REPTIL - Relativistic 3D Space Charge Particle Tracking Using the Fast Multipole Method

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

DESY & TEMF Meeting - Winter 2018

15.11.2018, DESY, Hamburg

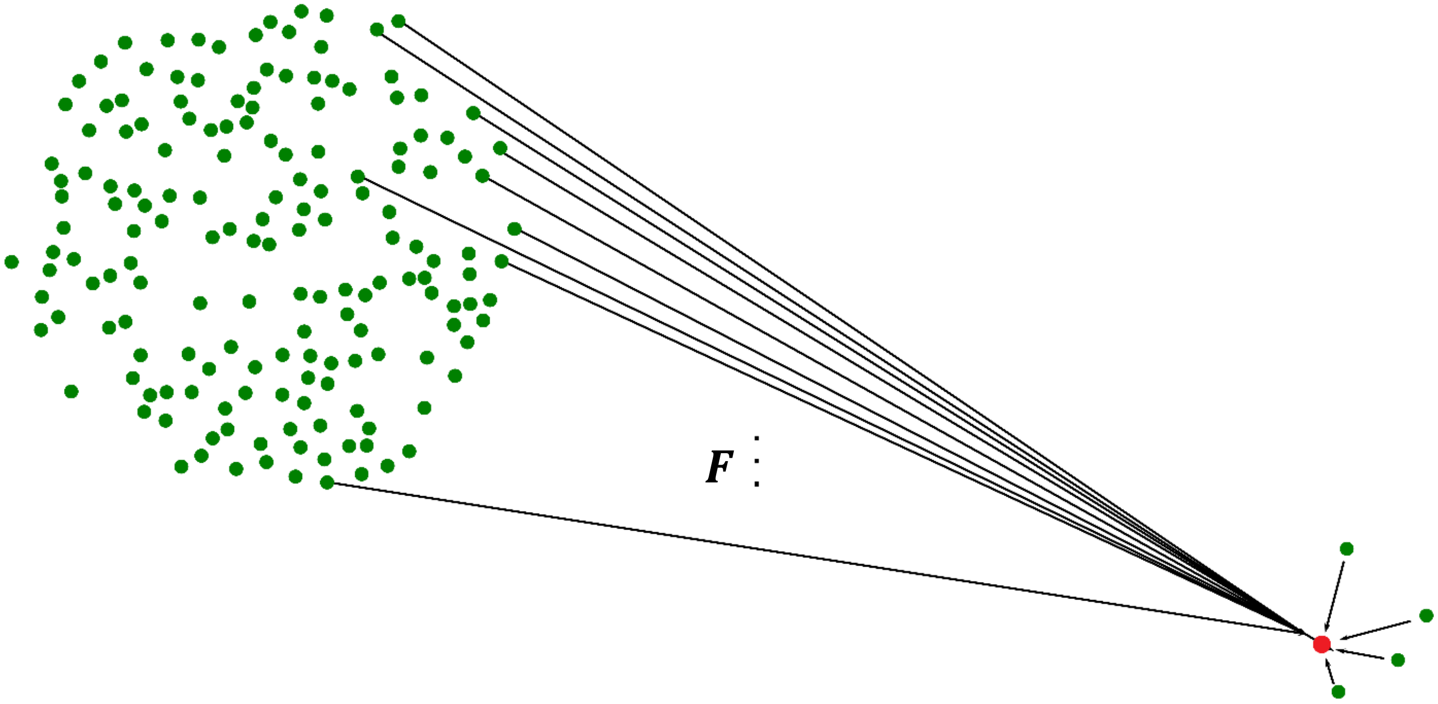
Structure

I. Fast Multipole Methods
II. Tree Construction
III. Numerical Convergence and Performance
   i. Particle Based Fast Multipole Method
   ii. Mesh Based Fast Multipole Method
IV. Simulation of the PITZ Injector
V. Outlook

Fast Multipole Methods
The Concept

Problem:

Efficient way to compute many-body interaction needed
→ Reduce complexity to less than $O(N^2)$



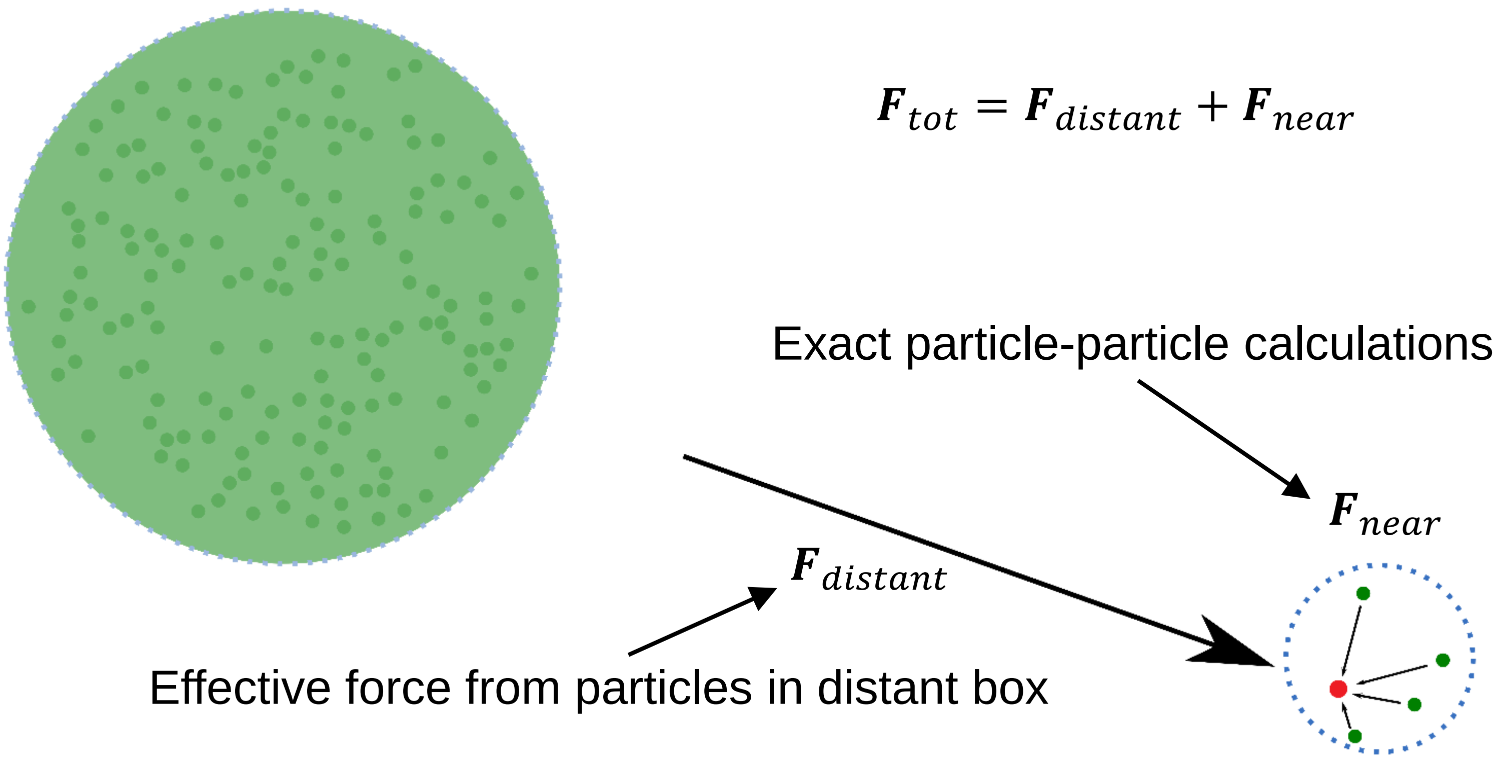
Fast Multipole Methods
The Concept

Solution:

Approximation of force for distant particles ($\theta \leq \boldsymbol{\theta_{max}}$)

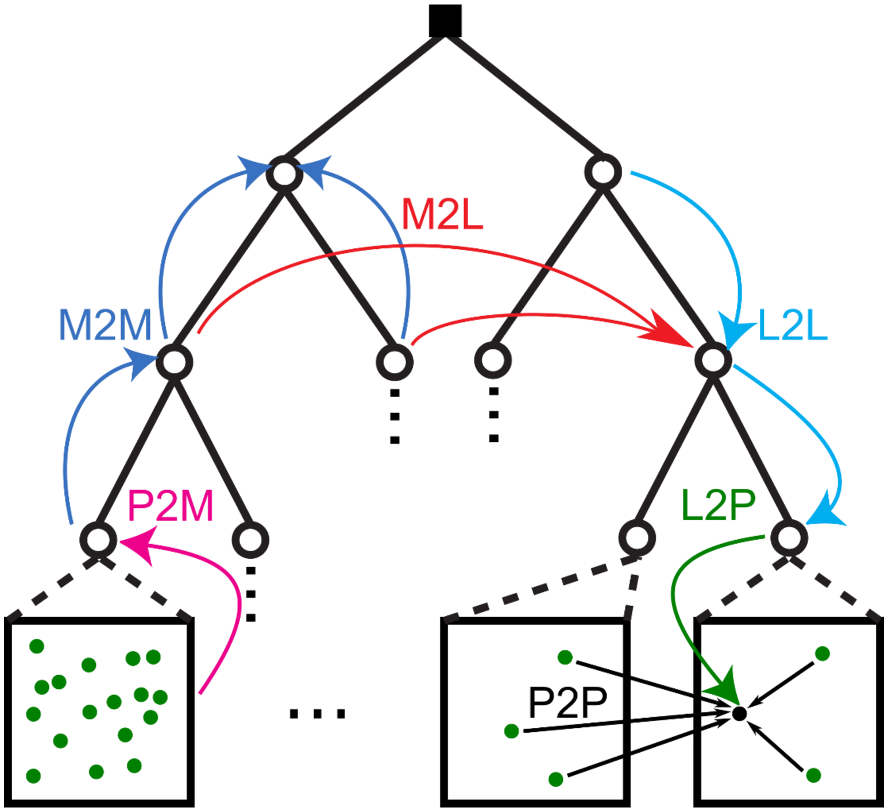
Direct computation of force for near particles

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



Fast Multipole Methods
3. Evaluate Interaction: Tree Traversal

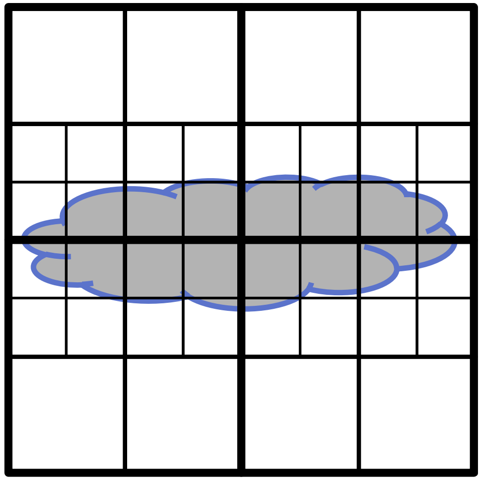
1. Compute multipole expansion of particles contained in each leaf box.
2. Express multipoles in parent node. Sum contributions from child nodes.
3. Translate approximation of distant distribution to local parent node.
4. Express multipole expansion in the local coordinates of the child nodes.
5. Evaluate $F_{distant}$ and F_{near} for each particle in the leaf.



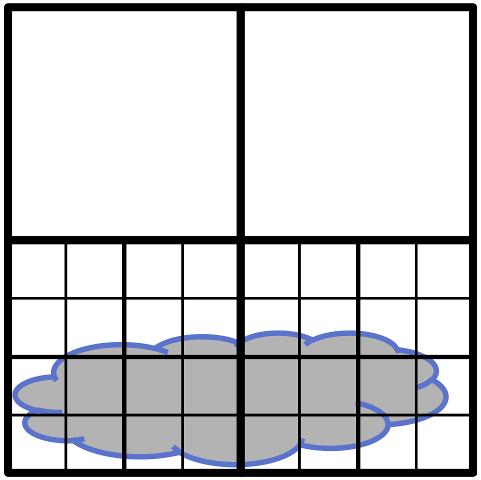
(Plot based on: R. Yokota, ExaFMM User's Manual, 2011)

Tree Construction
Spatial Sectioning Methods

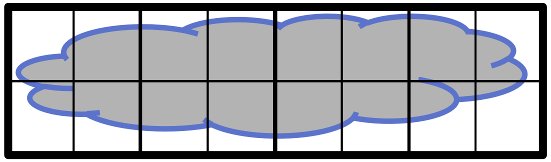
Centered 8-Section:



Shifted 8-Section:



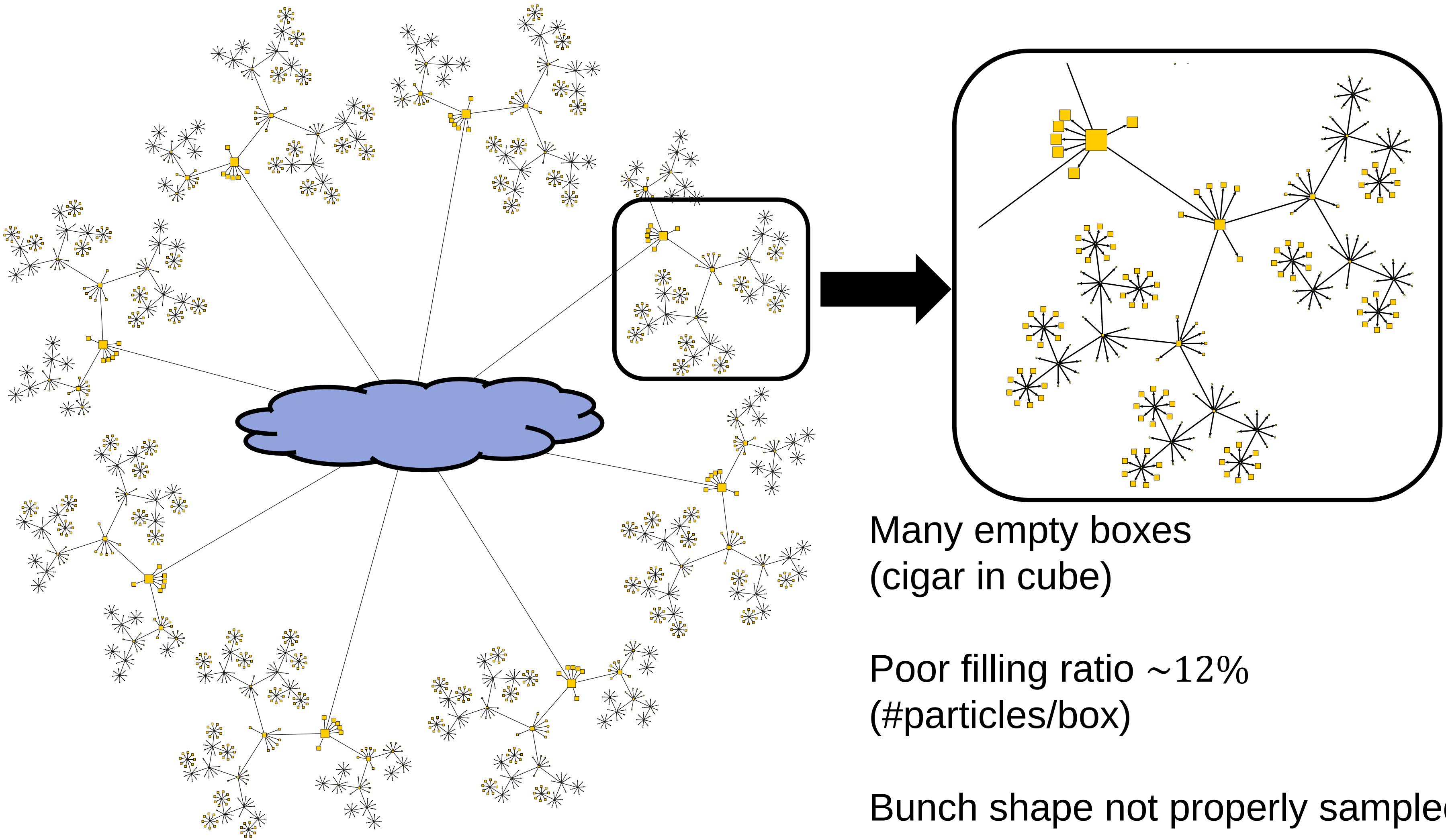
Adaptive 2^N-Section:



Centered 8-Section	Shifted 8-Section	Adaptive 2^N-Section
Common center	Tree shifted w.r.t bunch	Root box reshapes bunch
Isotropic refinement	Isotropic refinement	Non-isotropic refinement
Cubical boxes	Cubical boxes	Approx. cubical boxes

Tree Construction
Centered 8-Section for Prolate Bunch

TECHNISCHE UNIVERSITÄT DARMSTADT

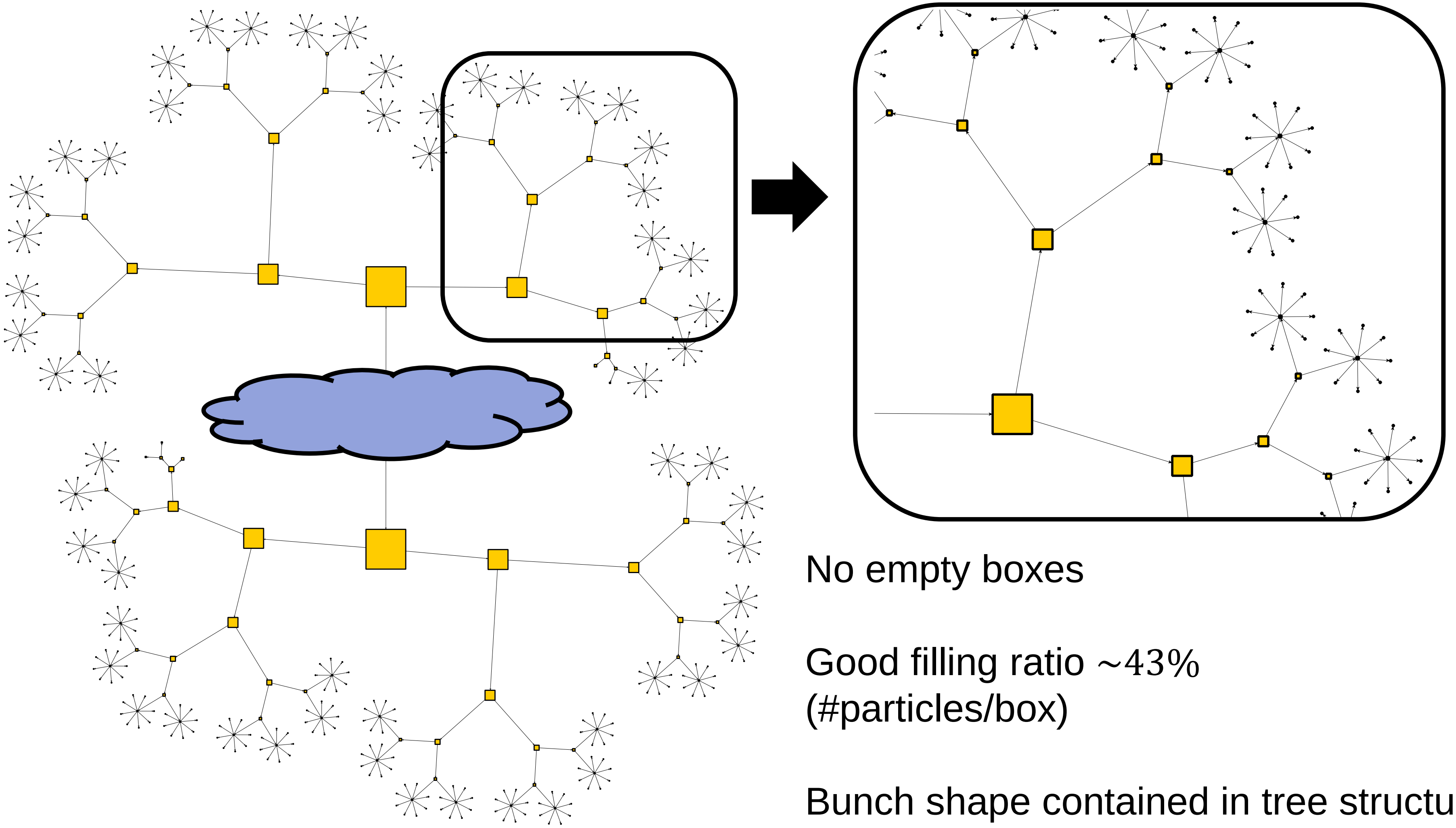


Many empty boxes
(cigar in cube)

Poor filling ratio ~12%
(#particles/box)

Bunch shape not properly sampled

Tree Construction
Adaptive 2^N-Section for Prolate Bunch



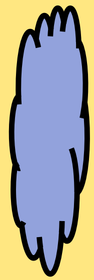
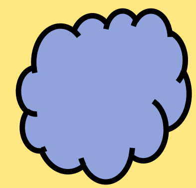
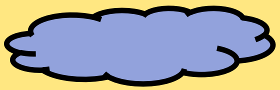
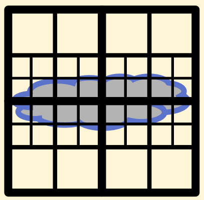
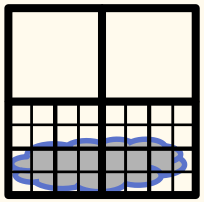
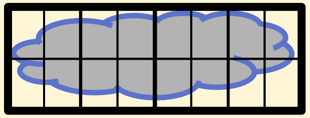
No empty boxes

Good filling ratio ~43% (#particles/box)

Bunch shape contained in tree structure

Tree Construction

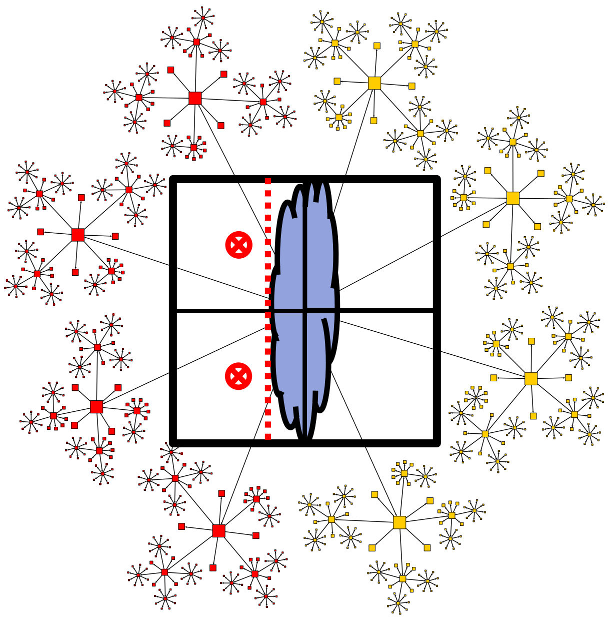
Speedup and Error of Sectioning Methods

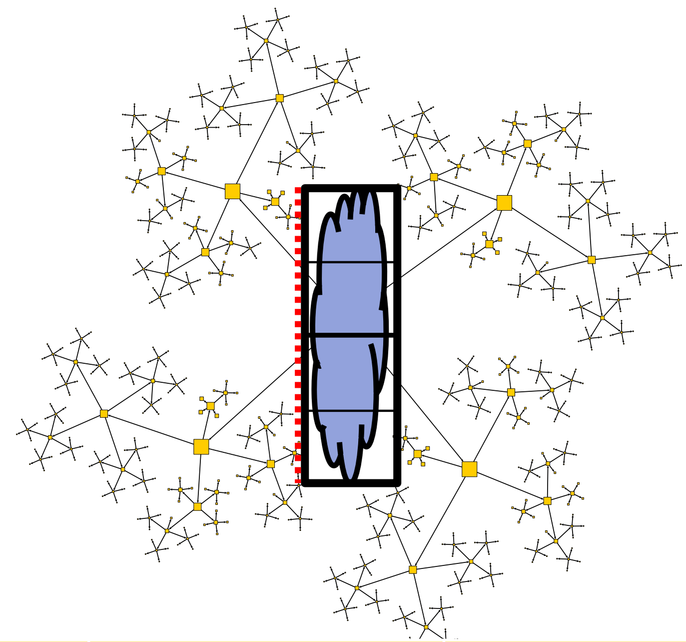
Speedup: $S := \frac{t_{PPM}}{t_{FMM}}$ Error: $\delta := \frac{\lvert E_{PPM} - E_{FMM} \rvert}{\lvert E_{PPM} \rvert}$			
	$\boldsymbol{S = 1.9}$ $\boldsymbol{\delta \sim 10^{-7}}$	$S = 1.3$ $\delta \sim 10^{-7}$	$\boldsymbol{S = 2.6}$ $\boldsymbol{\delta \sim 10^{-7}}$
	$S = 2.4$ $\delta \sim 10^{-7}$	$S = 1.4$ $\delta \sim 10^{-7}$	$S = 4.5$ $\delta \sim 10^{-8}$
	$\boldsymbol{S = 2.9}$ $\boldsymbol{\delta \sim 10^{-7}}$	$S = 1.4$ $\delta \sim 10^{-8}$	$\boldsymbol{S = 5.4}$ $\boldsymbol{\delta \sim 10^{-8}}$

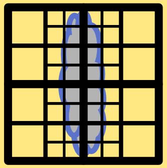
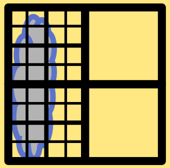
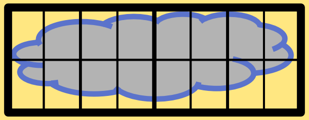
Tree Construction

Computation of Mirror Charge Interaction

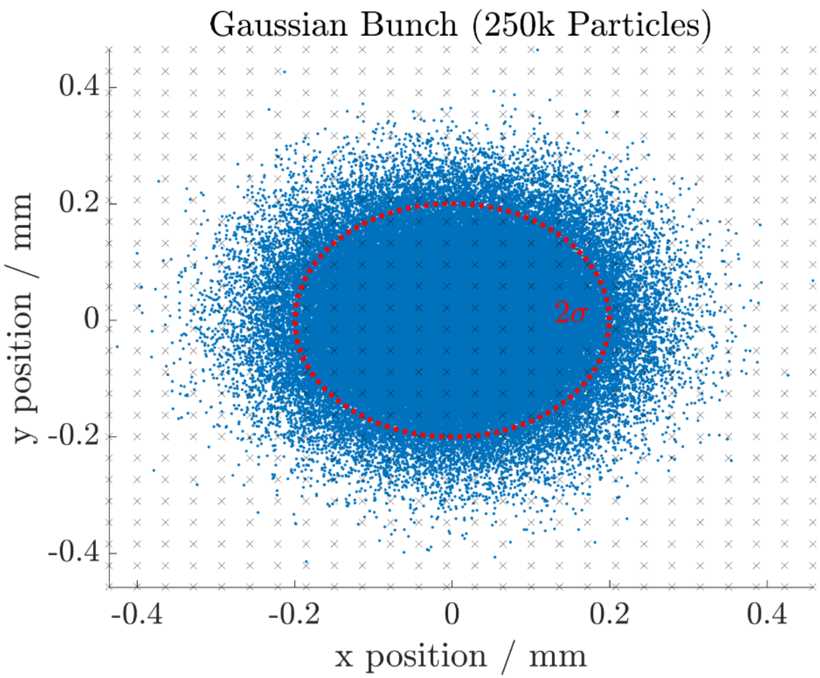
TECHNISCHE UNIVERSITÄT DARMSTADT

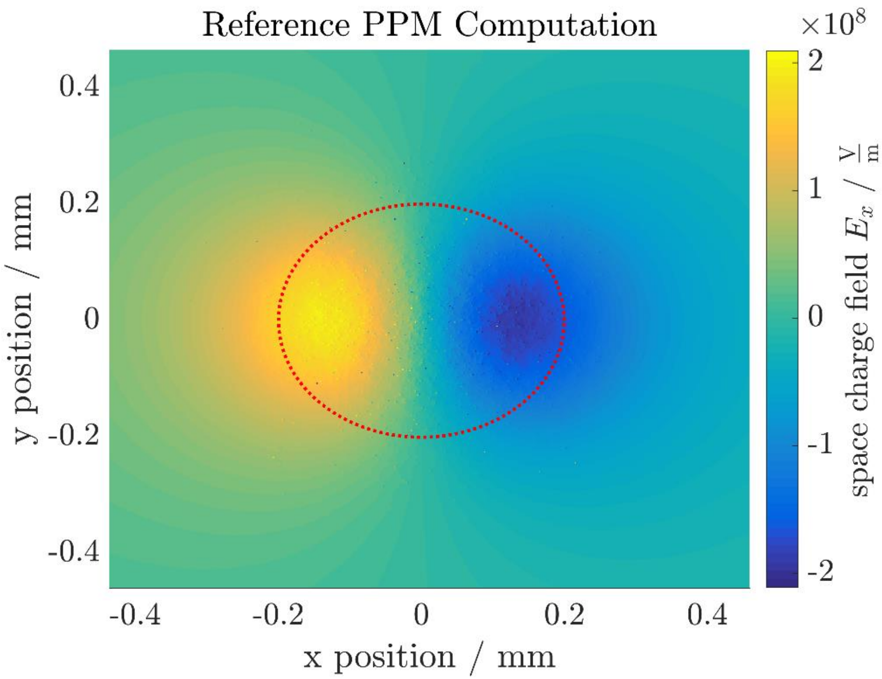




			
Speedup: $S := \frac{t_{PPM}}{t_{FMM}}$ **Error:** $\delta := \frac{\lvert E_{PPM} - E_{FMM} \rvert}{\lvert E_{PPM} \rvert}$	$S = 2.9$ $\delta \sim 10^{-6}$	$S = 20.6$ $\delta \sim 10^{-7}$	$S = 22.4$ $\delta \sim 10^{-7}$

Convergence and Performance
Particle FMM: Gaussian Bunch





<u>Test case:</u>

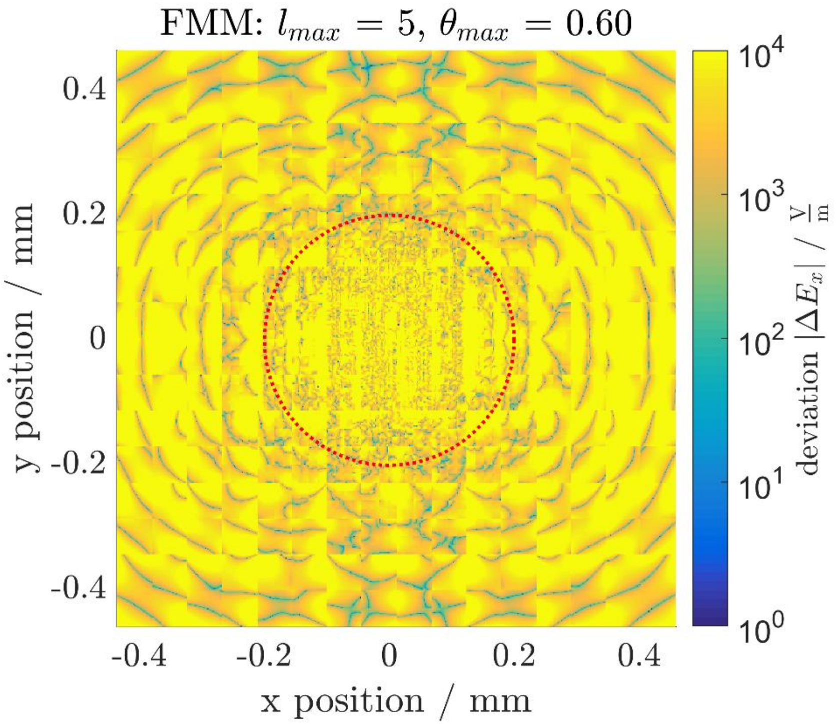
Truncated Gaussian bunch,
$N = 250\text{k}$, $\sigma_i = 0.1$ mm, $Q = 1.0$ nC,
501×501 probe points at $z = \mu_z$

Electrical field E_x:

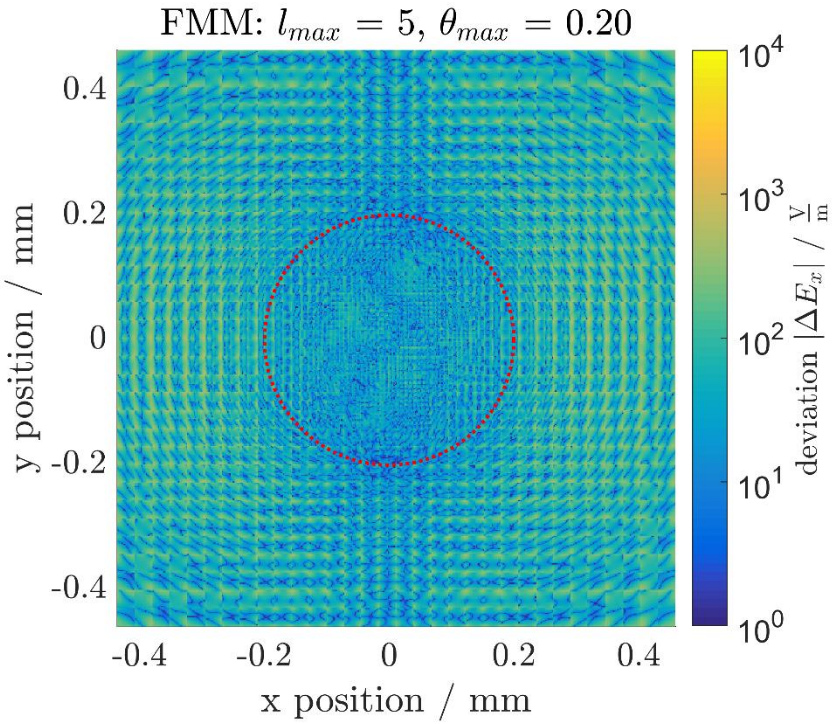
$$E_x = E_x^{gauss} + E_x^{near} \sim 10^8 \frac{V}{m}$$

Convergence and Performance
Particle FMM: Admissibility Parameter θ_{max}

$\theta_{max} = 0.6$
$\Rightarrow \sigma(E_x) \sim 10^5\ V/m$



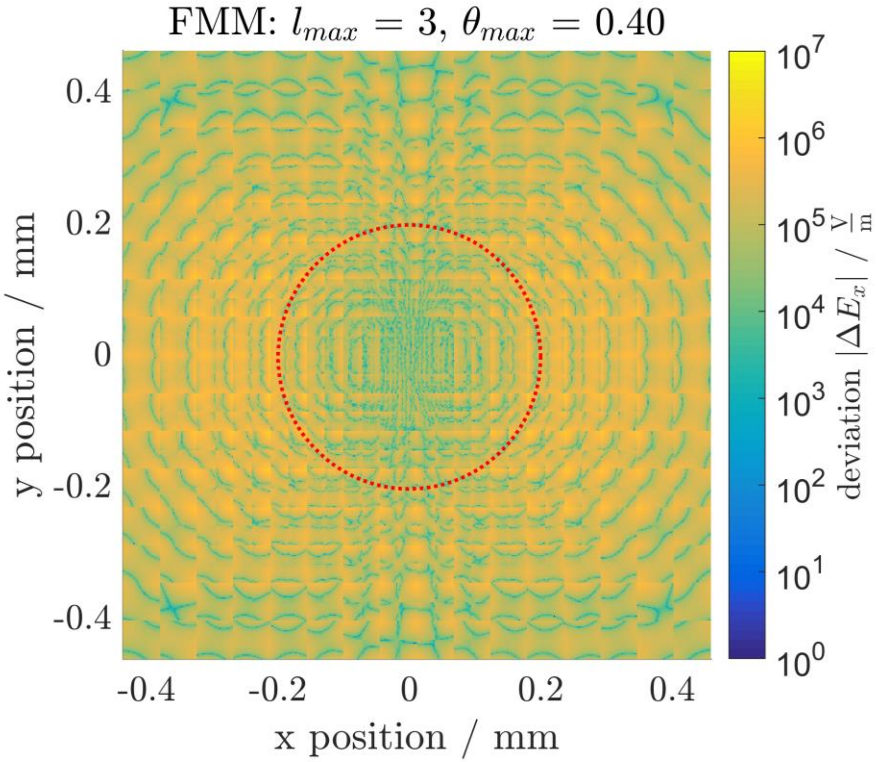
$\theta_{max} = 0.2$
$\Rightarrow \sigma(E_x) \sim 10^2\ V/m$

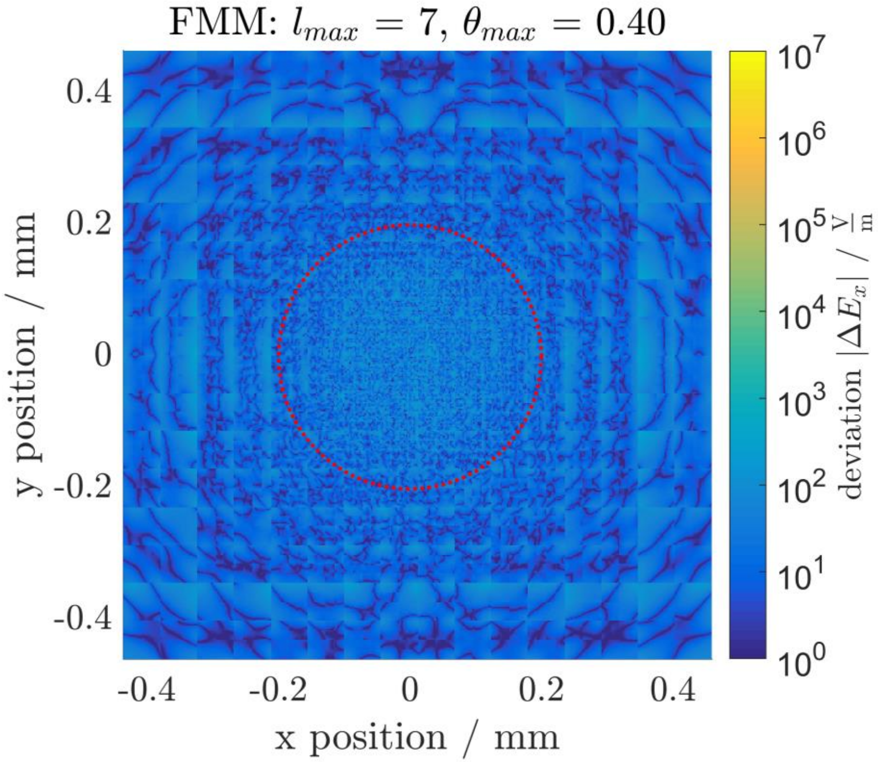


Convergence and Performance
Particle FMM: Multipole Expansion Order l_{max}

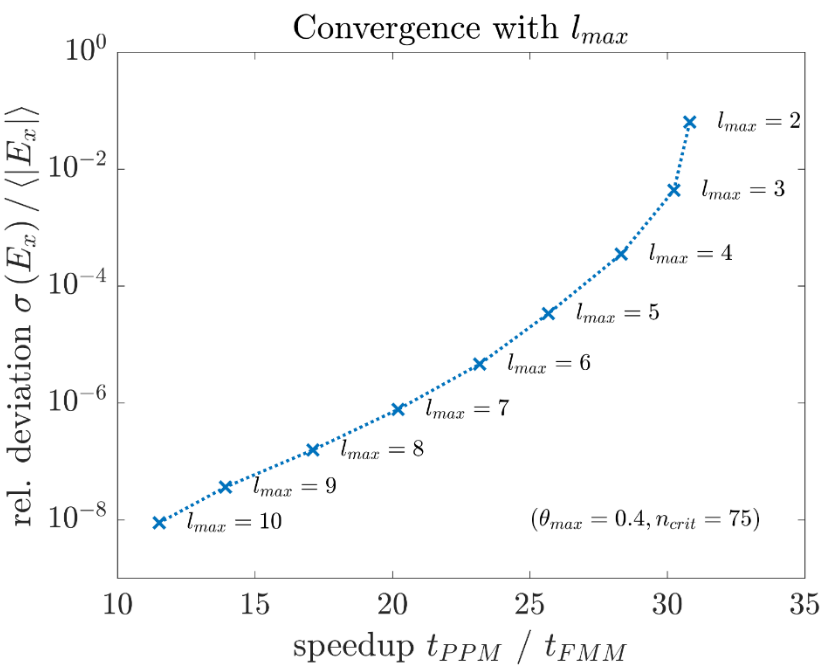
$$l_{max} = 3$$
$$\Rightarrow \sigma(E_x) \sim 10^6\ V/m$$

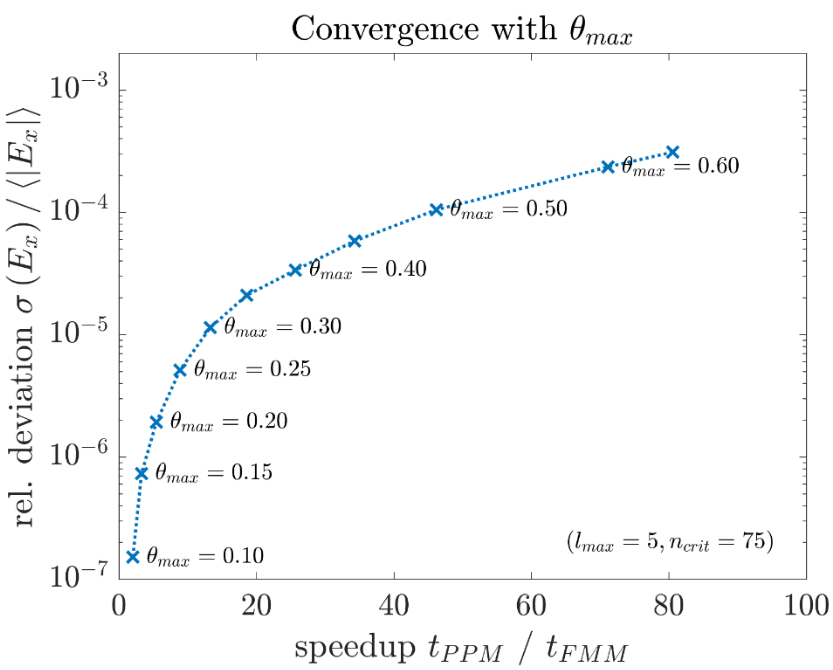
$$l_{max} = 7$$
$$\Rightarrow \sigma(E_x) \sim 10^2\ V/m$$





Convergence and Performance
Particle FMM: Numerical Convergence Study





<u>Speedup vs. Multipole Order:</u>

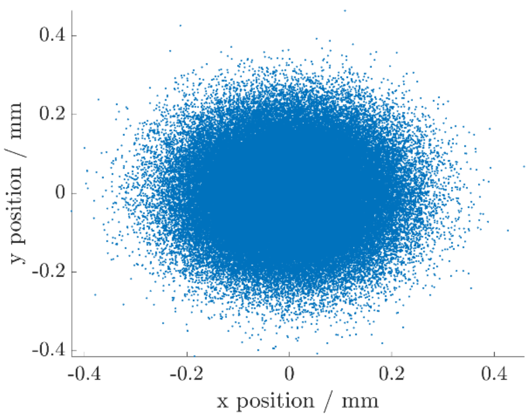
Exponential convergence in $\boldsymbol{l_{max}}$
Adds comp. cost of $O(\boldsymbol{l_{max}^2})$ to $O(\boldsymbol{l_{max}^4})$

<u>Speedup vs. Admissibility Criterion:</u>

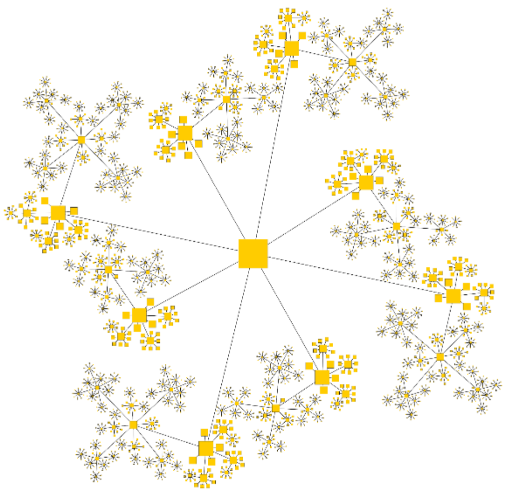
Ratio of direct particle-particle computations increases with $\frac{1}{\boldsymbol{\theta_{max}}}$

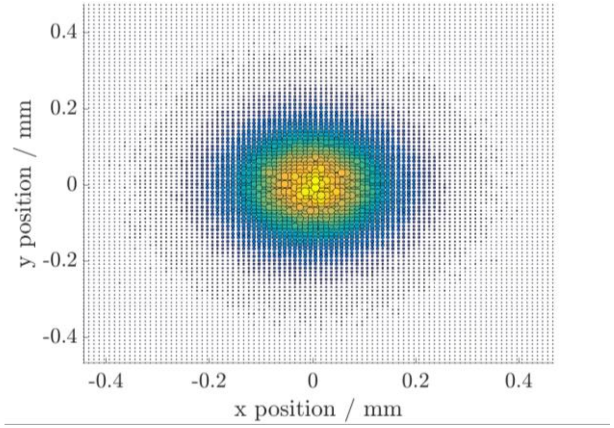
→ Parameters $\boldsymbol{l_{max}}$, $\boldsymbol{\theta_{max}}$ trade off speedup against accuracy

Convergence and Performance
Mesh FMM: Charge Deposition & Tree Structure

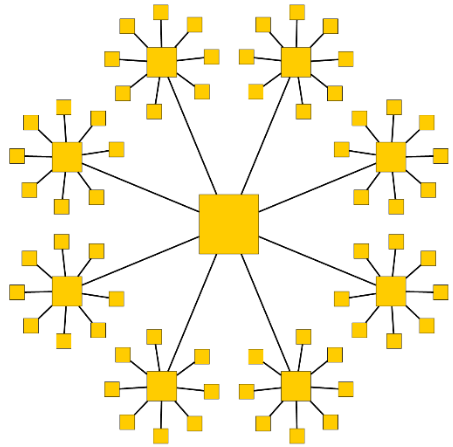


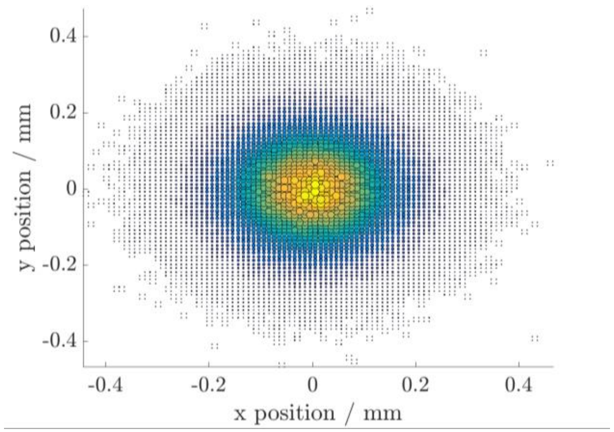
Particle FMM



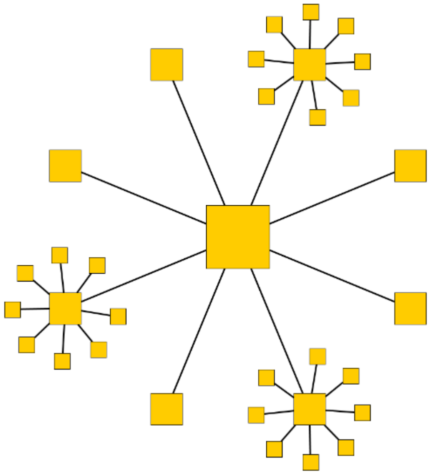


Mesh FMM





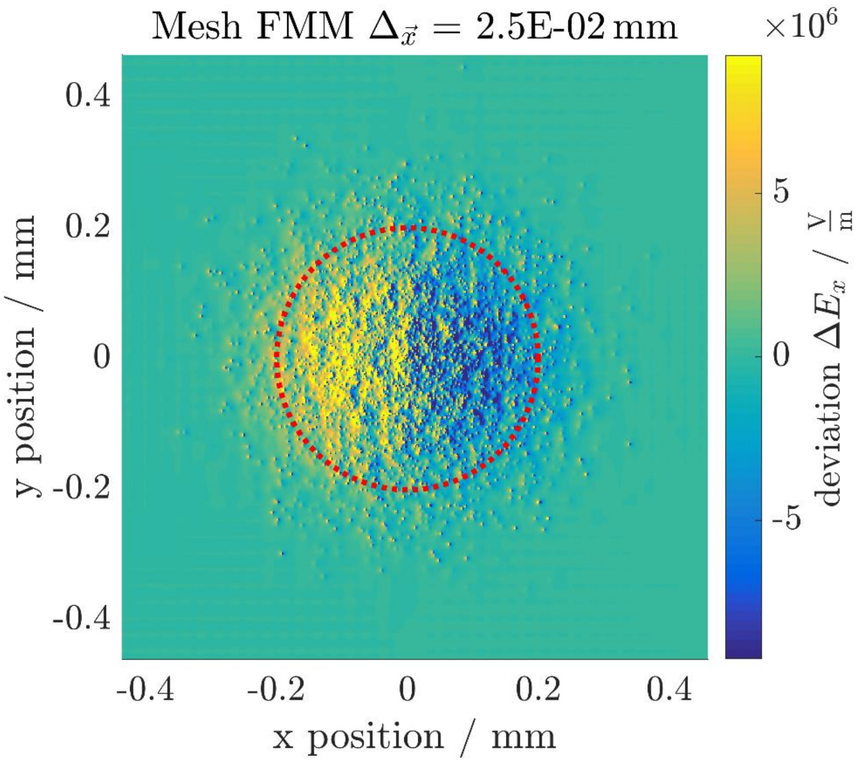
Reduced Mesh FMM

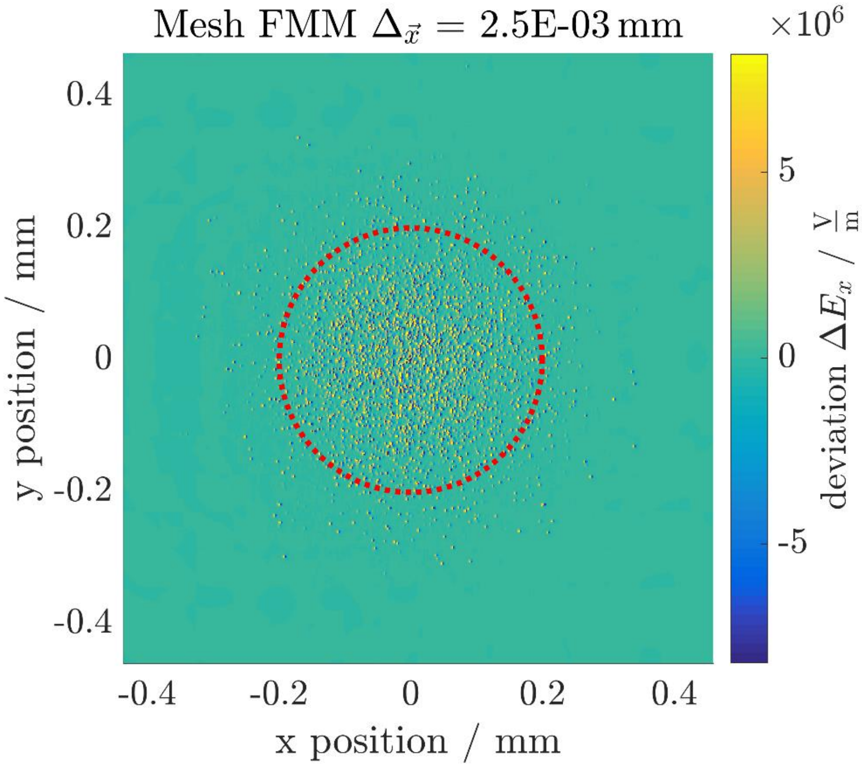


Convergence and Performance
Mesh FMM: Smoothening Single Particle Noise

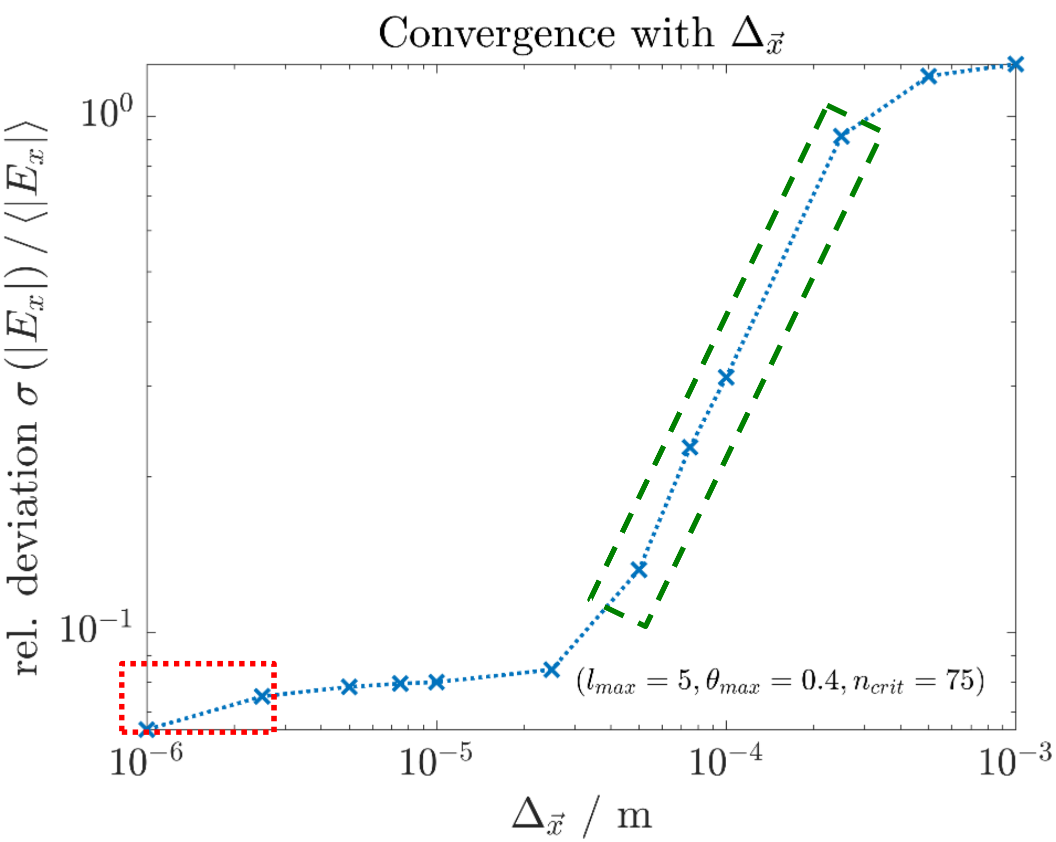
$\boldsymbol{\Delta_{\vec{x}} = 2.5 \cdot 10^{-5}}$ **m**
$\Rightarrow \sigma(E_x) \sim 10^6\, V/m$

$\boldsymbol{\Delta_{\vec{x}} = 2.5 \cdot 10^{-6}}$ **m**
$\Rightarrow \sigma(E_x) \sim 10^6$ V/m





Convergence and Performance
Mesh FMM: Numerical Convergence Study



<u>Convergence of mesh FMM:</u>

$$\sigma(E_x) = \sigma\left(E_x^{gauss}\right) + \sigma(E_x^{near})$$

Dimensions of particle bunch σ_{x_i}:

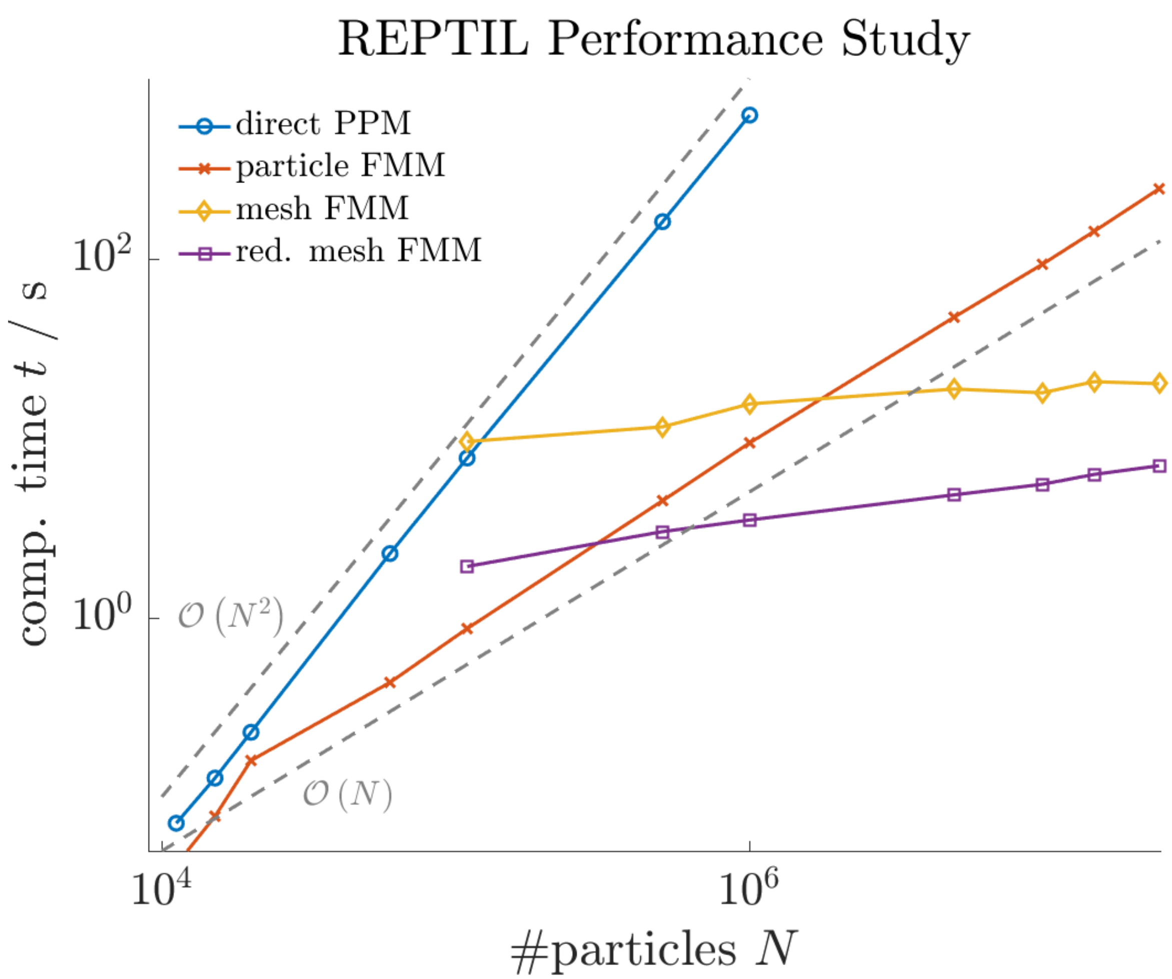
$$\Delta_{x_i} \ll \sigma_{x_i} \Rightarrow \sigma\left(E_x^{gauss}\right) \approx 0$$
$$\sigma_{x_i} \sim 10^{-4}\ \mathrm{m}$$

Distance of nearest neighbors Δ_{near}:

$$\Delta_{x_i} \ll \Delta_{near} \Rightarrow \sigma(E_x^{near}) \approx 0$$
$$\Delta_{near} \sim 10^{-6}\ \mathrm{m}$$

→ Smoothening of single particle noise if $\Delta_{near} \ll \Delta_{x_i} \ll \sigma_{x_i}$

Convergence and Performance
Performance Studies: PPM, FMM & Mesh FMM



Scaling with particle number:

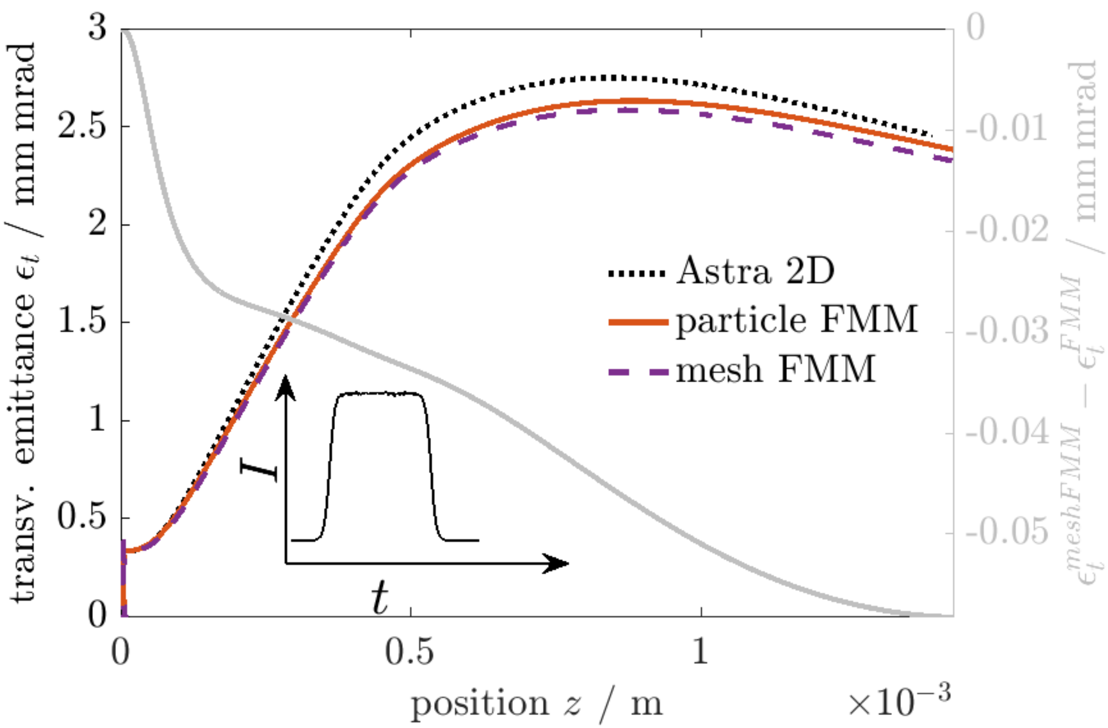
Particle-particle method:
$O(N^2)$

Fast multipole method:
$O(N)$ - $O(N \log N)$

FMM on mesh :
$FMM(N_{grid}) + O_{MESH}(N)$

Simulation of the PITZ Injector
Photoemission w/o Space Charge Limitation

TECHNISCHE UNIVERSITÄT DARMSTADT



<u>PITZ photoemission:</u>

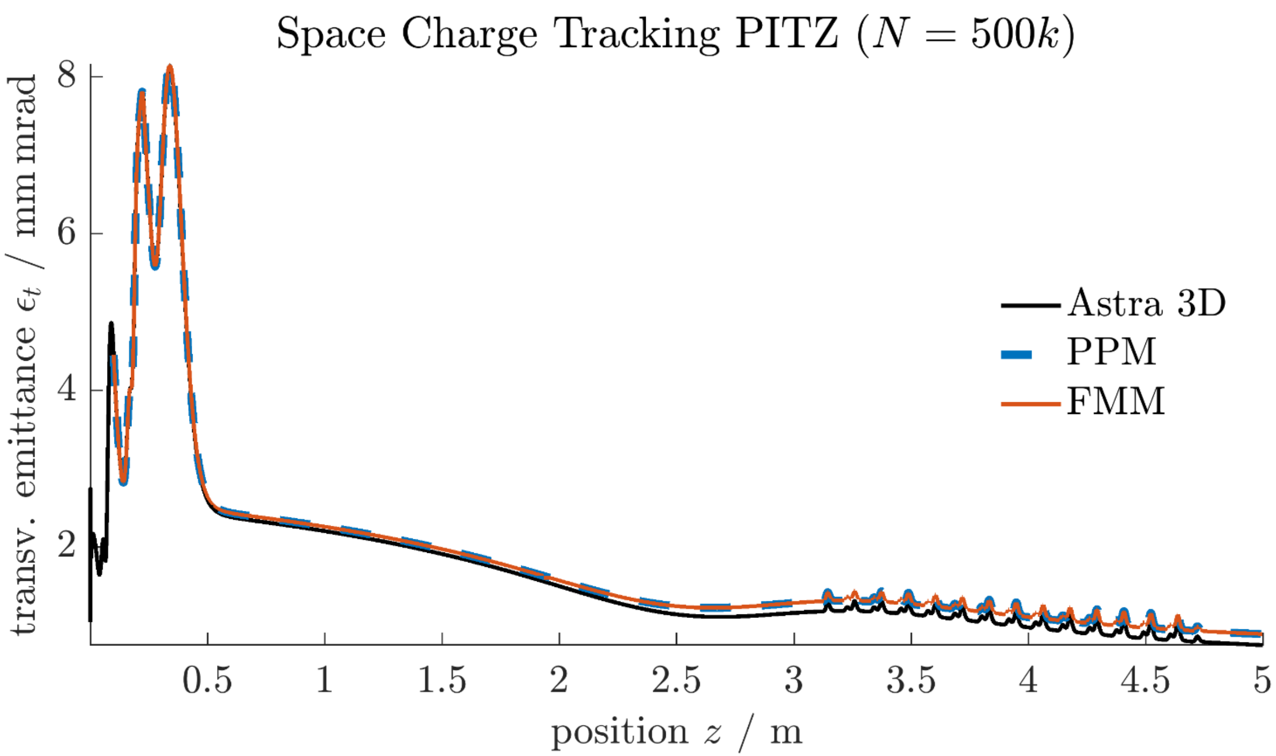
Bunch charge: $Q = 1\ \mathrm{nC}$
Laser spot size: $\sigma = 0.4\ \mathrm{mm}$
Pulse length: $\tau = 22\ \mathrm{ps}$
RF Field: $E_{RF} \sim 60\,\frac{\mathrm{MV}}{\mathrm{m}}$

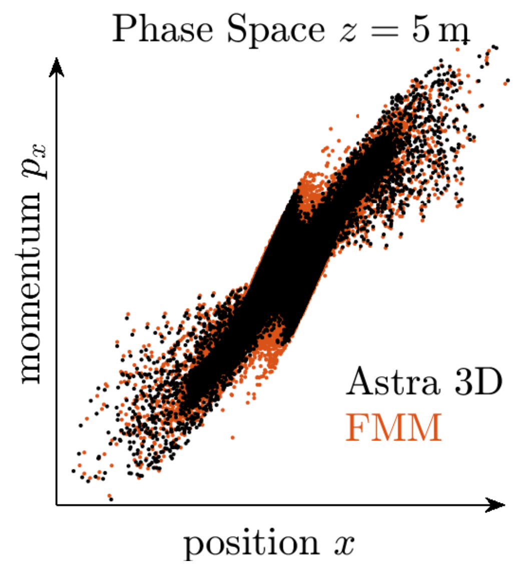
Smooth photo current $I(t)$ requires many particles $N \sim 10^6$

Image charge approach for boundary at cathode surface

#Particles: $N = 5000k$	Speedup: $S := t_{FMM} / t$	Deviation: $\delta := \lvert\epsilon_t - \epsilon_t^{FMM}\rvert$
Astra 2D	$\times\, 11$	$\sim 10^{-1}$ mm mrad
Mesh FMM ($\Delta_{\vec{x}} \sim 10^{-5}\ \mathrm{m}$)	$\times\, 6$	$\sim 10^{-2}$ mm mrad
Reduced mesh FMM	$\times\, 12$	$\sim 10^{-2}$ mm mrad

Simulation of the PITZ Injector
3D Space Charge Particle Tracking





#Particles: $N = 500k$	Speedup: $S := t_{PPM} / t$
Astra 3D	$\times 9$
FMM	$\times 27$

Single particle noise increases ϵ_t of FMM/PPM w.r.t. Astra 3D

→ <u>Ongoing work:</u> Investigate smoothening using mesh FMM
(Emission with Astra 2D, 3D tracking started at $z = 10$ cm)

Outlook
Agenda for the REPTIL FMM Code

Stats Quo:

+ Satisfactory performance results for REPTIL FMM simulations
- Non-optimized code segments slow down computation

Ongoing and Future Code Development:

- Optimization of REPTIL
- Implementation of 2D FMM kernel
- Investigation of relativistic interaction kernels

  Parallelized space charge tracking code for accelerator applications

- Step by step towards self consistent photo emission models

  Simulation of high current particle injectors