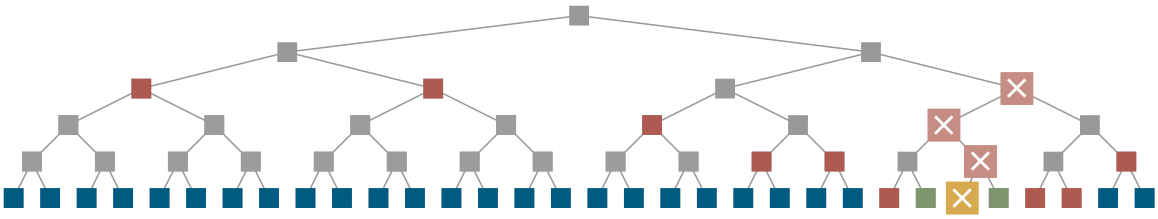
- Sequential view: full octree

Octree Workload Distribution



- Parallel view: full octree

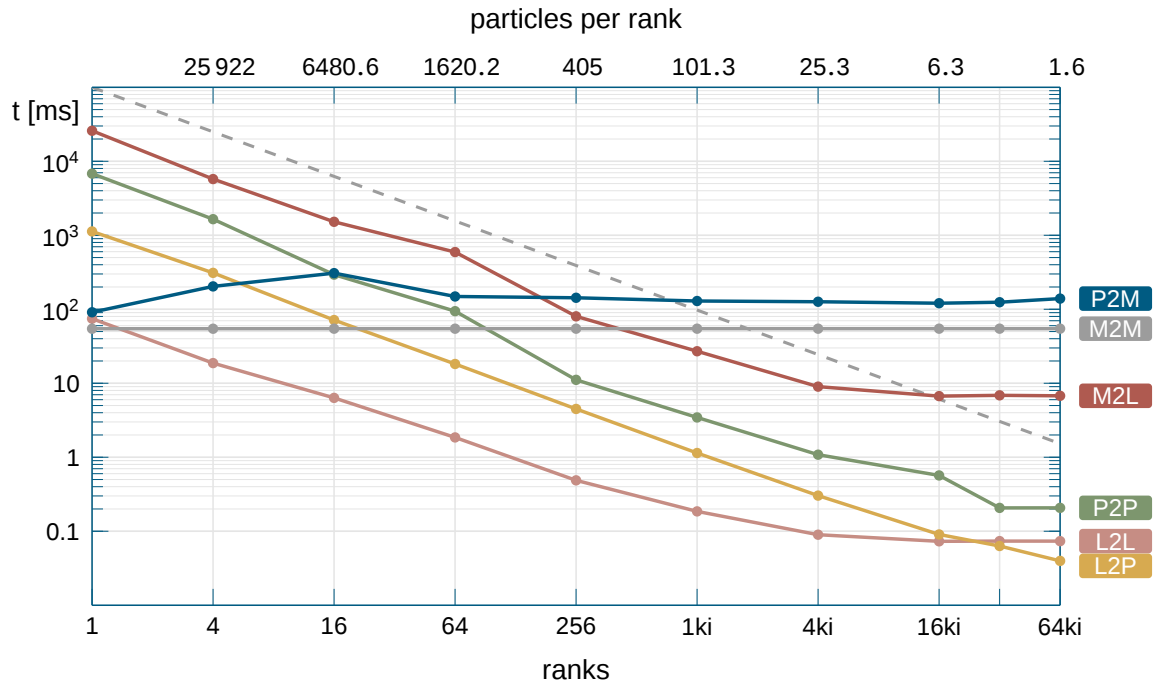
Octree Workload Distribution



- All target dependencies: P2M, M2M, M2L, L2L, L2P and P2P

Naïve Parallelization – Passes Scaling

Silicamelt (homogeneous) on JUQUEEN $N = 103680$, $d = 4$, $p = 5$



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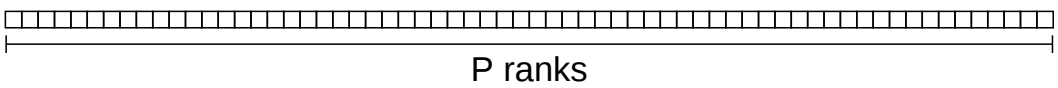
Communication-Avoiding Approach

Building teams

Starting with P processors and N particles.



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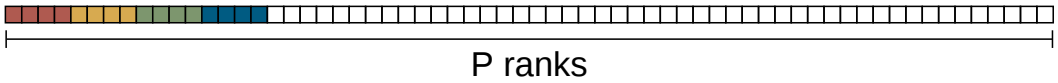
Communication-Avoiding Approach

Building teams

Divide processors into teams of size c



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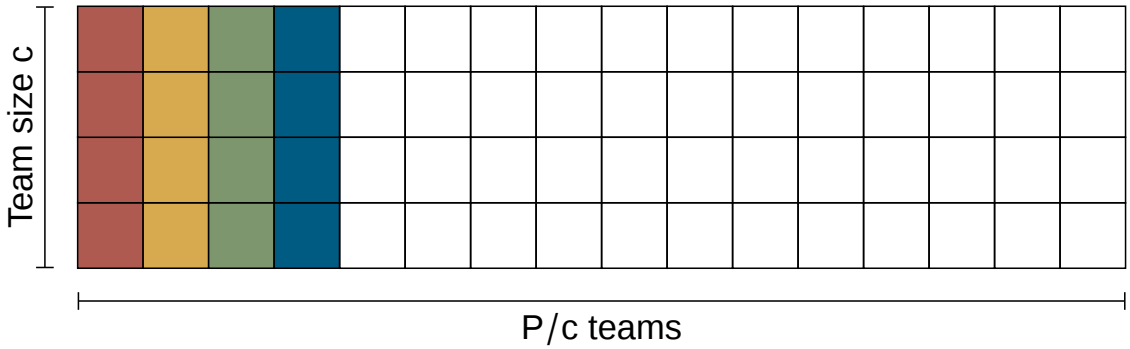
Communication-Avoiding Approach

Building teams

Now we have P/c teams arranged in a grid.



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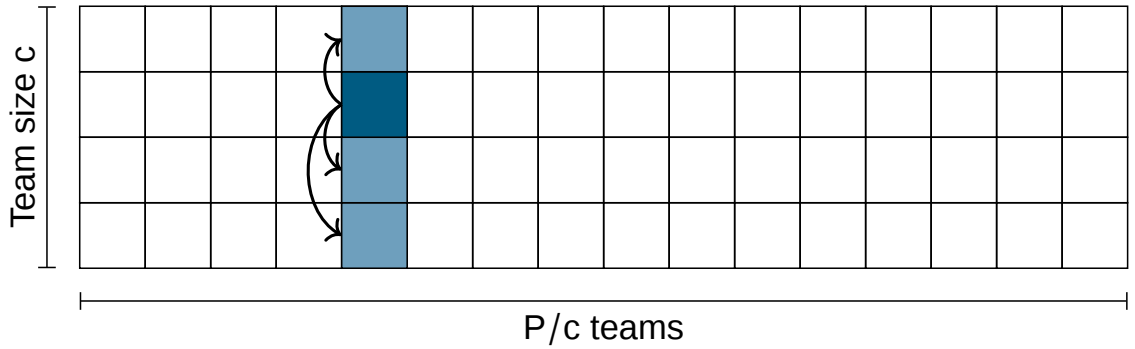
Communication-Avoiding Approach

First intra-team communication (particles)

Gather all team particles intra-team.



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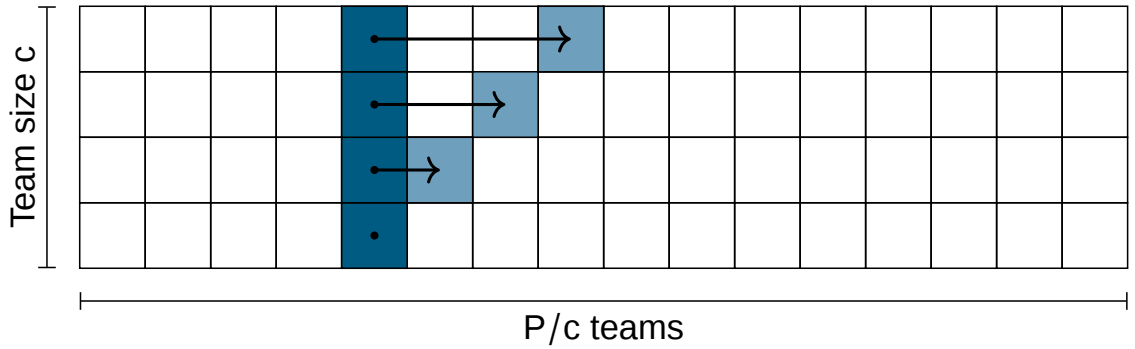
Communication-Avoiding Approach

Inter-team communication (particles)

Send the $c \cdot N/P$ team particles to P/c^2 interacting teams.



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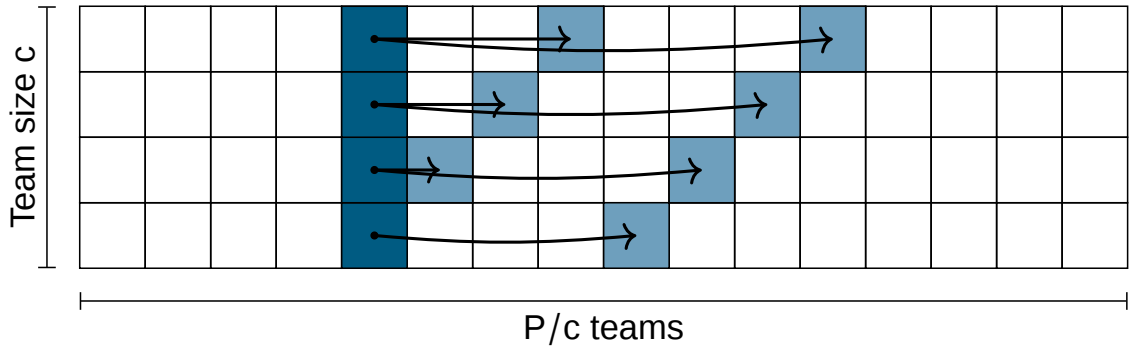

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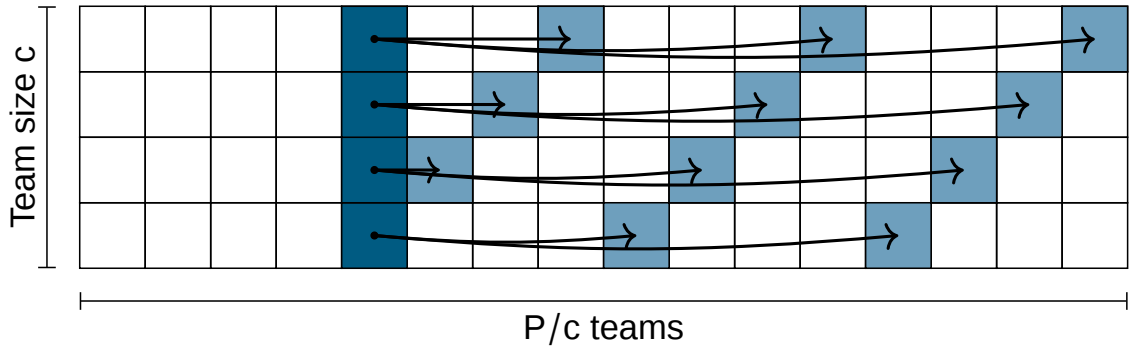

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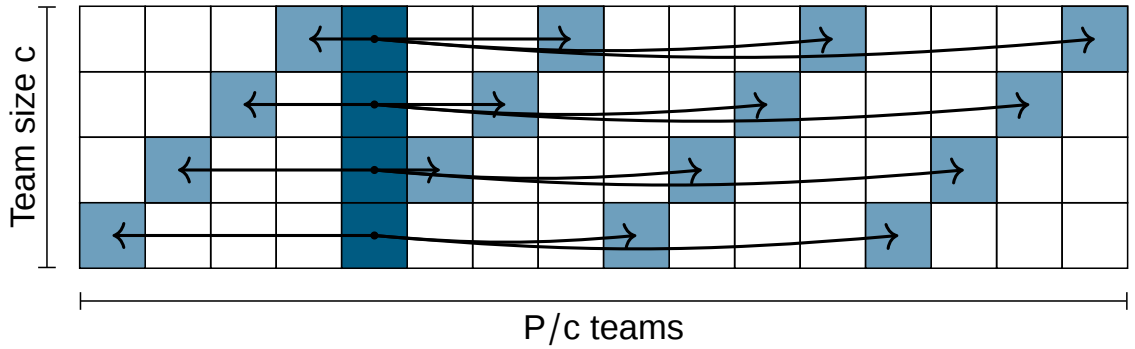

Each rank now has N/c particles. Compute multipoles for all particles.

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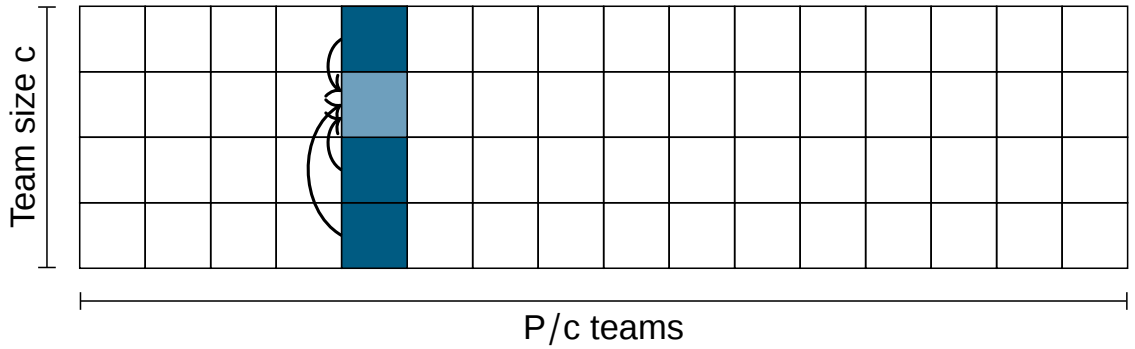
Communication-Avoiding Approach

Second intra-team communication (multipoles)

Gather all computed multipoles intra-team and reduce them.



All multipoles are available on each processor after this step.

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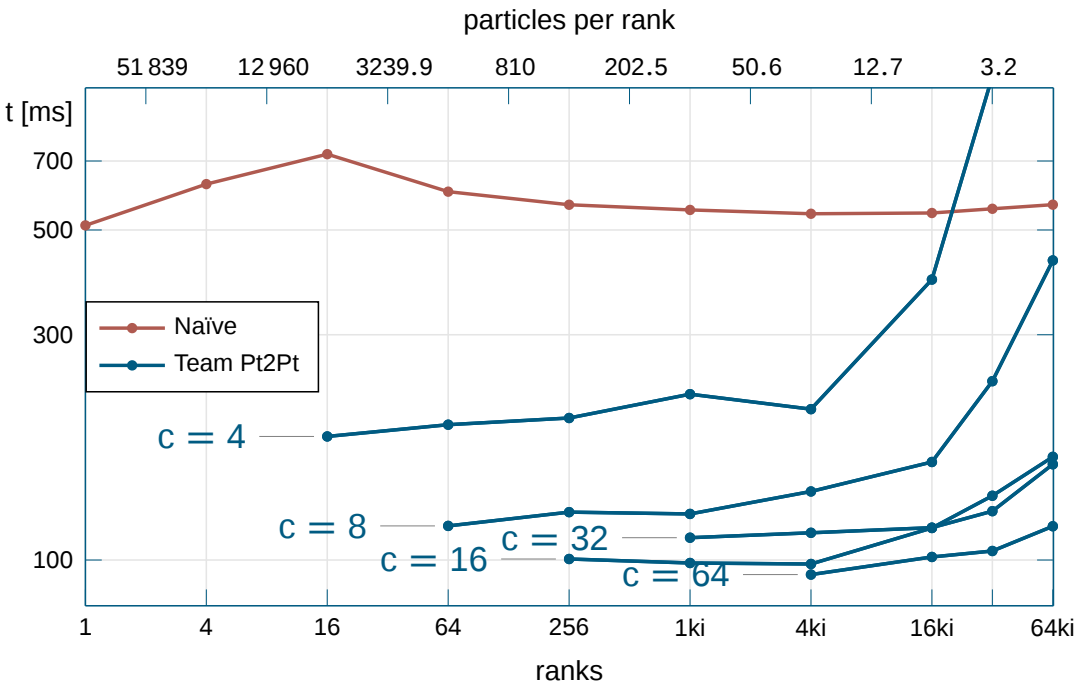
Benchmark – P2M

Silicamelt (homogeneous) on JUQUEEN $N = 103680$, $d = 4$, $p = 15$



Summary & Outlook

Summary

- Communication strategy from classical N-body can be reused
- Global communication can be hidden behind computation
- Available memory can be used to overlap comm/comp even more
- Strong scaling limit shifted to even lower particle numbers

Outlook

- Parallelize full first pass (M2M shift parallelization missing)
- Combine with optimized p^3 kernels
- Explore different MPI techniques (e.g. neighbor/partial collectives)

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