Advanced space charge tracking methods for high brilliance electron sources

S. Schmid, E. Gjonaj, and H. De Gersem
Institut für Theorie Elektromagnetischer Felder, TU Darmstadt

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Structure

- Introduction
- Fast Multipole Methods
- Numerical Analysis of the Method
- Preliminary Results for the PITZ Gun
- Outlook

Introduction
Numerical Methods for Photogun Modeling

Simulation of electron bunch dynamics
→ Solve equations of motion for N-body interaction problem

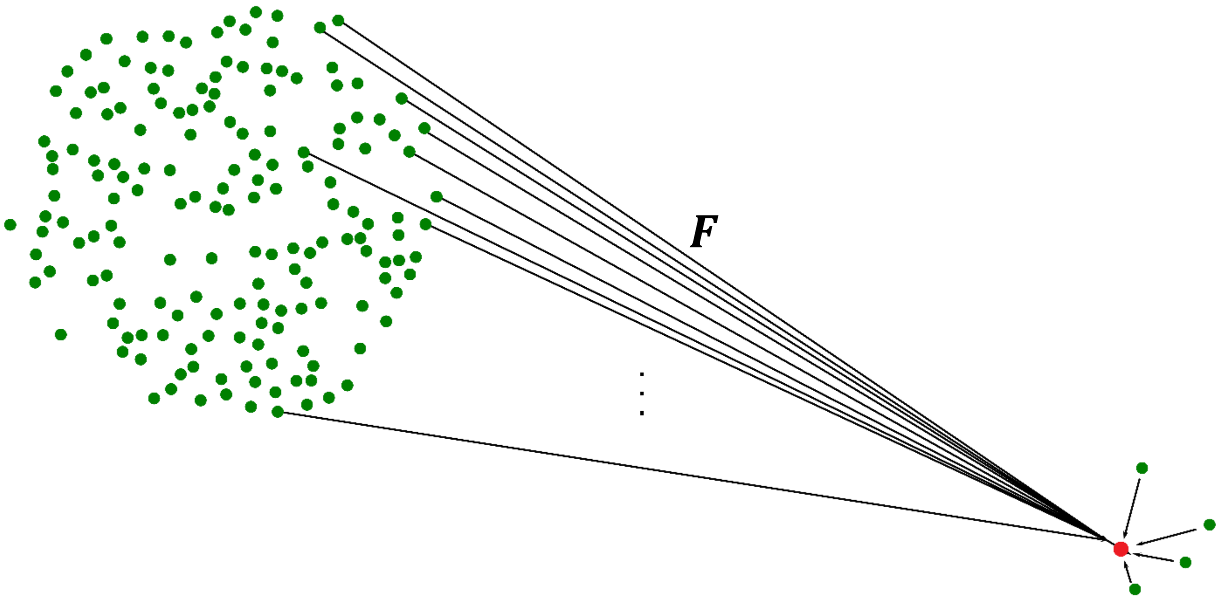
Particle-Particle Method	Particle-Mesh Methods
Brute force approach: → Compute N^2 interaction term	Deposit charges on mesh: → Poisson-FFT, FEM, E-M-PIC, etc…
• Open boundaries intrinsically matched • Flexible choice of interaction model • No aliasing	• Faster and more efficient • Fully electromagnetic solvers exist • Control resolution via mesh parameters
• Computational complexity $\propto N^2$ → Runtime limitation for large N → Large hardware requirements	• Complicated boundary conditions • Interpolations, smoothing, adaptive grids, etc. needed • Errors from spatial discretization (aliasing)

Use a hybrid approach for space charge calculations

→ Fast Multipole Methods

Fast Multipole Methods
The Concept

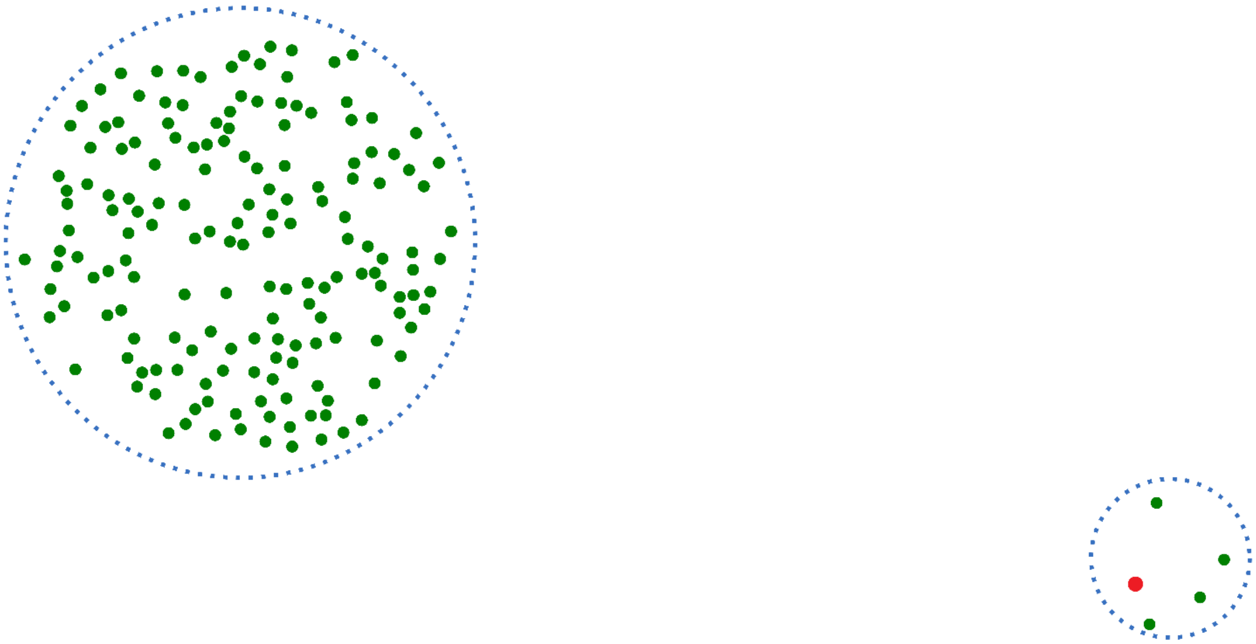
Aim: Find an efficient way to compute many-body interaction
→ Reduce complexity to less than $O(N^2)$



Fast Multipole Methods
The Concept

Aim: Find an efficient way to compute many-body interaction
$\rightarrow$ Reduce complexity to less than $O(N^2)$

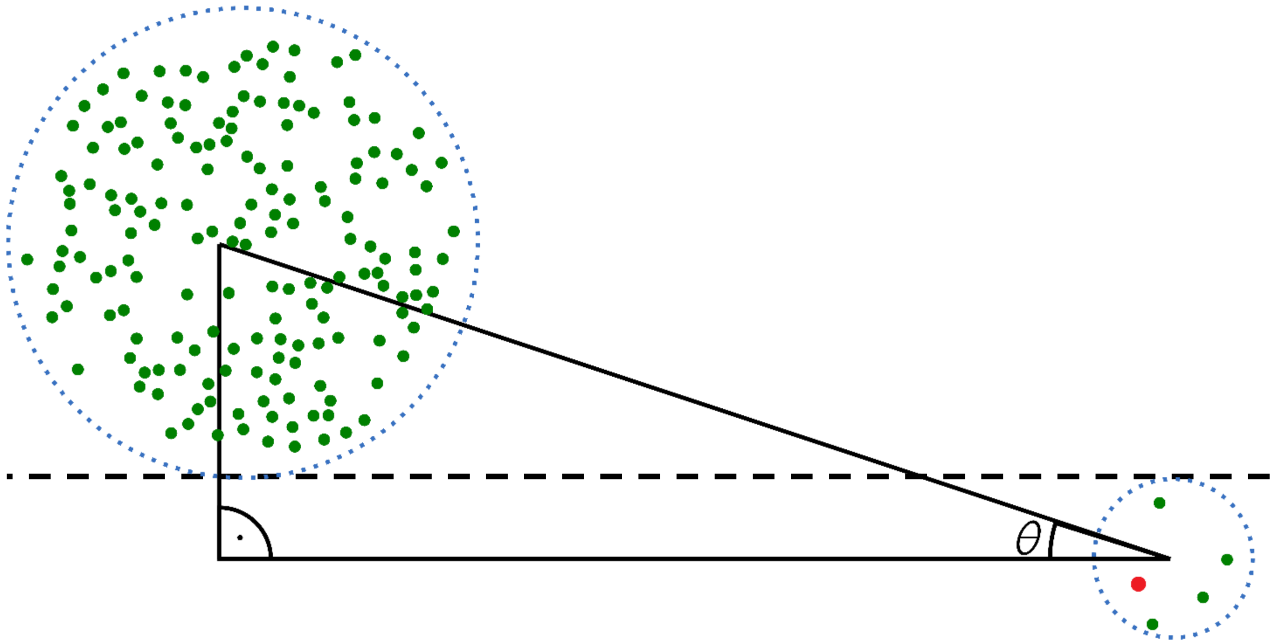
Idea: Internal structure of distant agglomerations less important
$\rightarrow$ Subdivide particle distribution into boxes



Fast Multipole Methods
The Concept

Idea: Internal structure of distant agglomerations less important
→ Subdivide particle distribution into boxes

Parameter $\boldsymbol{\theta_{max}}$: Define minimum spatial resolution
→ $\theta \leq \boldsymbol{\theta_{max}}$ ⇒ Use effective force $\boldsymbol{F}_{distant}$ for distant boxes



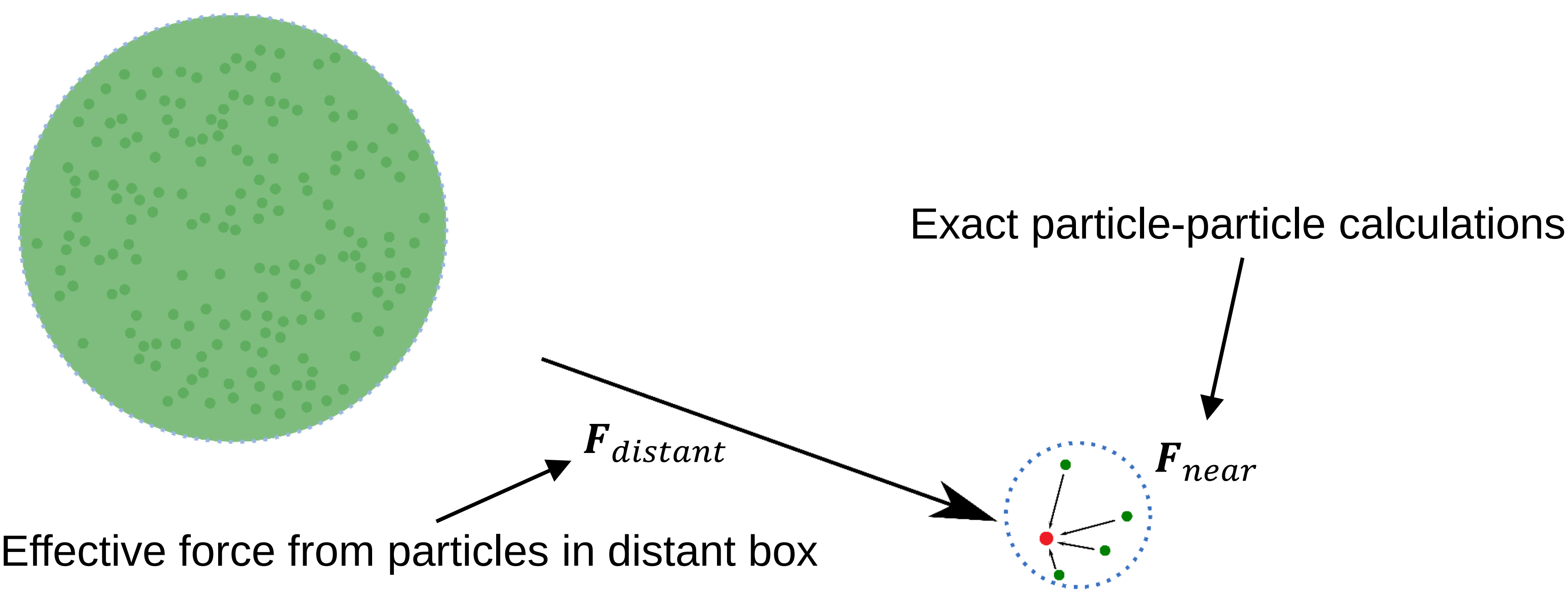
Fast Multipole Methods
The Concept

Parameter $\boldsymbol{\theta_{max}}$: Define minimum spatial resolution

$\rightarrow \theta \leq \boldsymbol{\theta_{max}} \Rightarrow$ Use effective force $\boldsymbol{F}_{distant}$ for distant boxes

Evaluation: Compute total interaction force

$$\rightarrow \boldsymbol{F}_{tot} = \boldsymbol{F}_{distant} + \boldsymbol{F}_{near}$$



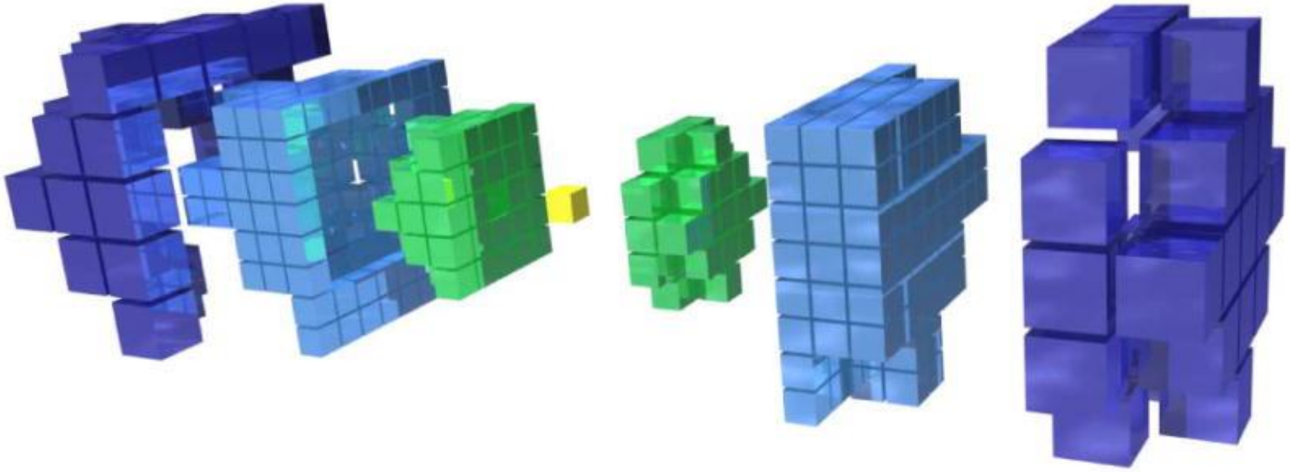
Fast Multipole Methods
The Concept

Evaluation: Compute total interaction Force

$\rightarrow \boldsymbol{F}_{tot} = \boldsymbol{F}_{distant} + \boldsymbol{F}_{near}$

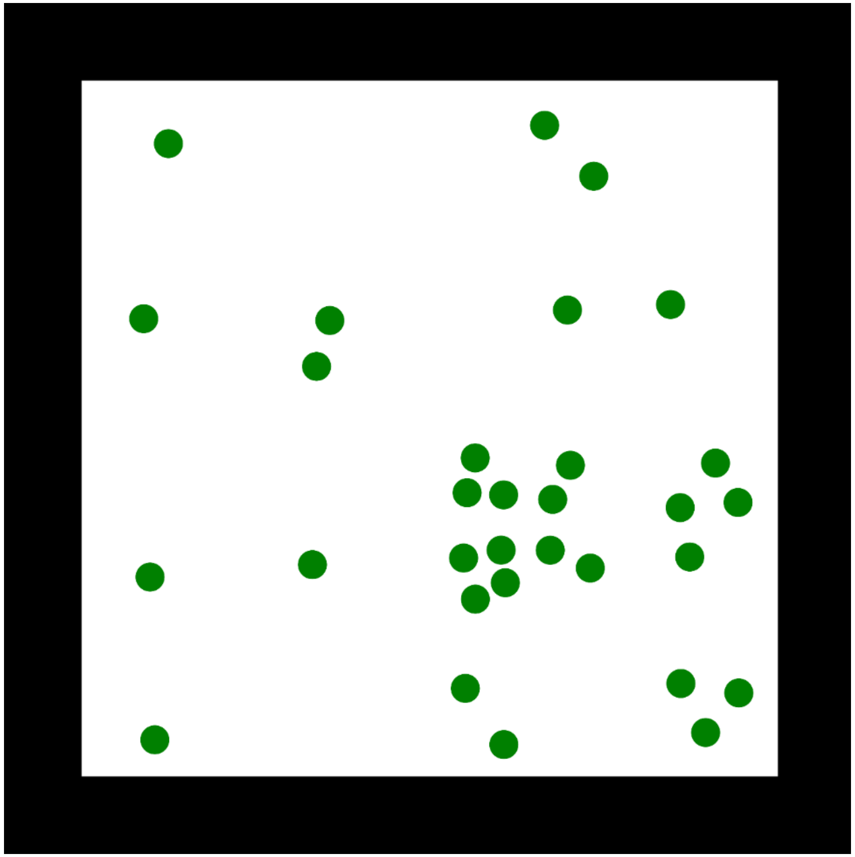
Next Step: Generalize concept for whole bunch

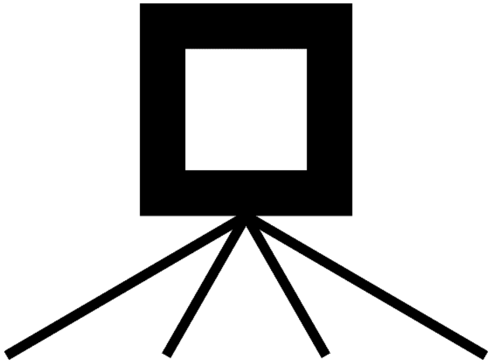
→ 1. Analyze spatial structure of particle distribution



(Plot from: J.Kurzak, et al., FMM for particle dynamics, 2006)

Fast Multipole Methods
1. Spatial Structure: Tree Construction





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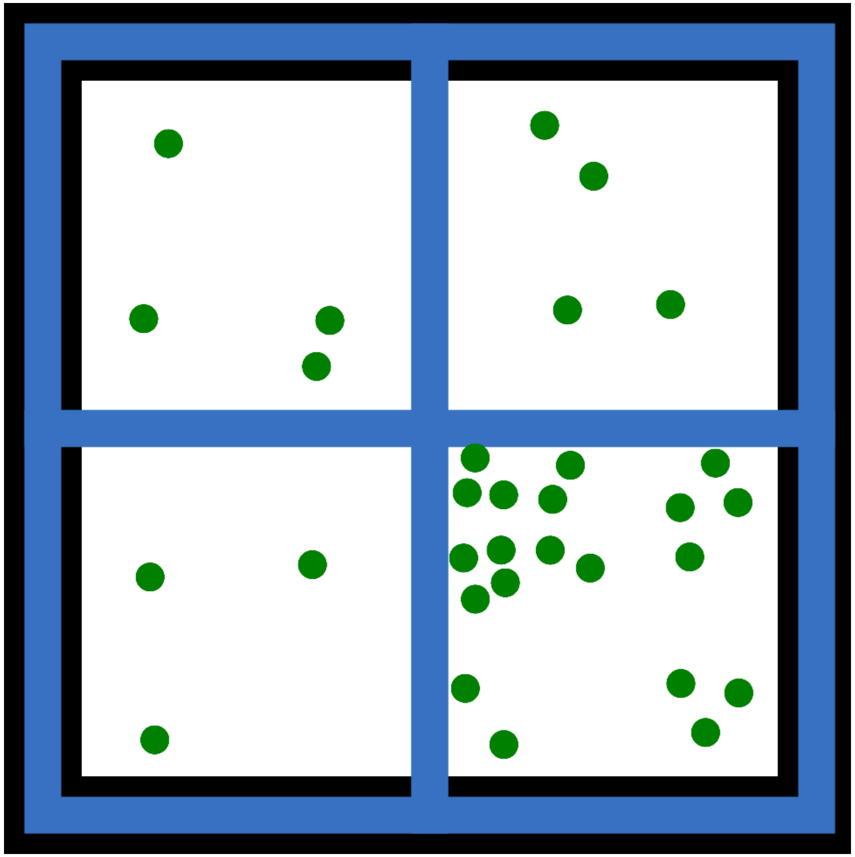

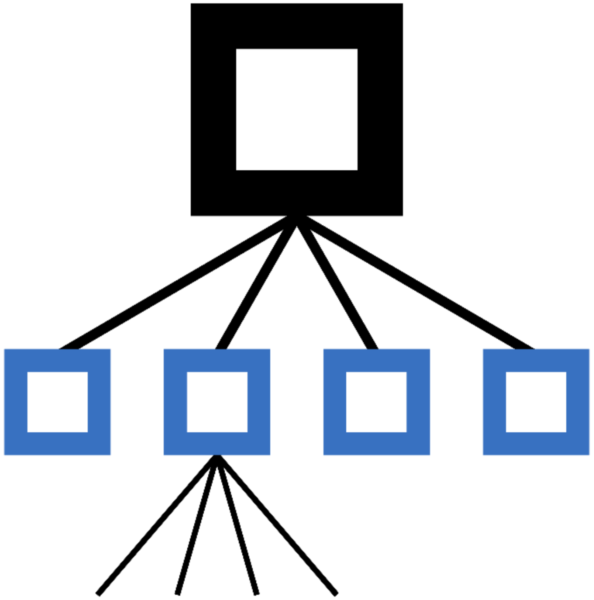

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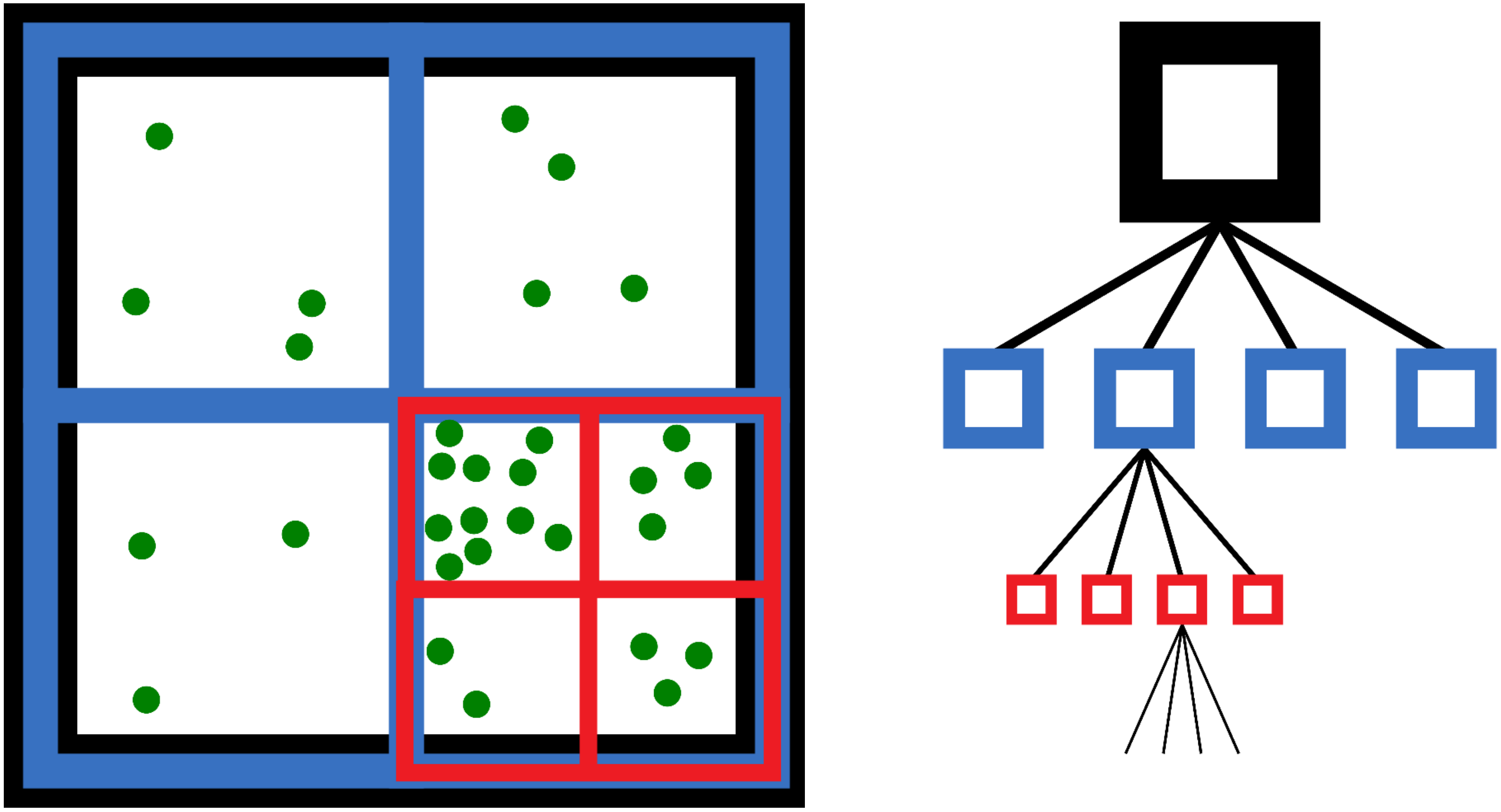

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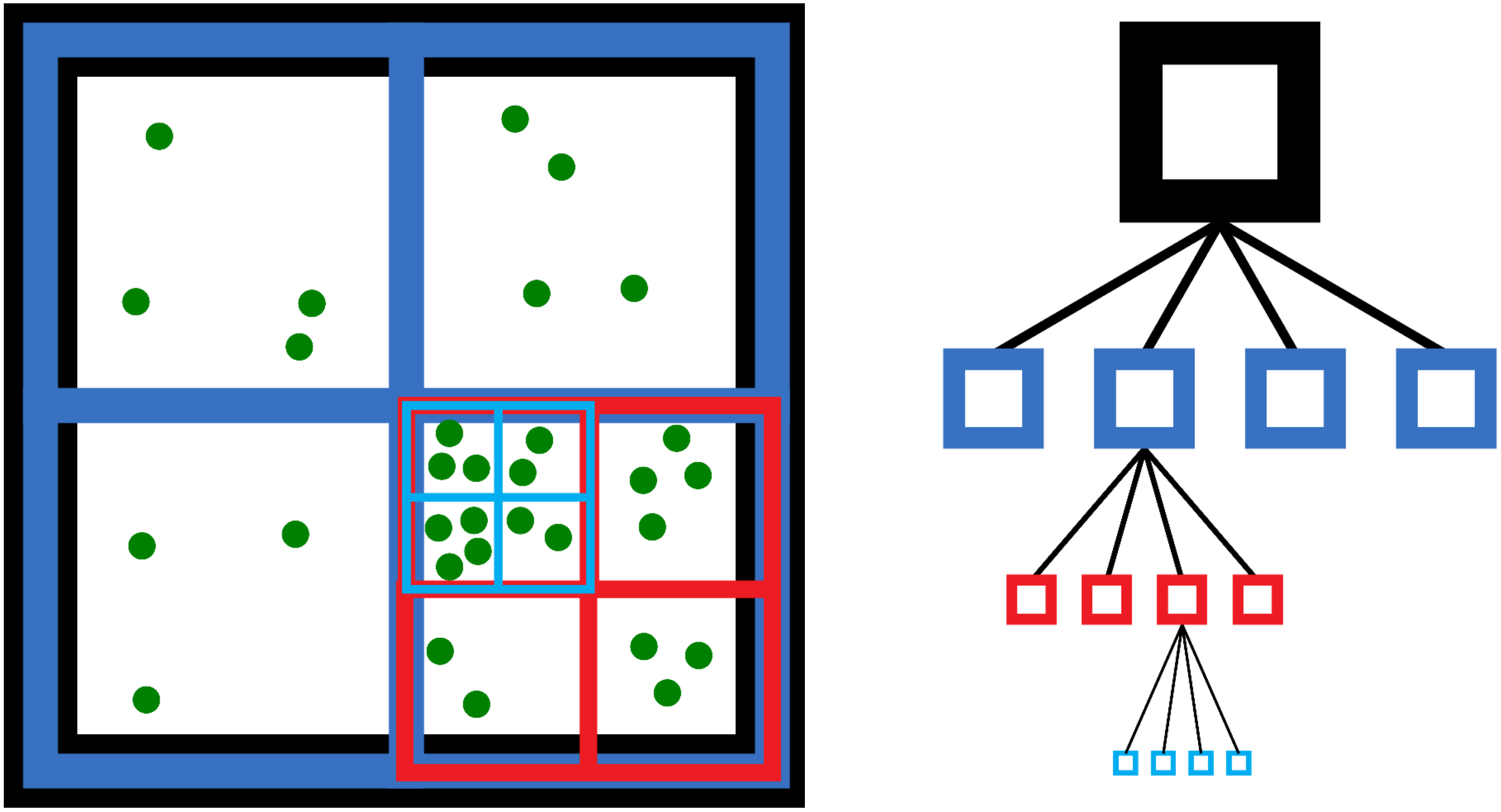
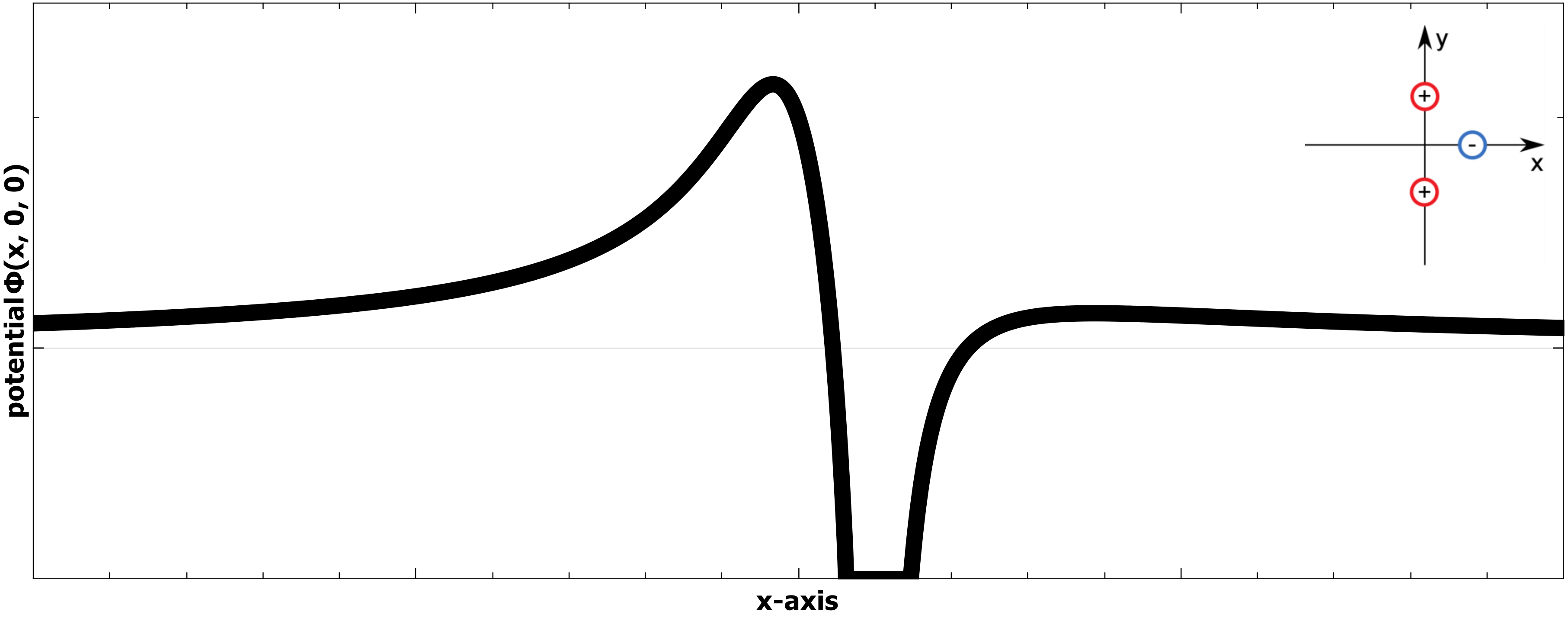


Result: Representation of bunch as a tree → Max. #particles per leaf: n_{crit}

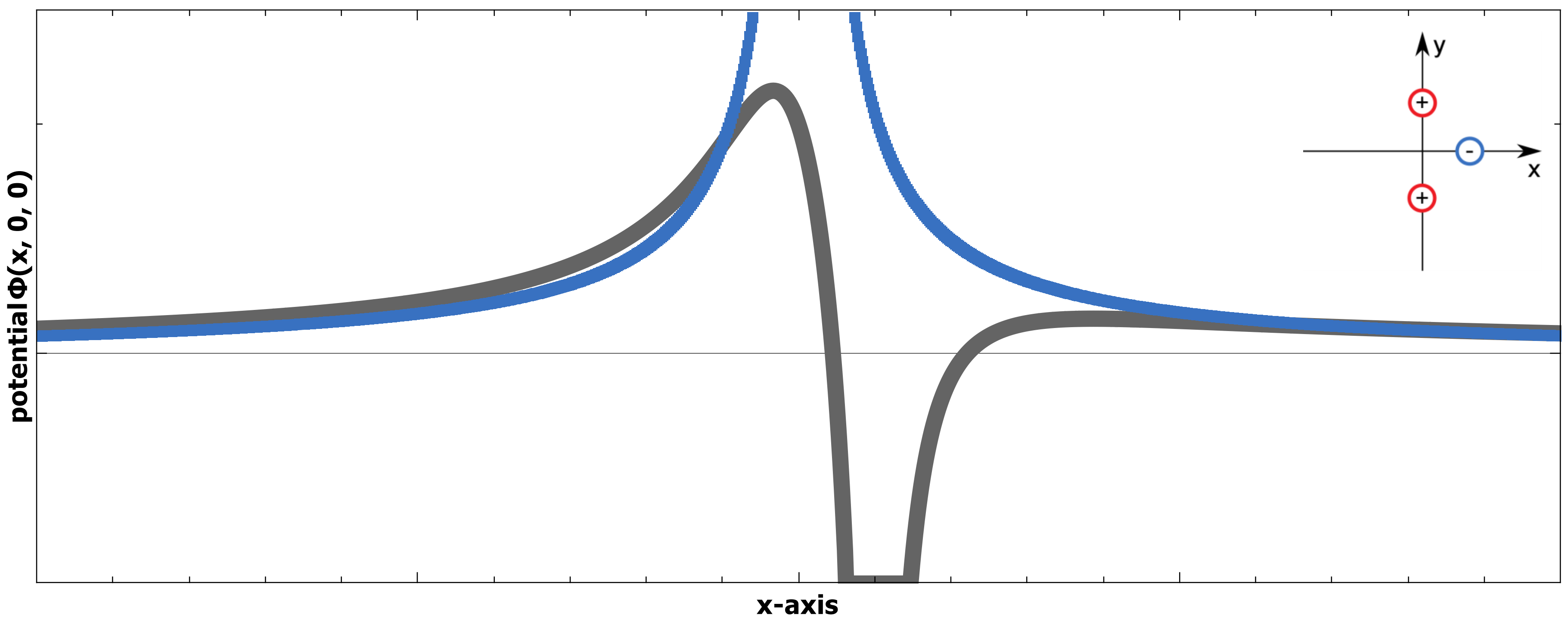
Example: Coulomb potential Φ_{exact} of three point charges (on x-axis)

$$\Phi_{exact}(x,0,0) \propto \frac{2}{\sqrt{x^2+1}} - \frac{1}{\sqrt{(x-1)^2}}$$



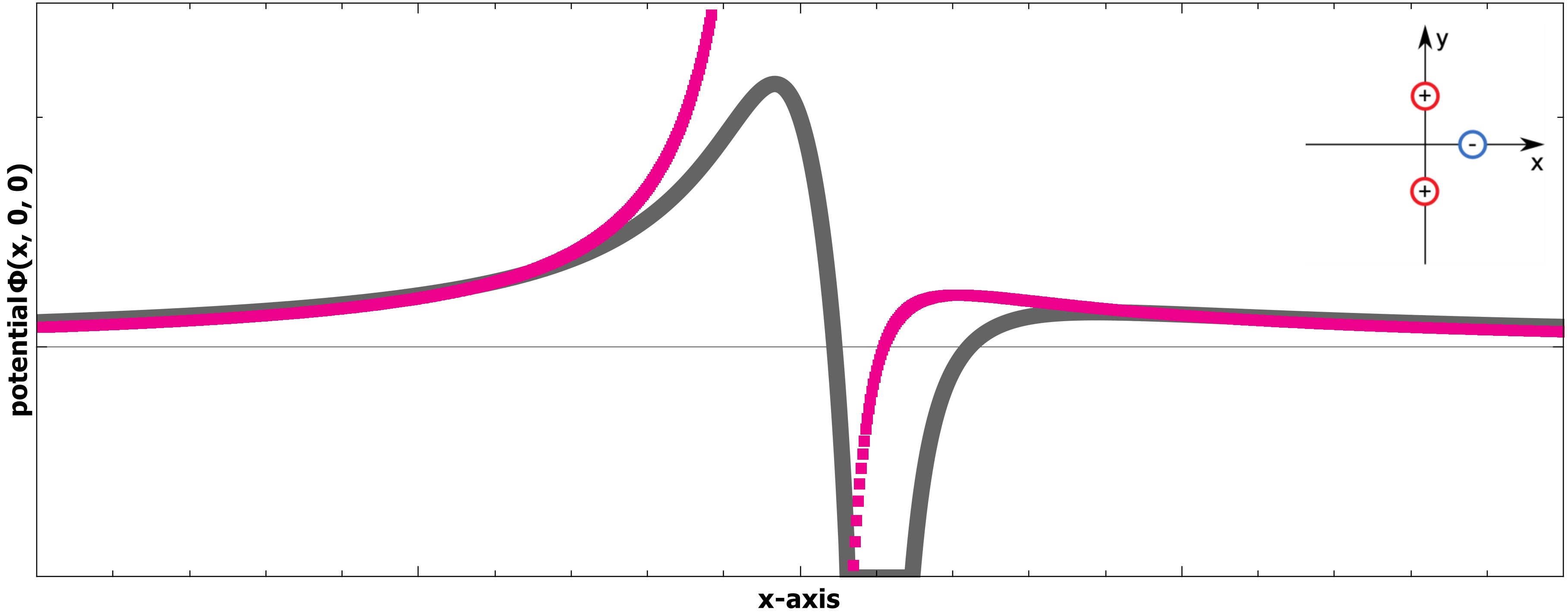
Fast Multipole Methods
2. Effective Force: Multipole Expansion

$$\Phi_{exact}(x,0,0) \propto \frac{2}{\sqrt{x^2+1}} - \frac{1}{\sqrt{(x-1)^2}} \;\mapsto\; \Phi_{monopole}(x,0,0) \propto \frac{1}{|x|}$$



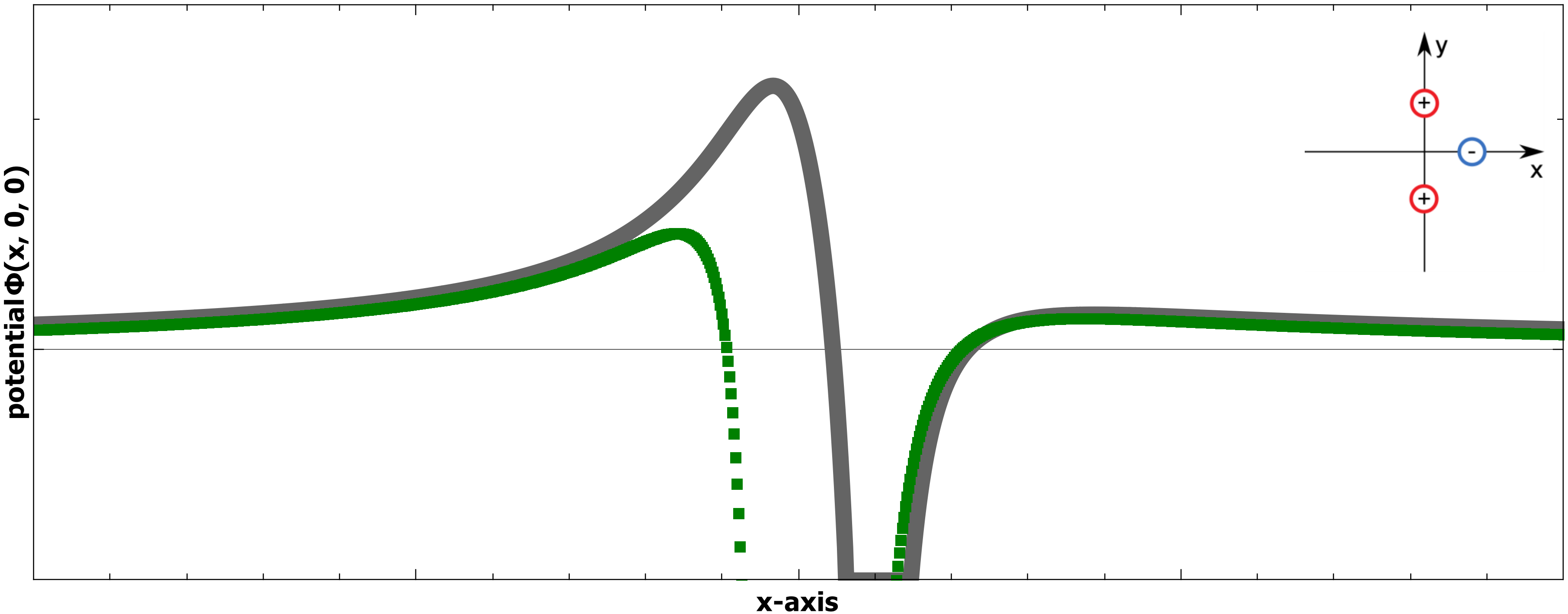
Fast Multipole Methods
2. Effective Force: Multipole Expansion

$$\Phi_{exact}(x,0{,}0) \propto \frac{2}{\sqrt{x^2+1}} - \frac{1}{\sqrt{(x-1)^2}} \;\longmapsto\; \Phi_{dipole}(x,0{,}0) \propto \frac{1}{|x|} - \frac{x/|x|}{|x|^2}$$



Fast Multipole Methods
2. Effective Force: Multipole Expansion

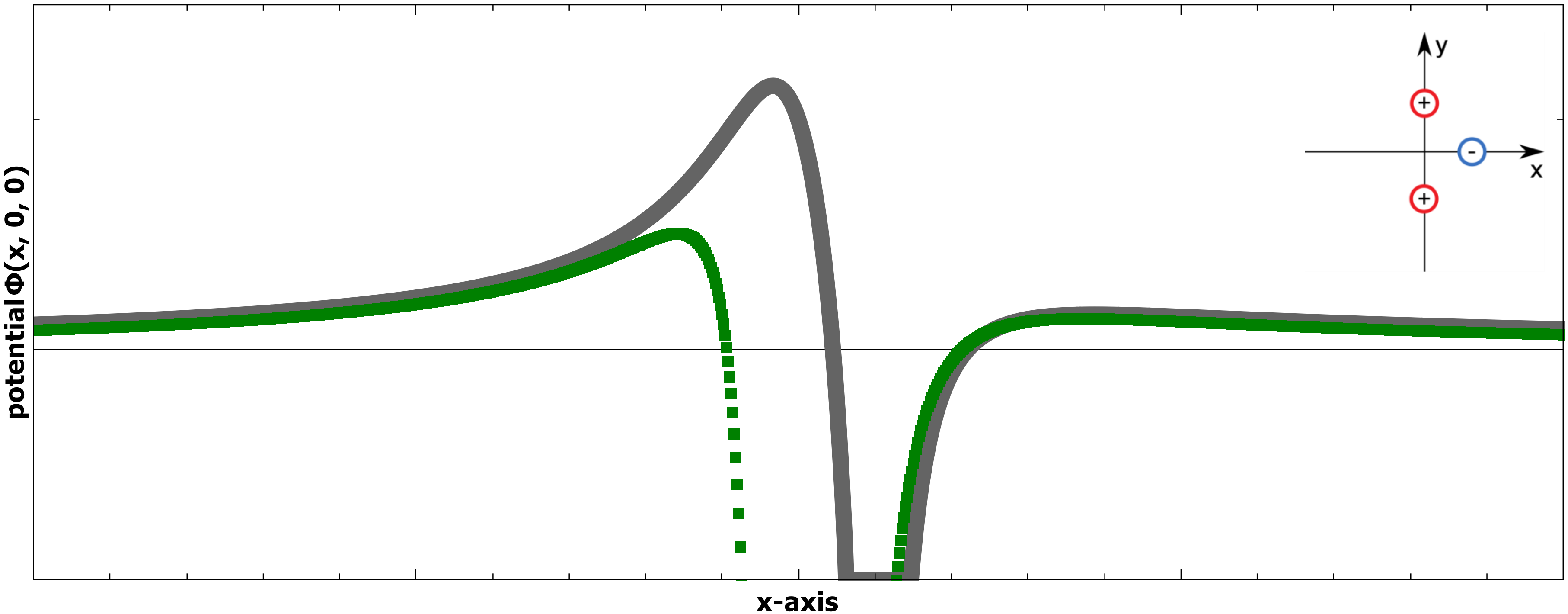
$$\Phi_{exact}(x,0,0) \propto \frac{2}{\sqrt{x^2+1}} - \frac{1}{\sqrt{(x-1)^2}} \mapsto \Phi_{quadrupole}(x,0,0) \propto \frac{1}{|x|} - \frac{x/|x|}{|x|^2} - \frac{2}{|x|^3} \dots$$



Fast Multipole Methods
2. Effective Force: Multipole Expansion

General case: Multipole expansion in spherical coordinates truncated at $\boldsymbol{l_{max}}$

$$\Phi(x) = \frac{1}{4\,\pi\epsilon_0} \cdot \sum_{i=0}^{N} \frac{q_i}{|x - x_i|} = \sum_{l=0}^{\boldsymbol{l_{max}}} \sum_{m=-l}^{l} \left(L_l^m\, r^l + \frac{M_l^m}{r^{l+1}} \right) Y_l^m(\theta, \phi) + O(l > \boldsymbol{l_{max}})$$

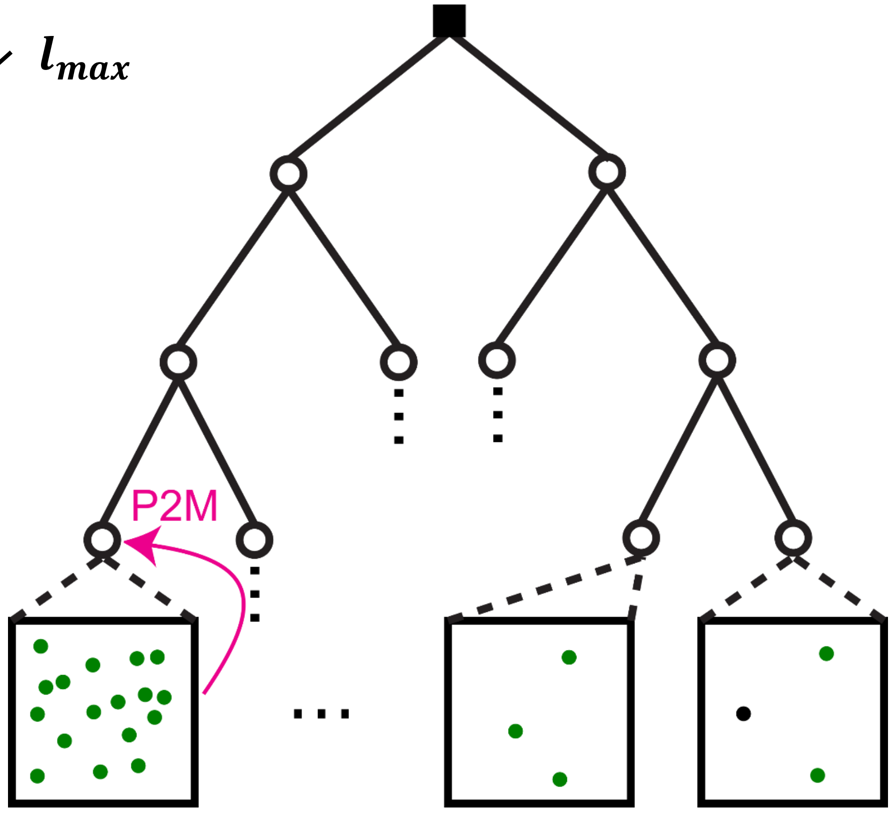


Fast Multipole Methods
3. Evaluate Interaction: Tree Traversal

How to get from $O(N^2)$ to $O(N)$?

1. Compute multipole expansion of particles contained in each leaf box.

l_{max}



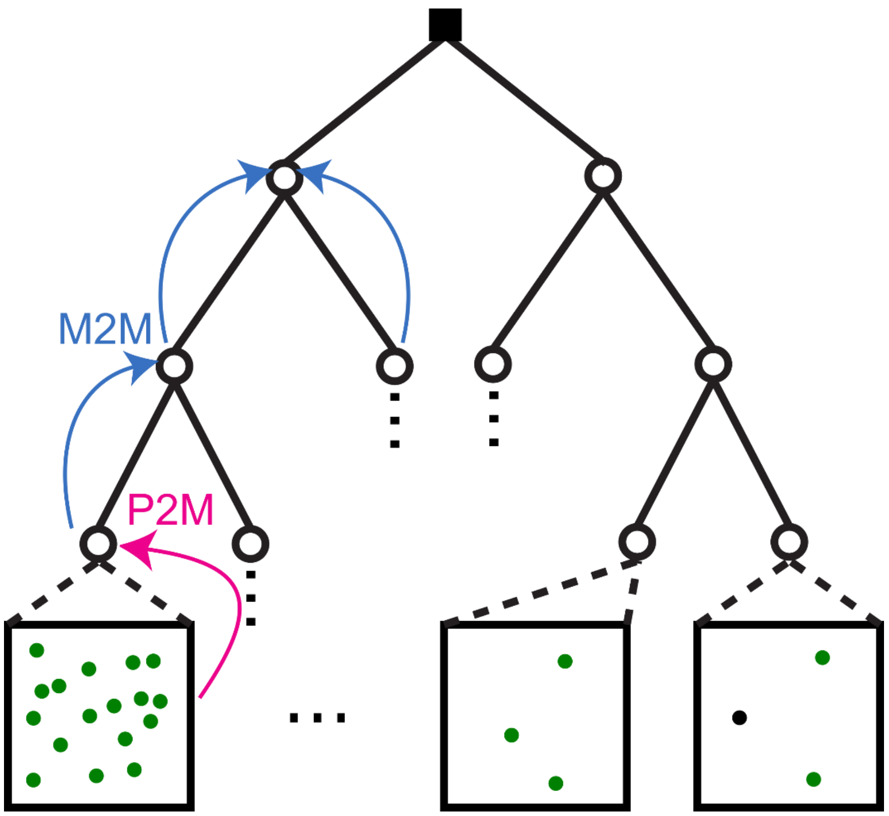
(Plot based on: R. Yokota, ExaFMM User's Manual, 2011)

Fast Multipole Methods
3. Evaluate Interaction: Tree Traversal

How to get from $O(N^2)$ to $O(N)$?

1. Compute multipole expansion of particles contained in each leaf box.

2. Express multipoles in parent node. Sum contributions from child nodes.



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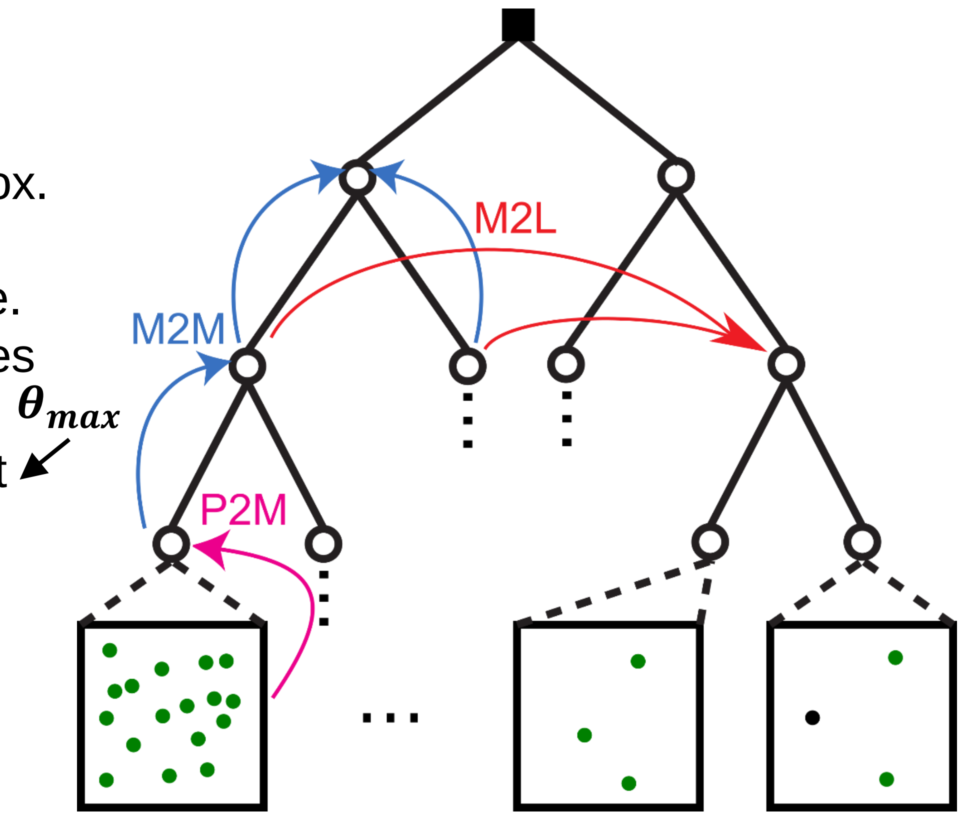
Fast Multipole Methods

3. Evaluate Interaction: Tree Traversal

How to get from $O(N^2)$ to $O(N)$?

1. Compute multipole expansion of particles contained in each leaf box.
2. Express multipoles in parent node. Sum contributions from child nodes
3. Translate approximation of distant distribution to local parent node.



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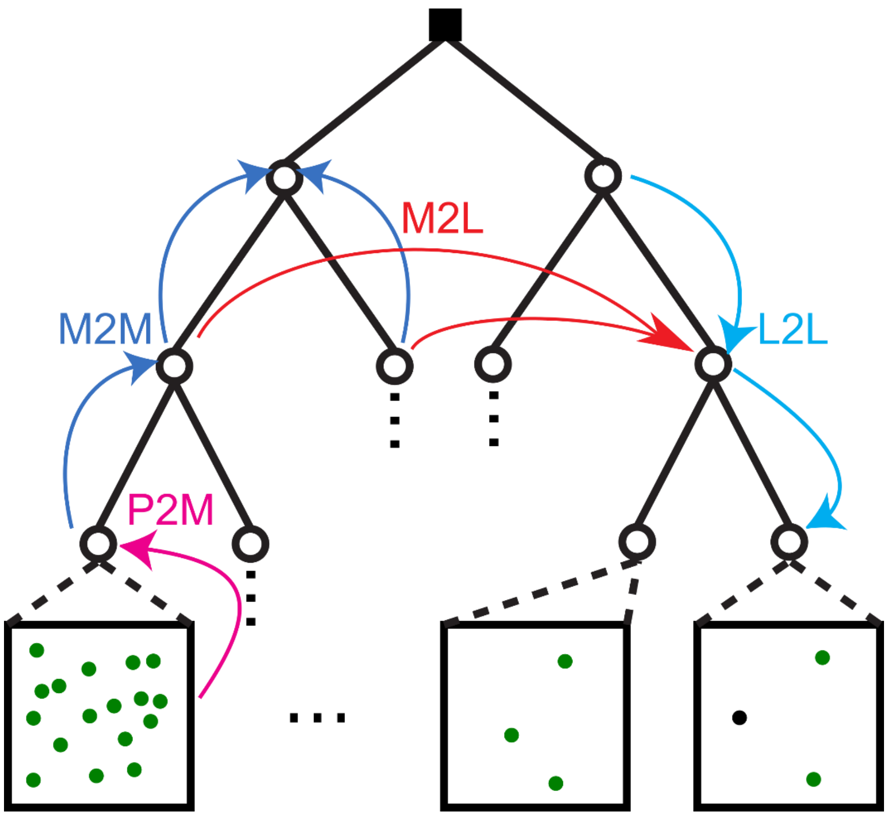
4. Express multipole expansion in the local coordinates of the child nodes.



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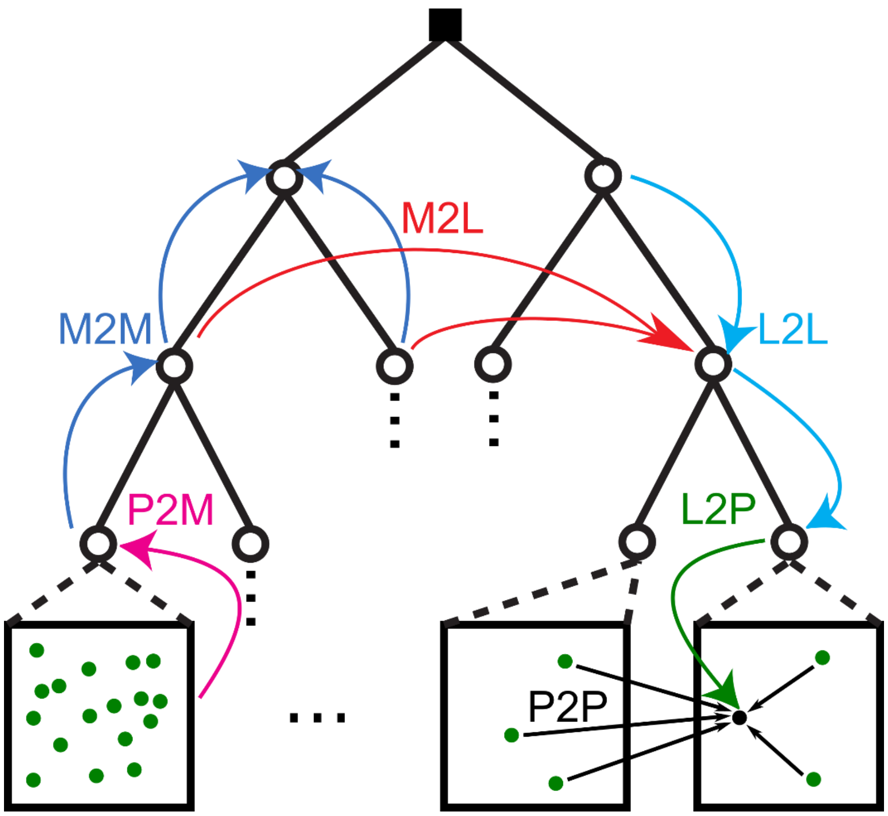
2. Express multipoles in parent node. Sum contributions from child nodes.
3. Translate approximation of distant distribution to local parent node.
4. Express multipole expansion in the local coordinates of the child nodes.
5. Evaluate $F_{distant}$ and F_{near} for each particle in the leaf.
   $\rightarrow O(N)$ scaling



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Numerical Analysis of the Method
Implementation: Overview of FMM Codes

TECHNISCHE UNIVERSITÄT DARMSTADT

Strategy:
Use an existing FMM code as a basis to extend our in-house particle tracker

Overview of available codes:

Code	Comments
Exafmm (C++) (George Washington University & Tokyo Institute of Technology)	**FMM code developed for exa-scale computing** • **MPI parallelization and GPU acceleration** • **Issues with certain particle distributions**
Tapas (C++) (Tokyo Institute of Technology)	Implicitly parallel programming framework • Flexible template framework • Under development, No mature version available
Scafacos/PEPC (C++, F90) (BMBF, DFG Project of German research groups)	Parallel library to solve electrostatic problems • Established code • No GPU version

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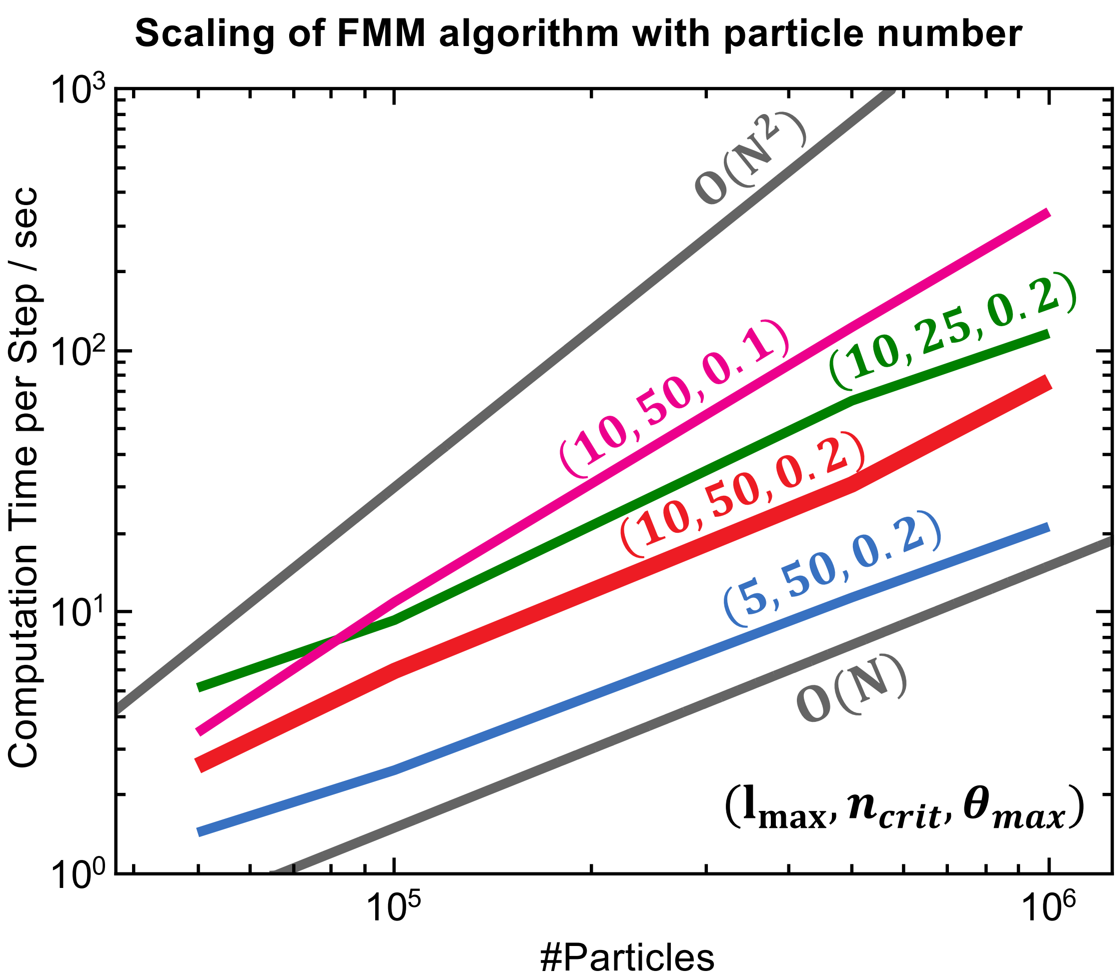
Our Choice:

Exafmm - MPI & GPU parallelization, C++ (LW-code in C), best documentation

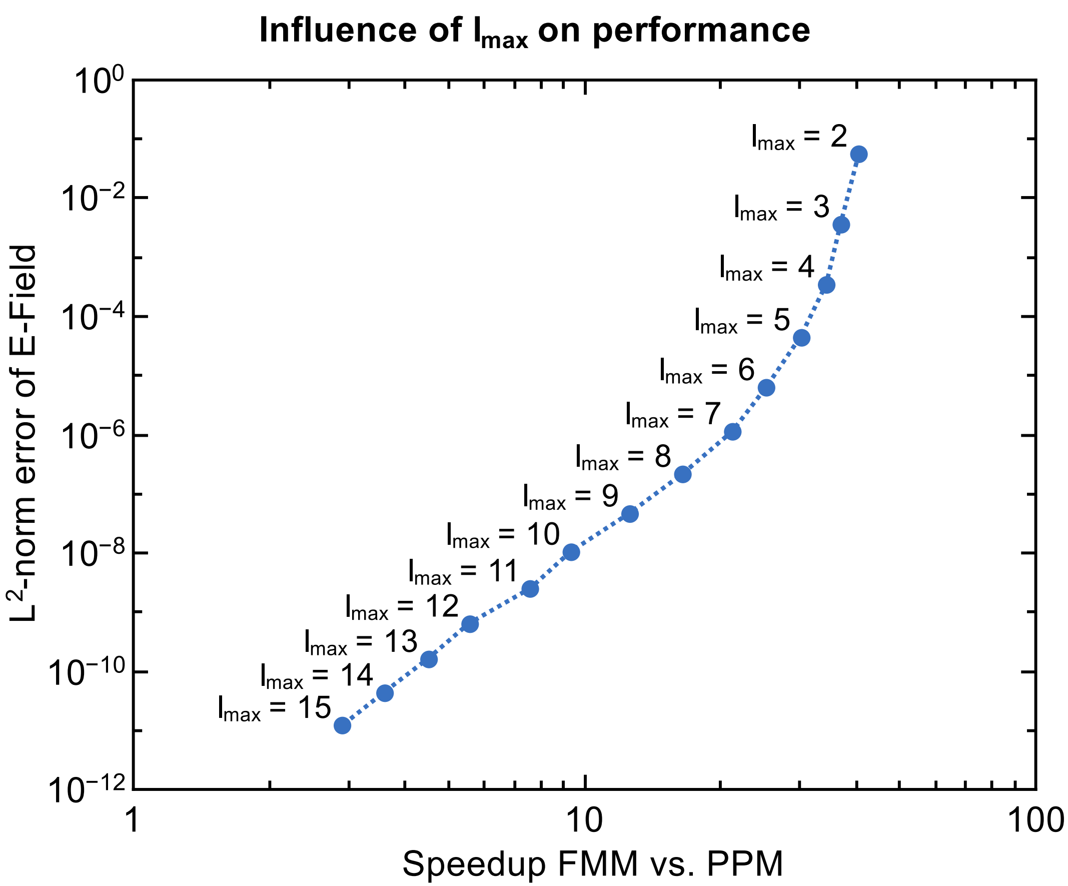
Numerical Analysis of the Method
Approximation Errors and Speedup



- Electrostatic interaction
- Freely propagating bunch
- 100 processes on cluster
- Average over ~40 time steps

Scaling: $O(N)$ up to $O(N^2)$
(depends on $l_{max}, n_{crit}, \theta_{max}$)

Numerical Analysis of the Method
Approximation Errors and Speedup

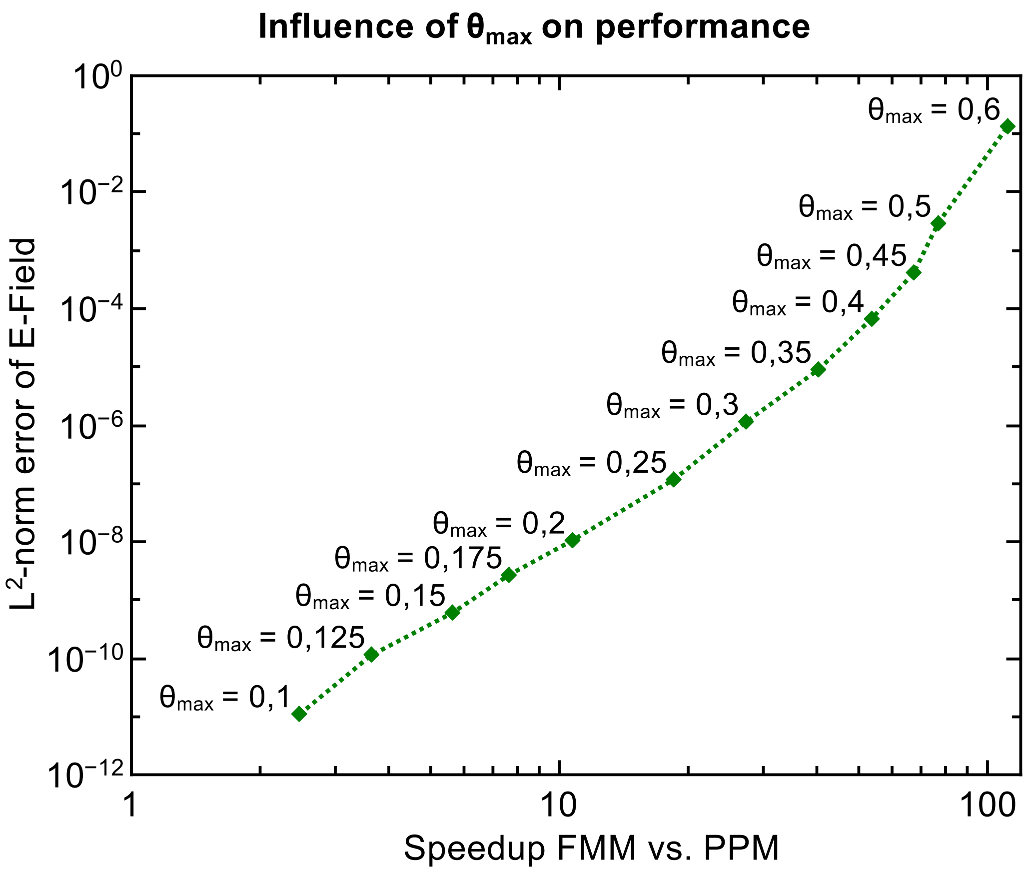


- Electrostatic interaction
- 500k propagating particles
- 60 processes on cluster
- Average over ~40 time steps
- $\boldsymbol{\theta_{max} = 0.2}$
  $\boldsymbol{n_{crit} = 50}$
  $\boldsymbol{l_{max} \in [2, 15]}$

Tradeoff: Error vs. speedup

Numerical Analysis of the Method

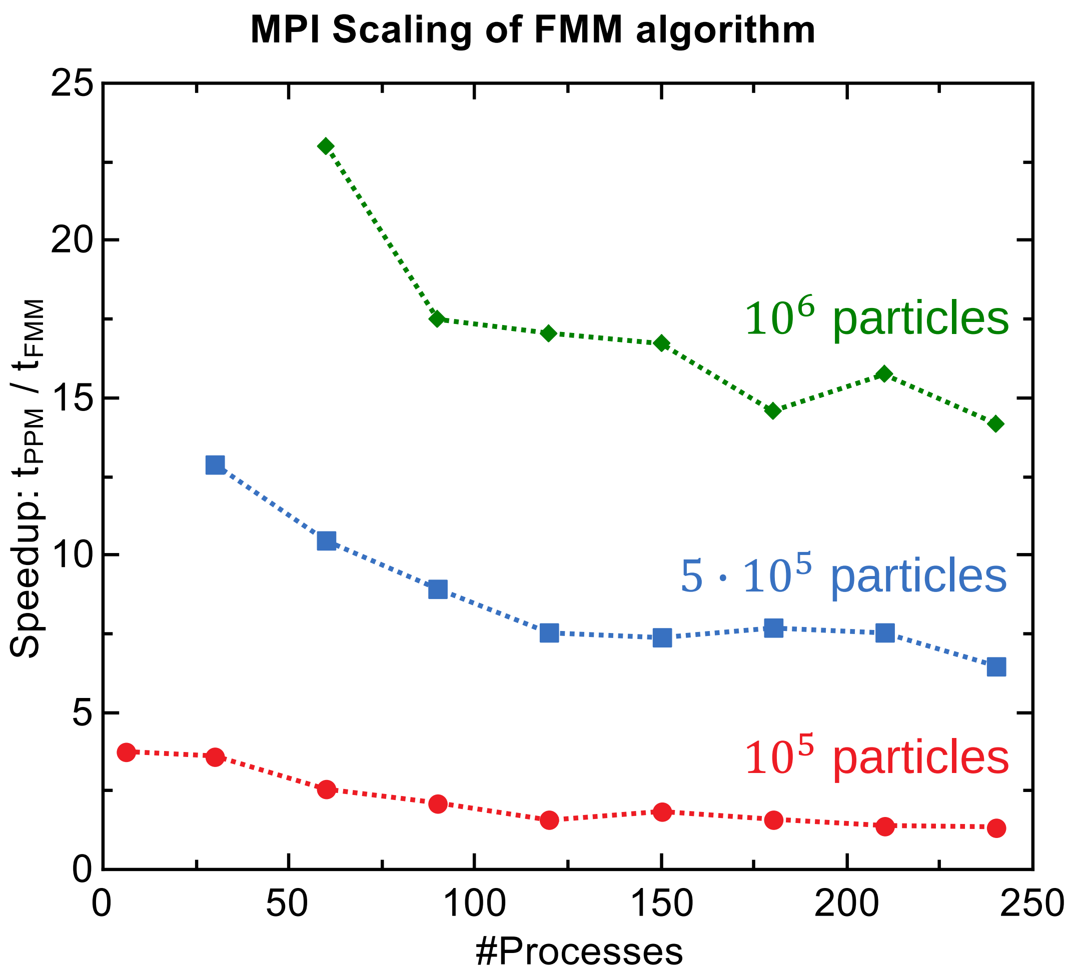
Approximation Errors and Speedup



- Electrostatic interaction
- 500k propagating particles
- 60 processes on cluster
- Average over ~ 40 time steps
- $\boldsymbol{l_{max} = 10}$
  $\boldsymbol{n_{crit} = 50}$
  $\boldsymbol{\theta_{max} \in [0.1, 0.6]}$

Tradeoff: Error vs. speedup

Numerical Analysis of the Method
Approximation Errors and Speedup

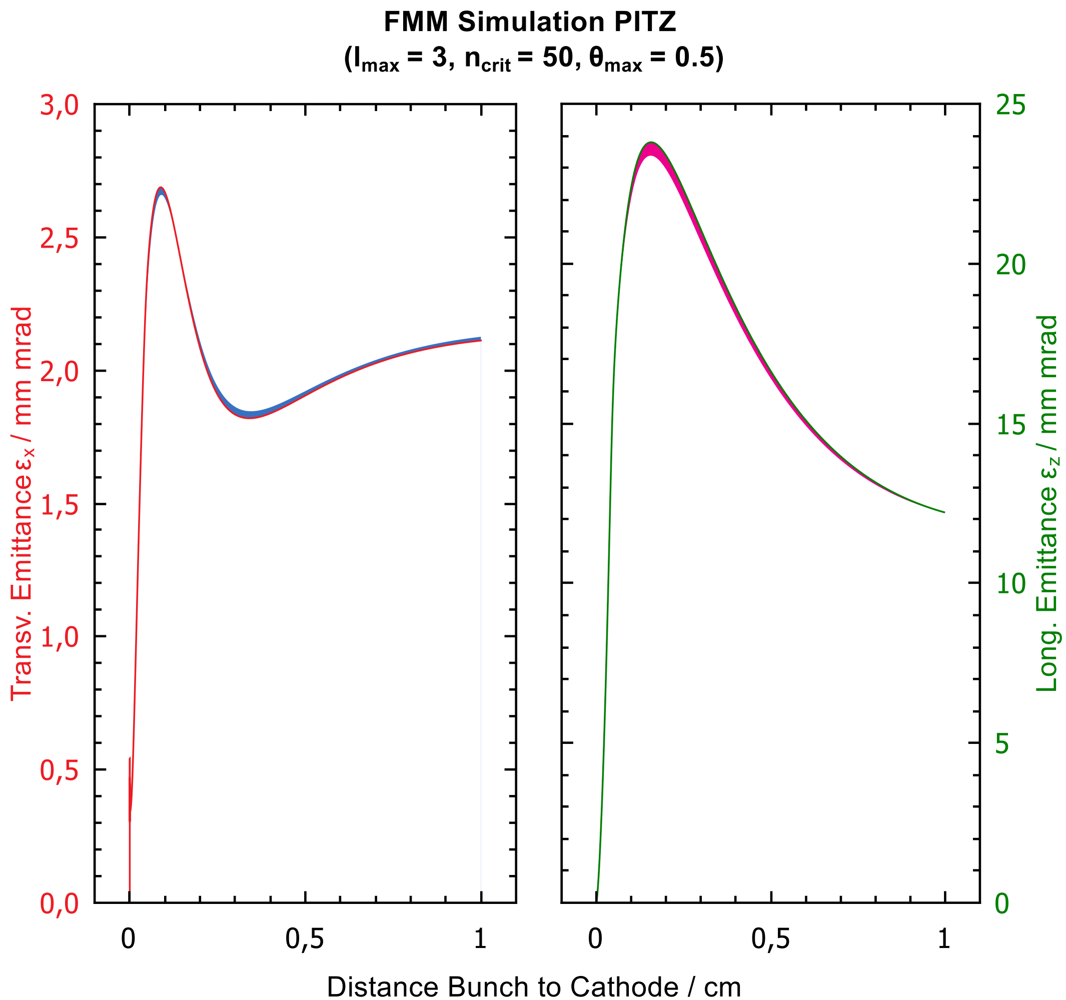


- Electrostatic interaction
- Identical compute nodes
- Average over ~ 40 time steps
- $$\boldsymbol{l_{max} = 10}$$ $$\boldsymbol{n_{crit} = 50}$$ $$\boldsymbol{\theta_{max} = 0.2}$$

MPI scaling of PPM code better than FMM code

Best FMM speedup for more particles and less processes

Preliminary Results for the PITZ Gun
Emittance study

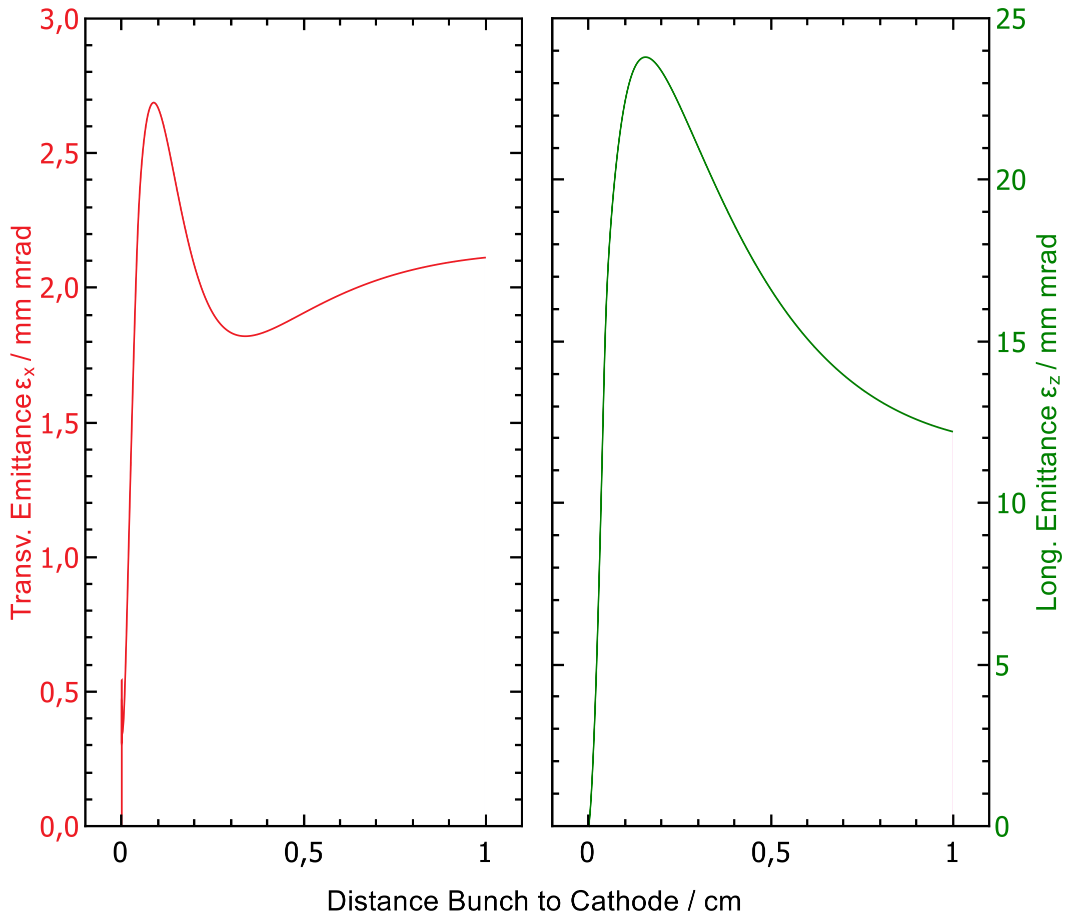


- Relativistic rest frame model
- #particles: $N = 500.000$
  $\sigma_r = 0.4\ \mathrm{mm}, \sigma_t = 22\ \mathrm{ps}$
- PPM: 234 processes on cluster
  Runtime: $T_{PPM} \sim 42\ \mathrm{h}\ 41\ \mathrm{min}$
- FMM: 8 processes on desktop
  Runtime: $T_{FMM} \sim 46\ \mathrm{min}$

Speedup $\sim\times$ 55
Max. Deviation $\sim 3.14\ \%$

Preliminary Results for the PITZ Gun
Emittance study

FMM Simulation PITZ
($l_{max} = 5$, $n_{crit} = 50$, $\theta_{max} = 0.4$)



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- FMM: 8 processes on desktop
  Runtime: $T_{FMM} \sim 1\ \mathrm{h}\ 37\ \mathrm{min}$

Speedup $\sim\times\ 26$
Max. Deviation $\sim 0.06\ \%$

Preliminary Results for the PITZ Gun
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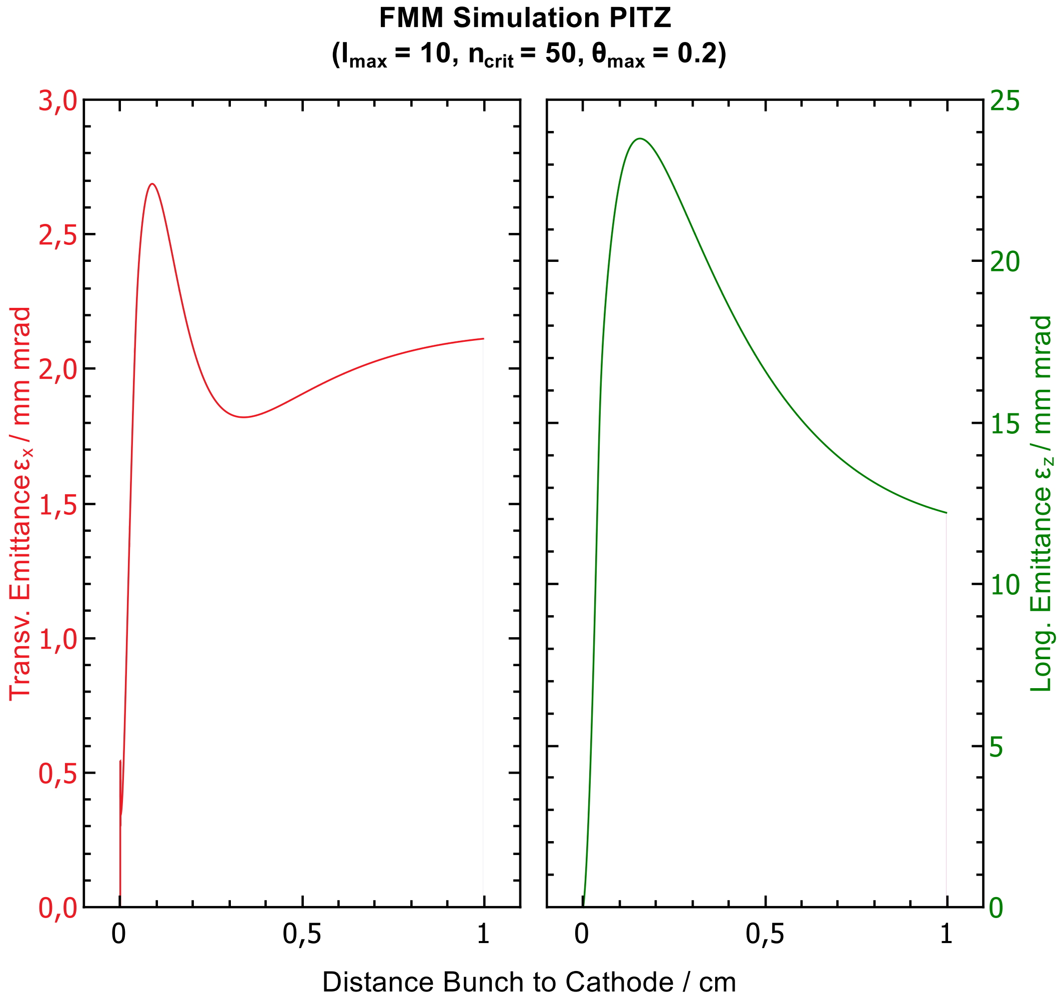

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- FMM: 8 processes on desktop
  Runtime: $T_{FMM} \sim 26\ \text{h}\ 50\ \text{min}$

Speedup $\sim\times\ 1.6$
Max. Deviation $\sim 9.8 \cdot 10^{-7}\ \%$

Outlook

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Status quo:

- ExaFMM merged with in-house particle tracking code
- Basic models (electrostatic, rel. rest frame, image charges) implemented
- Numerical studies with FMM: MPI-Scaling, Influence of $l_{max},\ n_{crit}, \theta_{max}$
- First particle tracking simulations for PITZ gun

Ongoing Work:

- Optimization of MPI communication
  $\rightarrow$ Achieve better scaling on cluster
- Investigate using GPU parallelization
  $\rightarrow$ Use tree-algorithms from graphics software for particle tracking
- Implementation of self-controlled models (e.g. Schottky effect)