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

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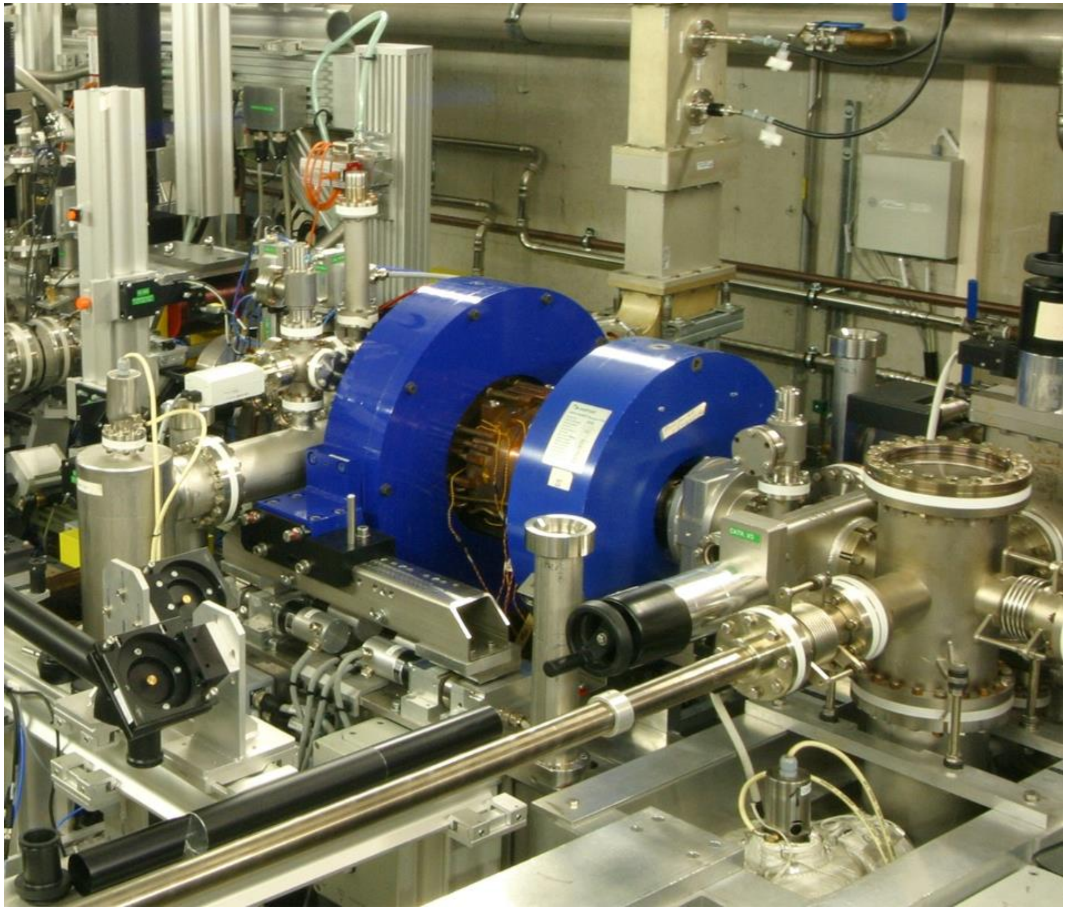
Motivation:
Simulation of High Brightness Photo Injectors



(Image source: http://pitz.desy.de/research_and_development/machine/)

Structure

I. Fast Multipole Methods

II. Numerical Convergence and Performance

  i. Particle Based Fast Multipole Method

  ii. Mesh Based Fast Multipole Method

III. Simulation of the PITZ Injector

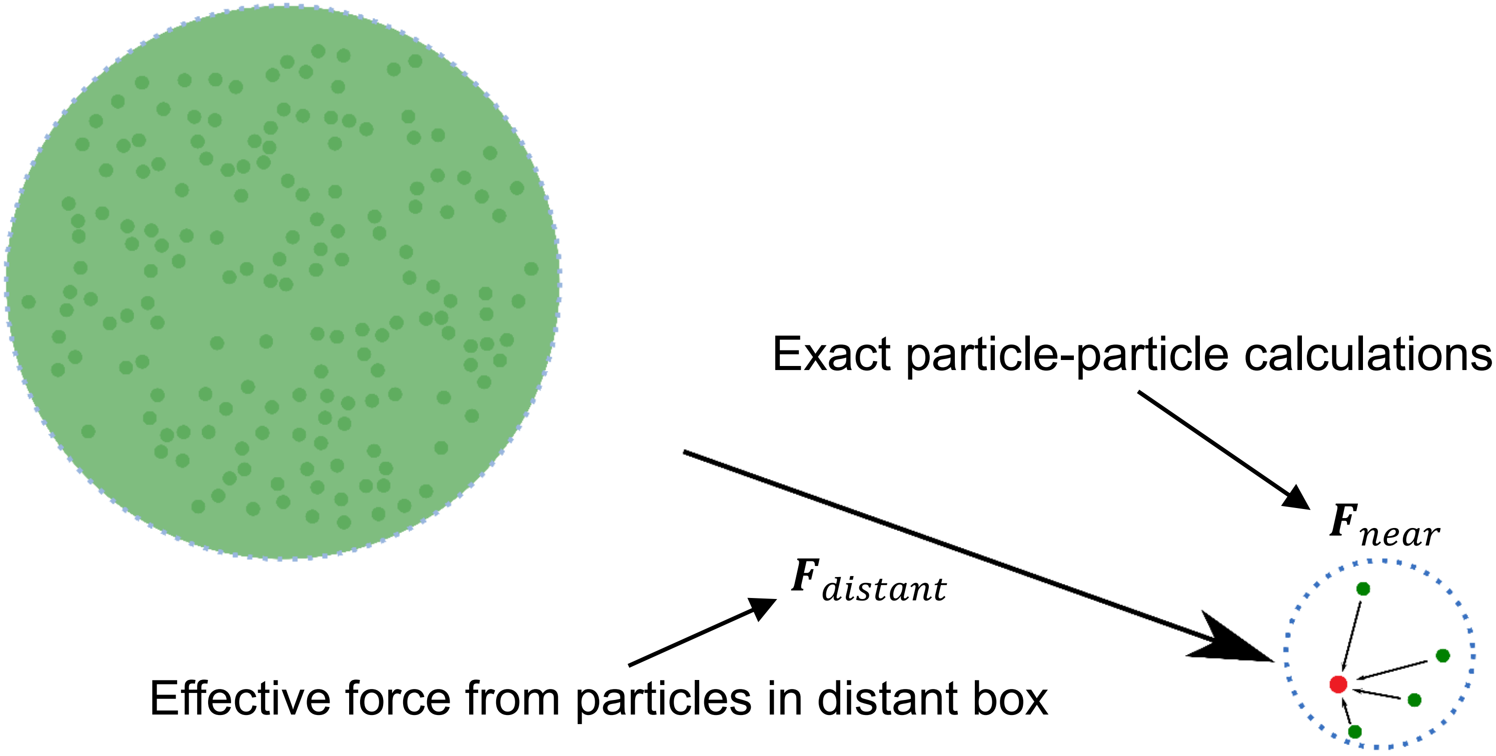
IV. Outlook

Fast Multipole Methods
The Concept

Approximation of far field contributions

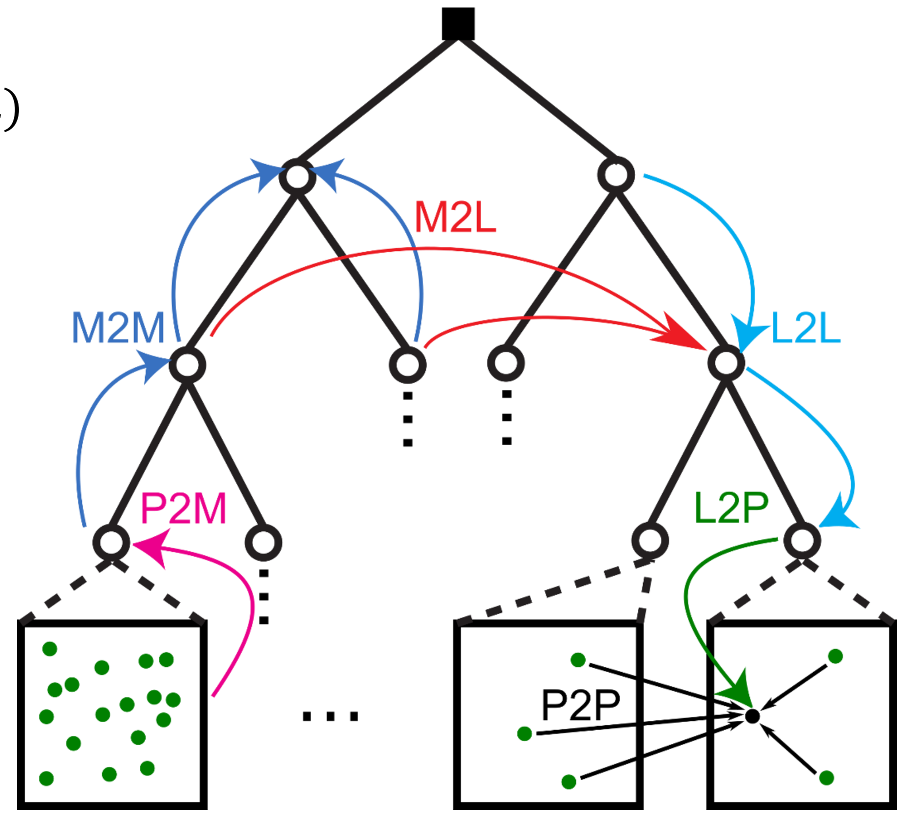
+

Direct computation of near field contributions



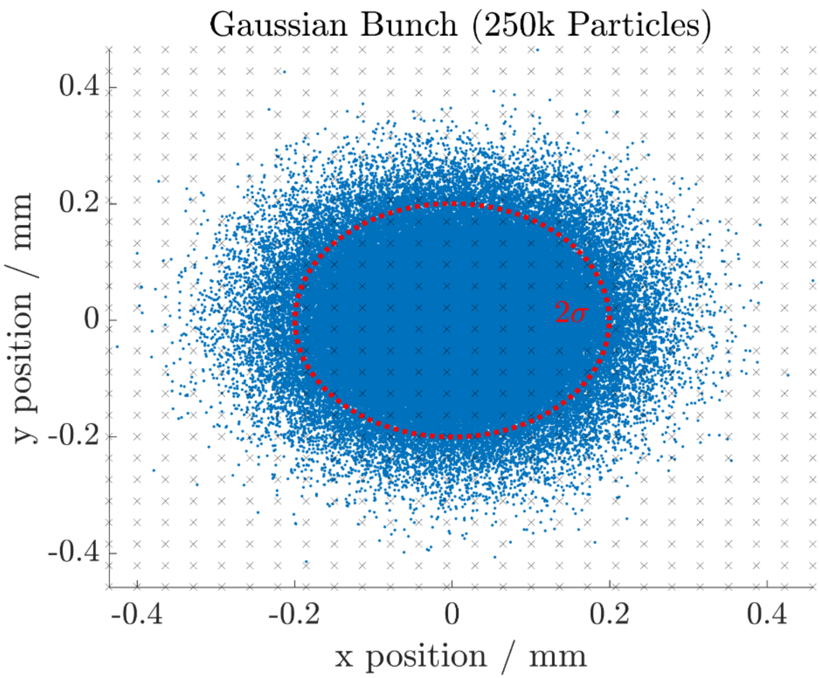
Fast Multipole Methods
The Concept

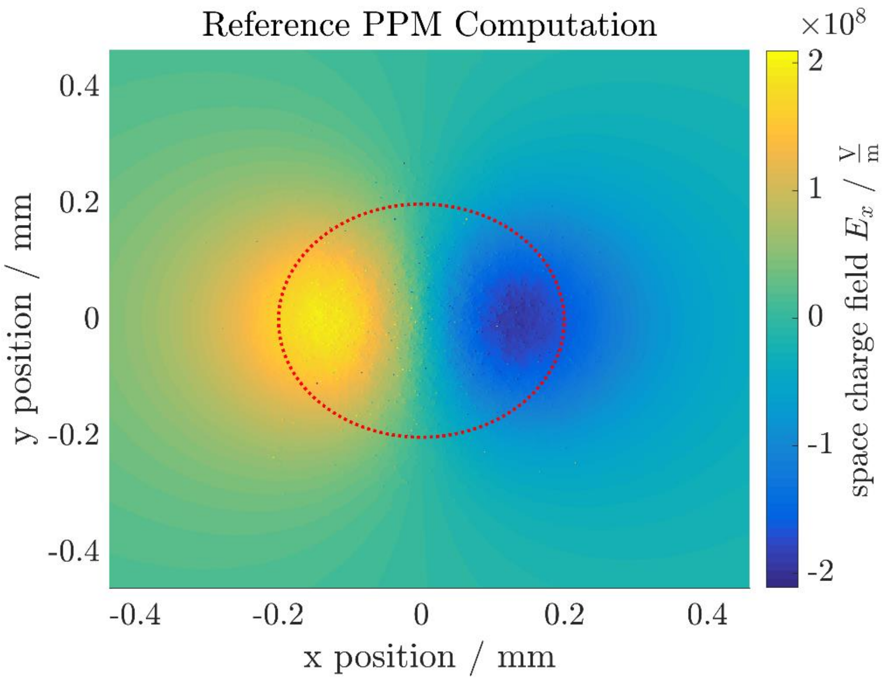
1. Compute multipole expansion $(\boldsymbol{l} \leq \boldsymbol{l_{max}})$ of particles contained in each leaf box.
2. Express multipoles in parent node as sum of contributions from child nodes.
3. Approximate distant $(\boldsymbol{\theta} \leq \boldsymbol{\theta_{max}})$ multipoles as local expansion.
4. Express local expansion in the coordinates of the child nodes.
5. Evaluate $\boldsymbol{F_{distant}}$ and $\boldsymbol{F_{near}}$ for each particle in the leaf.



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

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,

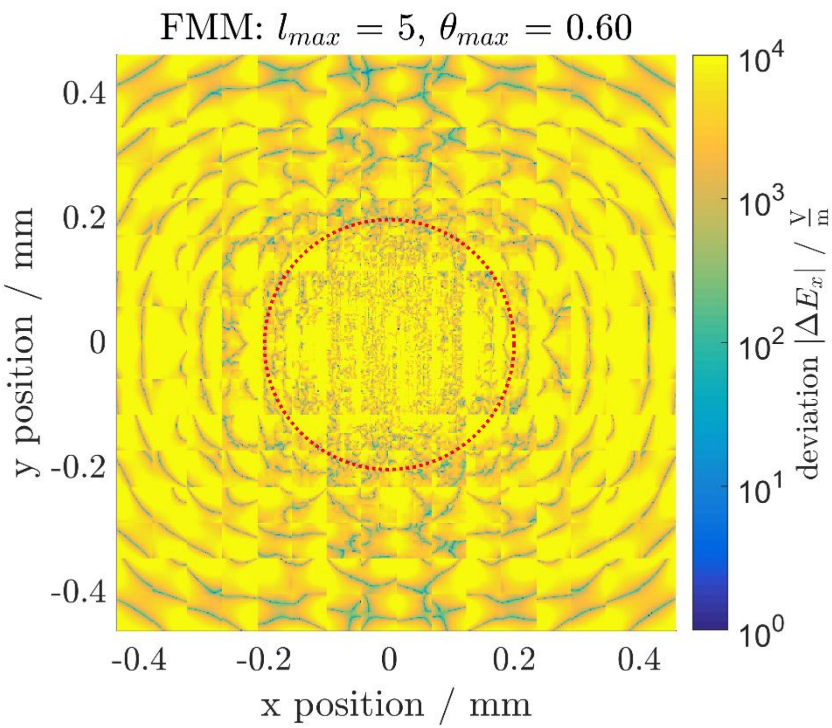
501×501 probe points at $z = \mu_z$

Electrical field E_x:

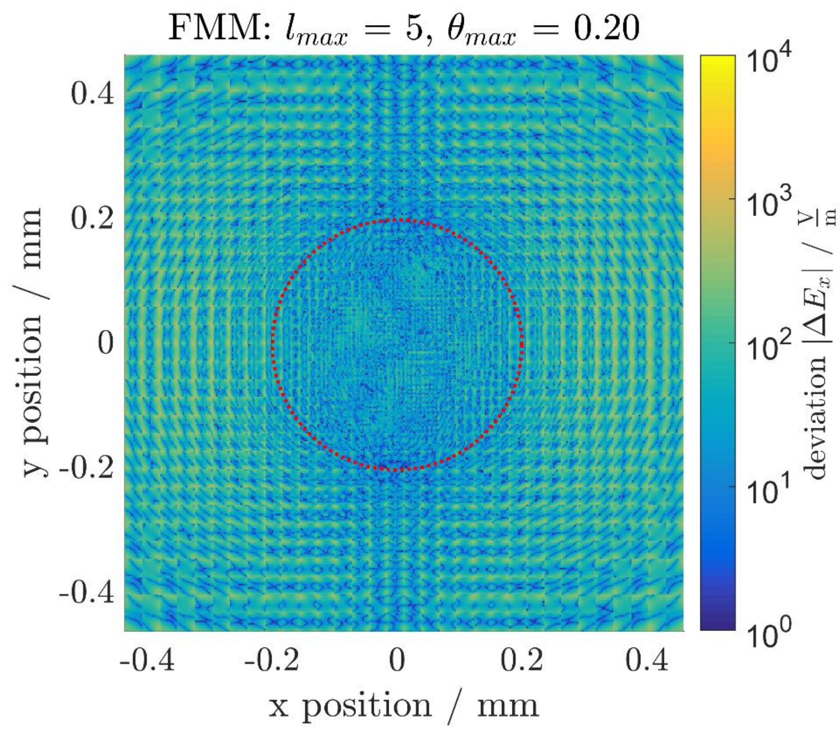
$$E_x = E_x^{gauss} + E_x^{near} \sim 10^8 \frac{V}{m}$$

Convergence and Performance
Particle FMM: Admissibility Parameter $\boldsymbol{\theta_{max}}$

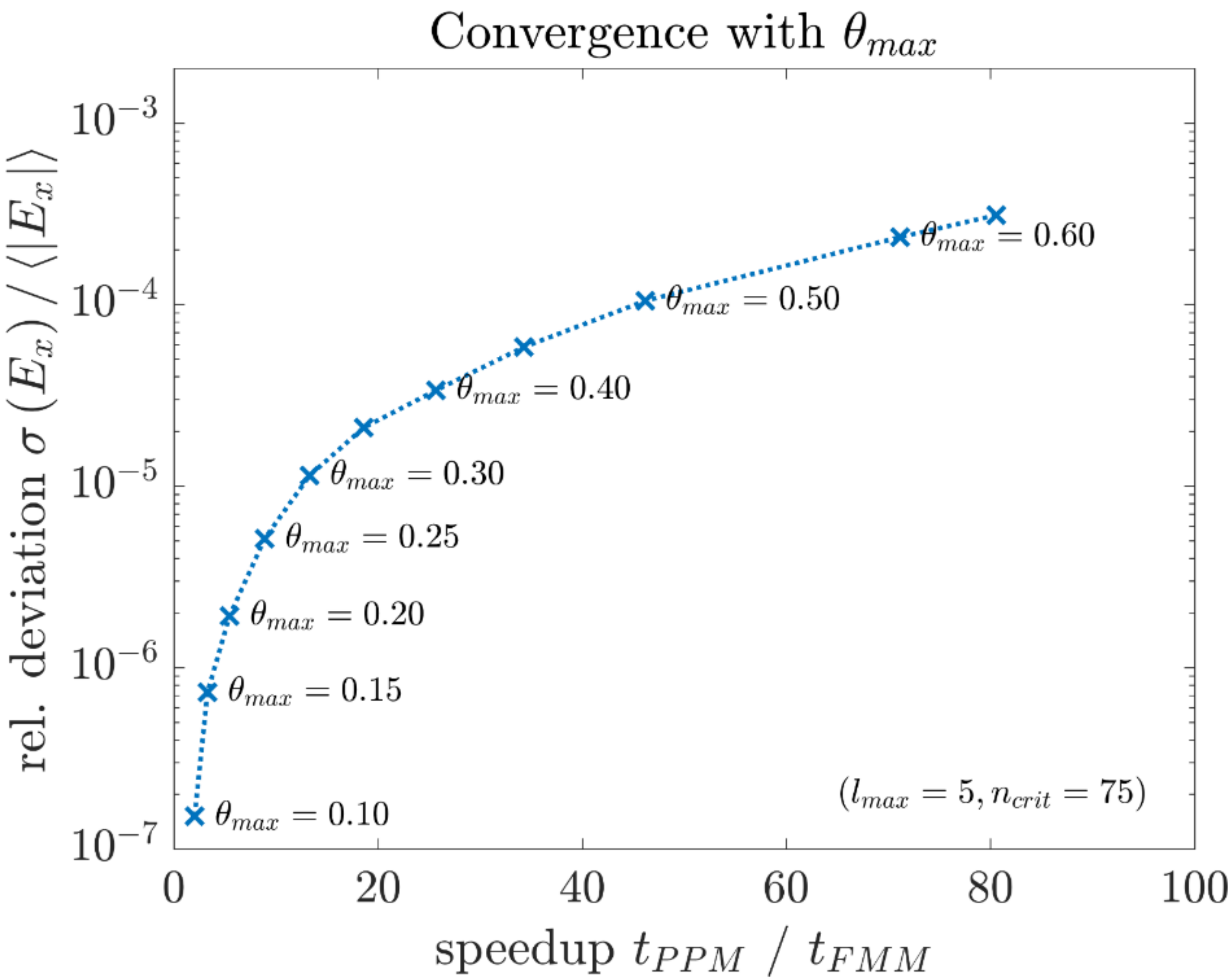
$\boldsymbol{\theta_{max} = 0.6}$
$\Rightarrow \sigma(E_x) \sim 10^5\ V/m$



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



Convergence and Performance
Particle FMM: Numerical Convergence Study



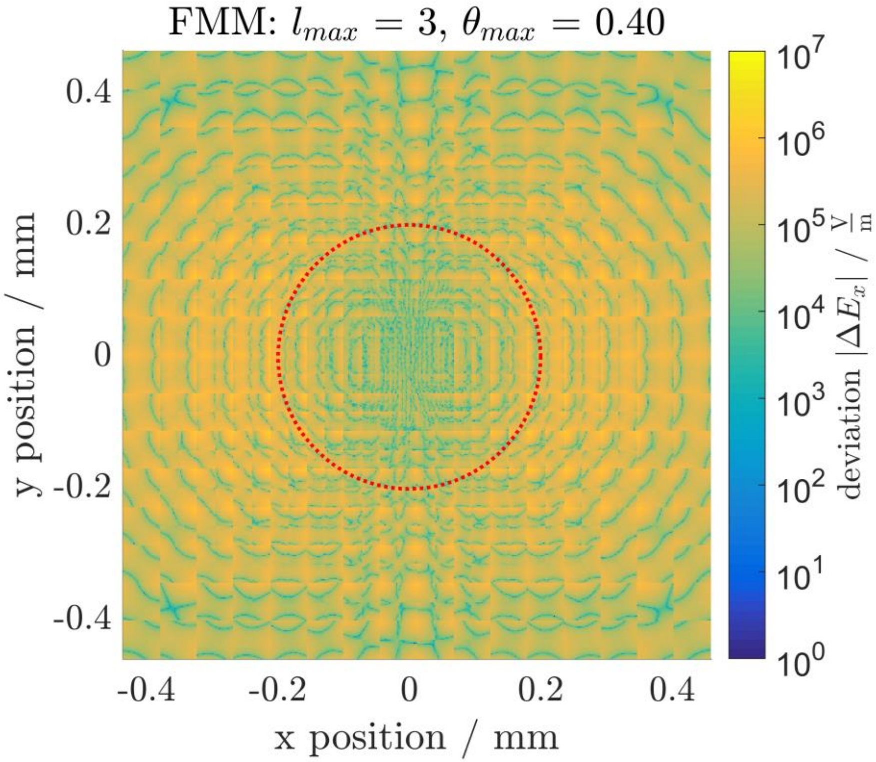
Speedup vs. θ_{max}:

Number of direct interactions

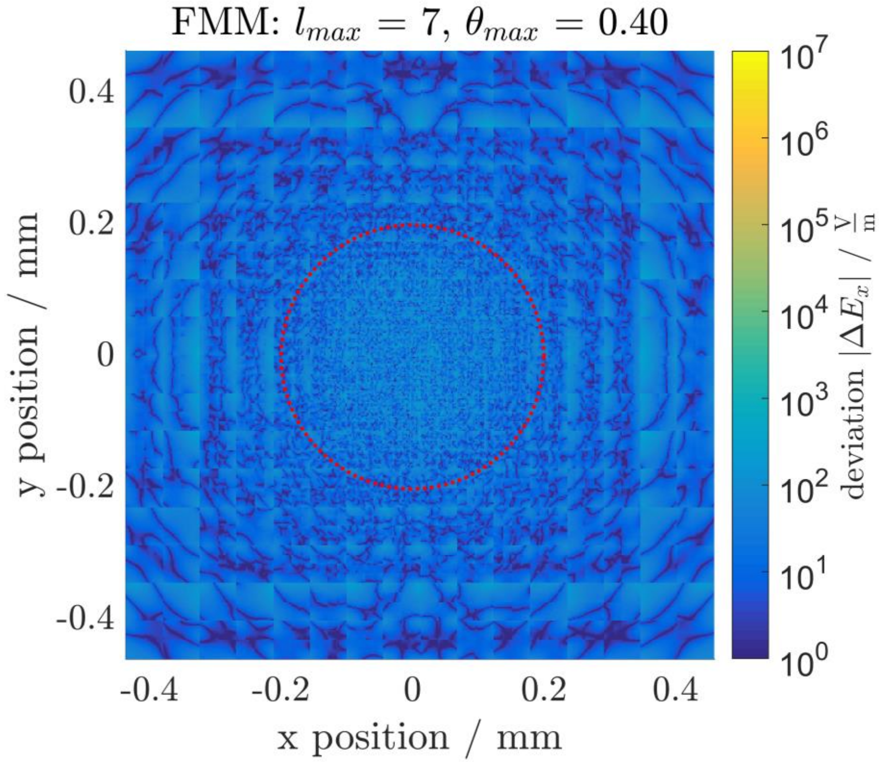
$$\sim \left(\frac{1}{\theta_{max}}\right)^x$$

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

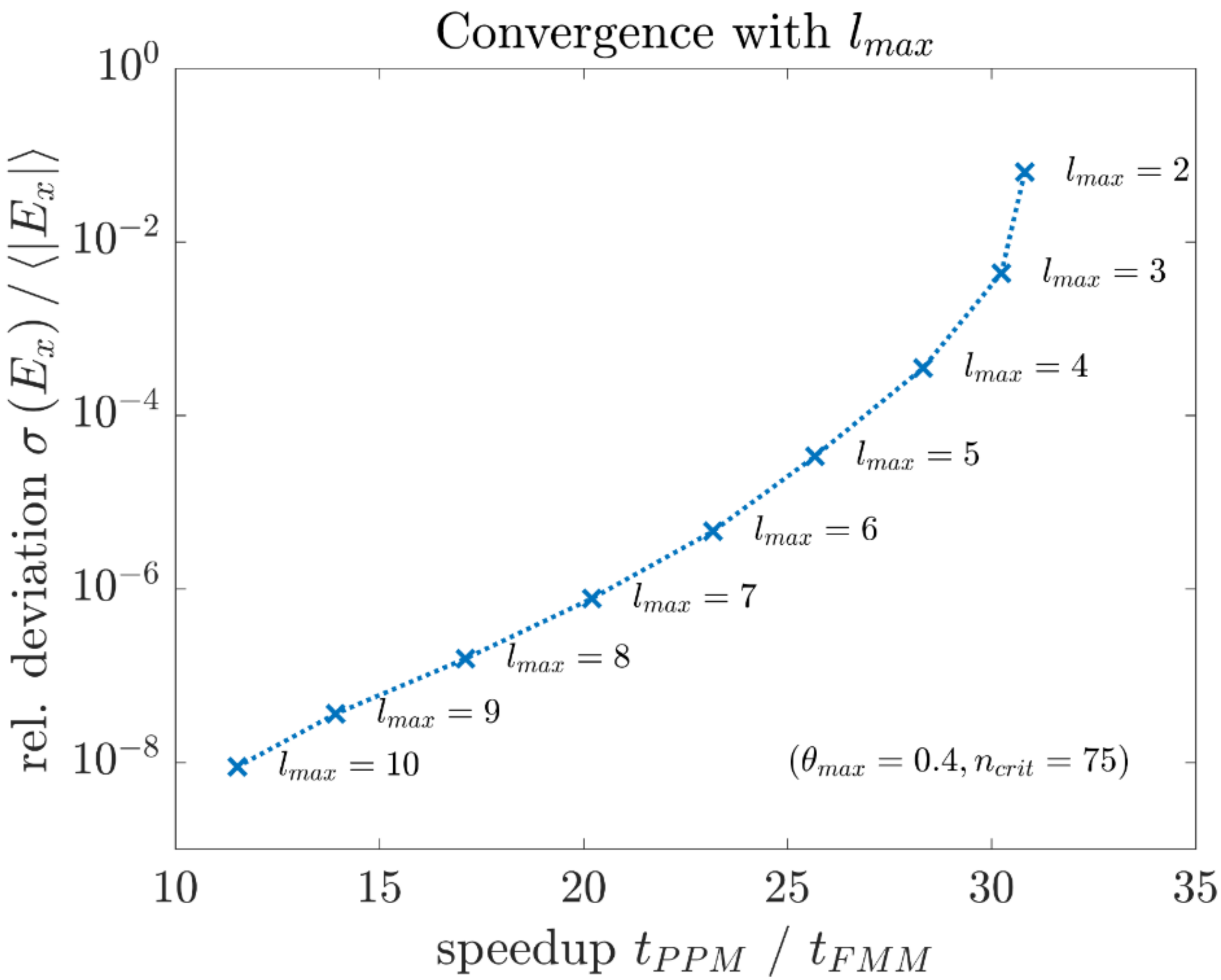
$\boldsymbol{l_{max} = 3}$
$\Rightarrow \sigma(E_x) \sim 10^6\ V/m$



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



Convergence and Performance
Particle FMM: Numerical Convergence Study



Speedup vs. l_{max}:

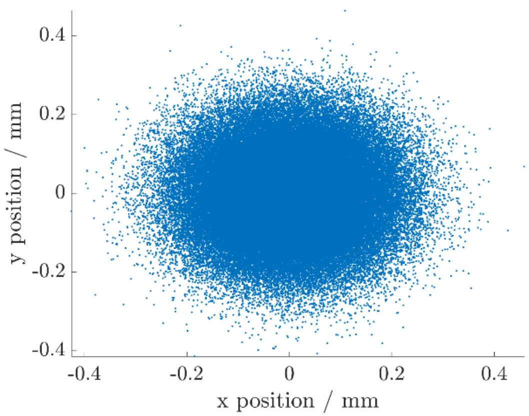
Convergence of error:

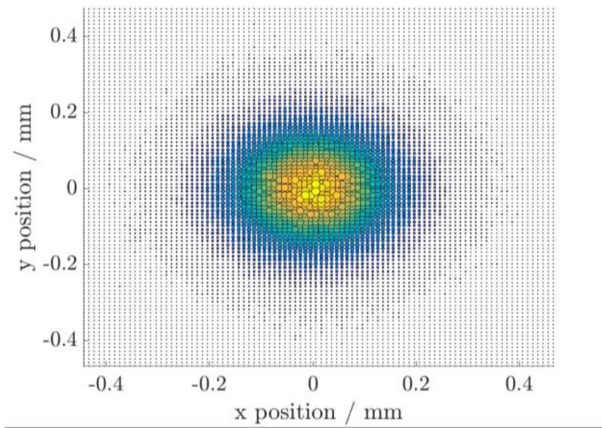
Exponential in l_{max}

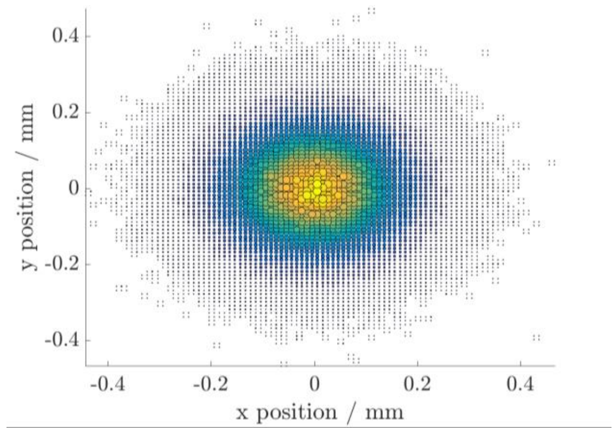
Inc. of computation time:

Expansions: $\mathcal{O}(l_{max}^2)$
Translations: $\mathcal{O}(l_{max}^4)$

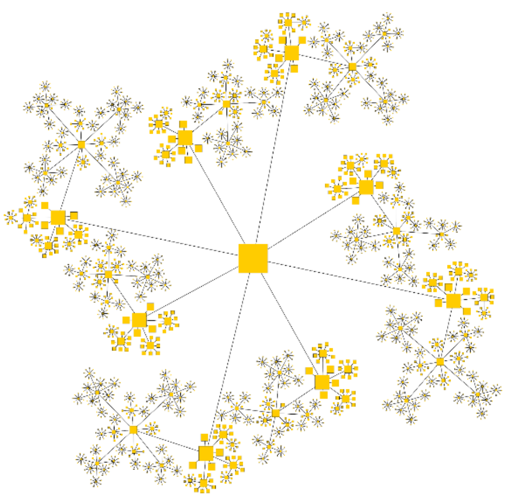
Convergence and Performance
Mesh FMM: Charge Deposition & Tree Structure

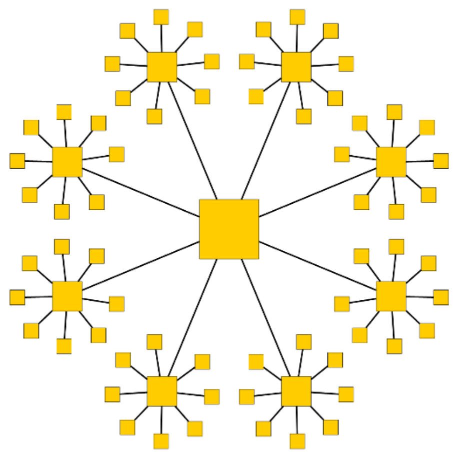


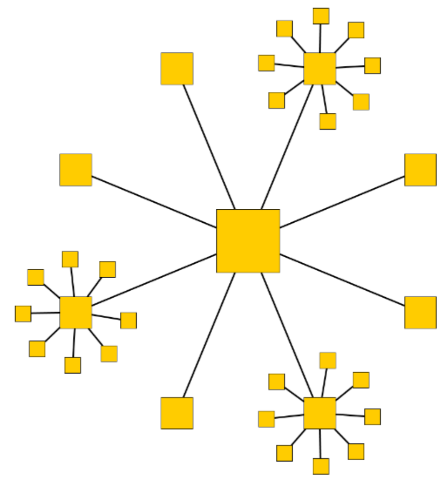




Particle FMM | **Mesh FMM** | **Reduced Mesh FMM**







Convergence and Performance
Mesh FMM: Smoothening Single Particle Noise

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

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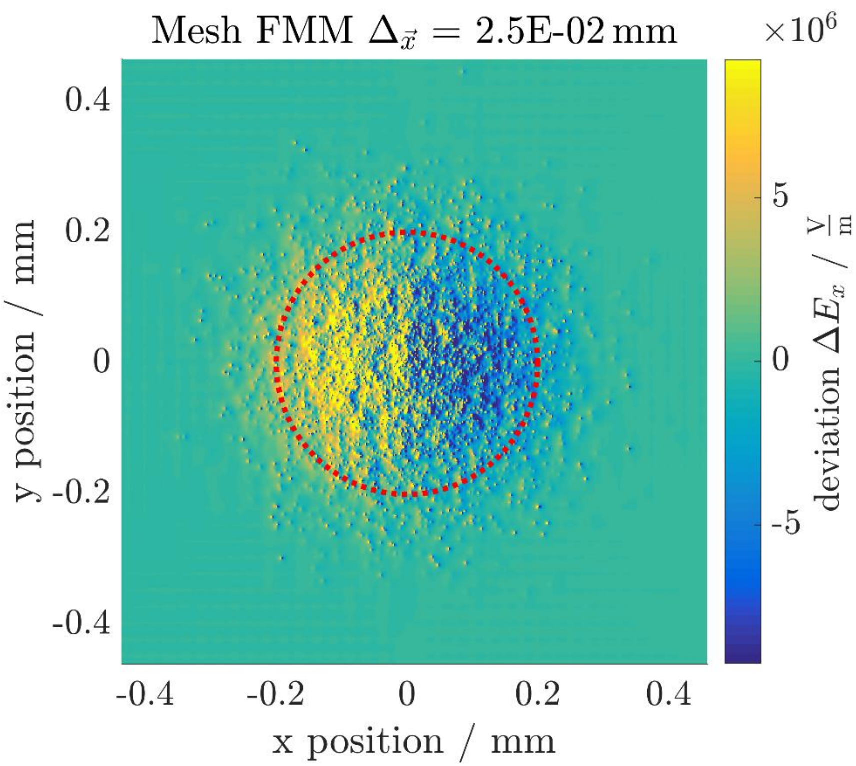
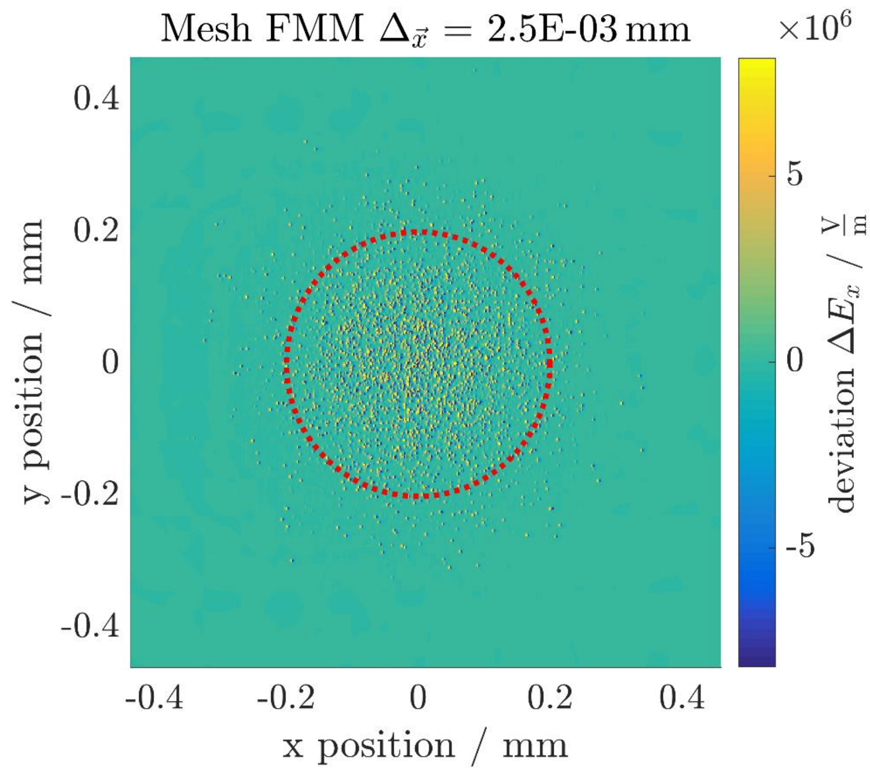
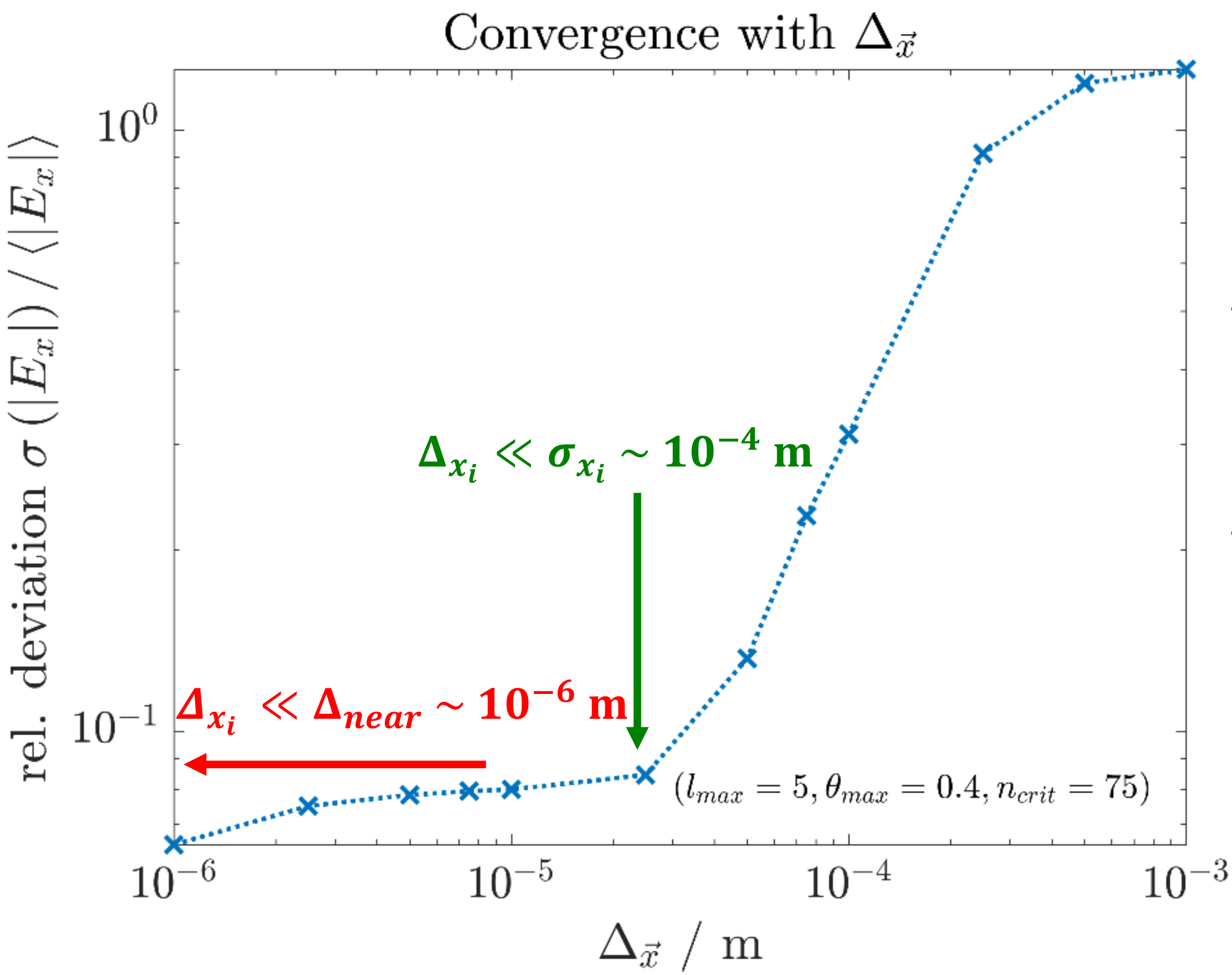




Convergence and Performance
Mesh FMM: Numerical Convergence Study



Mesh FMM:

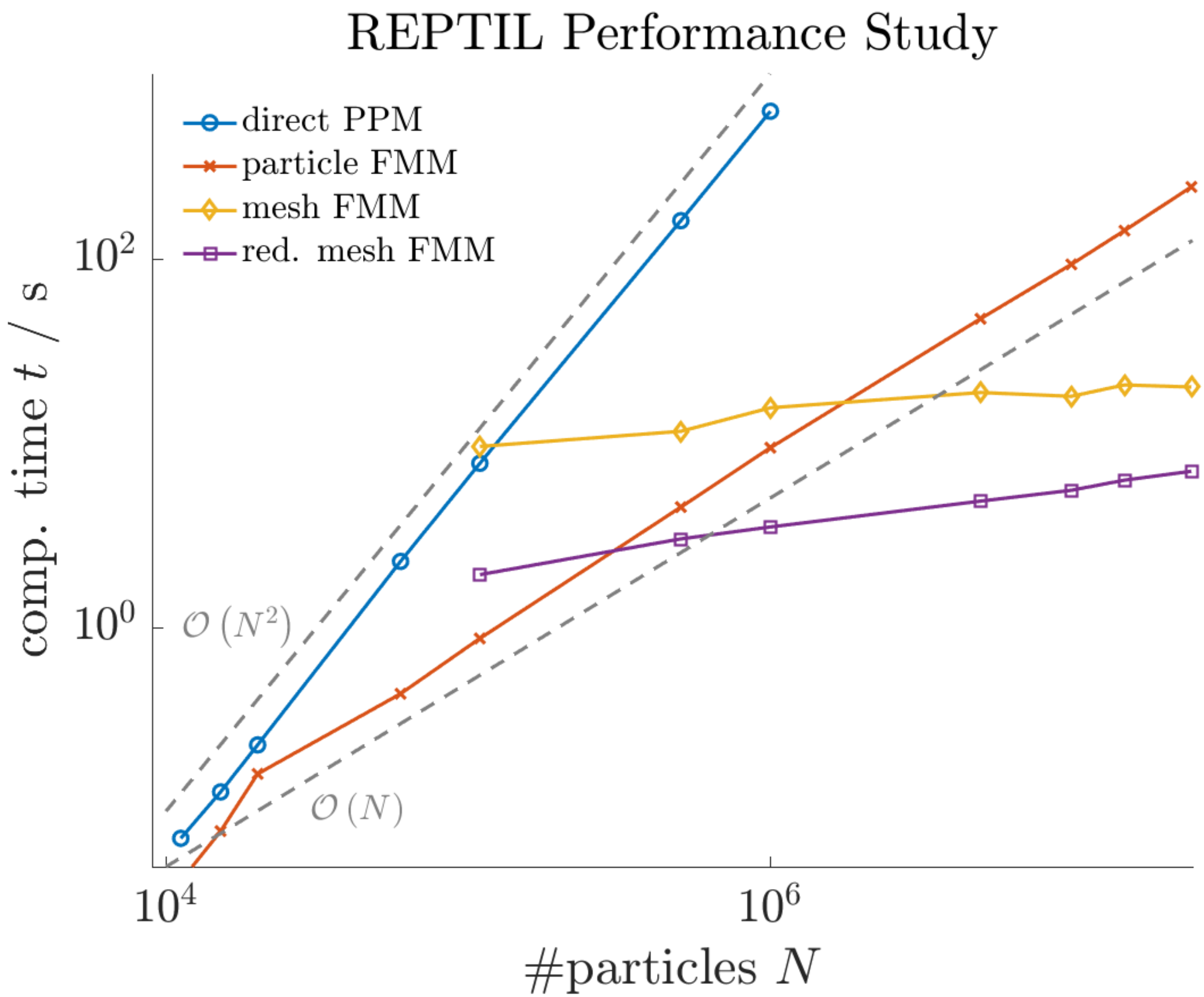
Error of approximation:

$$\sigma_{tot} = \sigma_{gauss} + \sigma_{near}$$

Smoothening:
(single particle noise)

$$\Delta_{near} \ll \Delta_{x_i} \ll \sigma_{x_i}$$

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



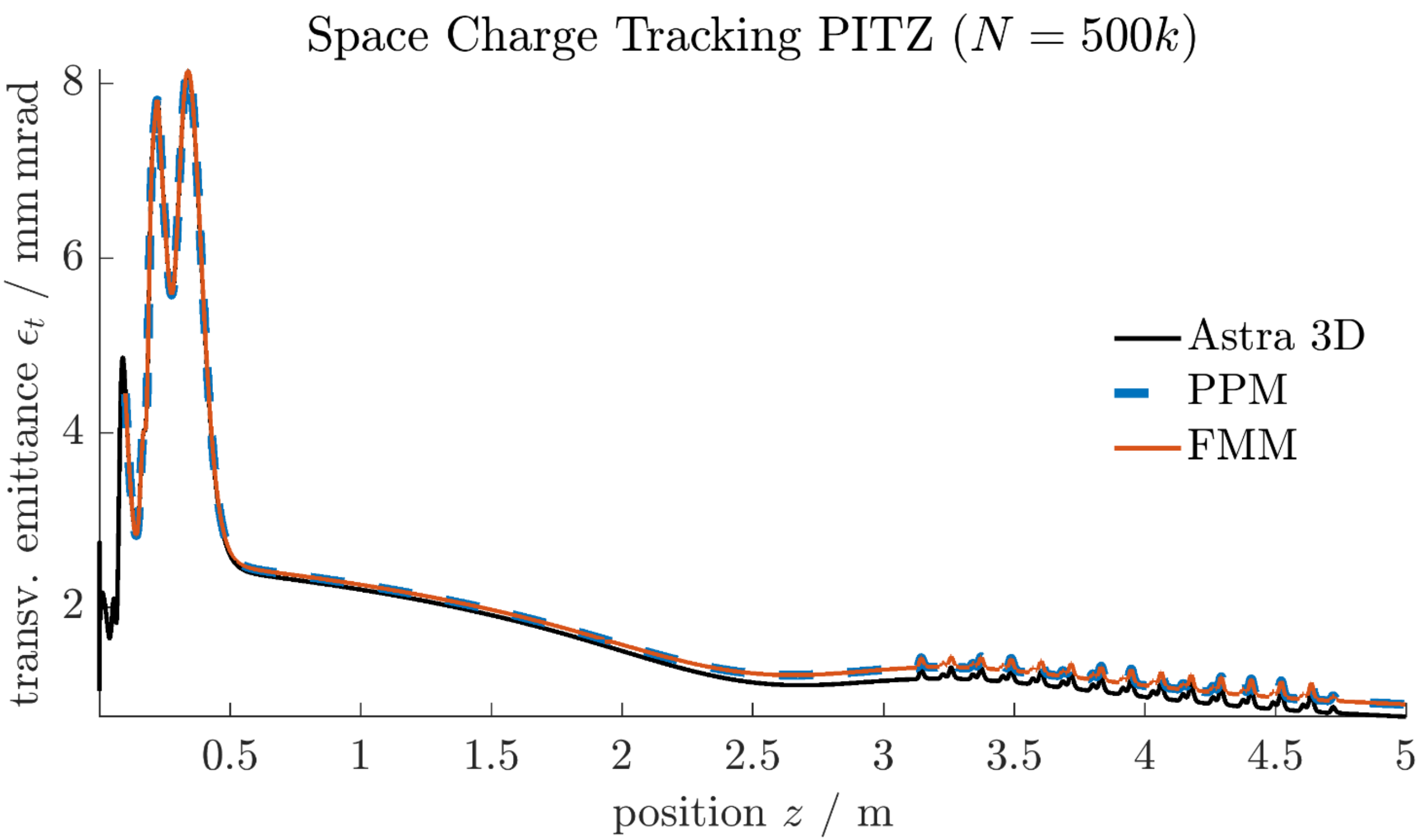
Scaling with #particles:

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

Fast multipole method:
$O(N)$

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

Simulation of the PITZ Injector
3D Space Charge Particle Tracking



<u>Astra 3D:</u>
(single core)

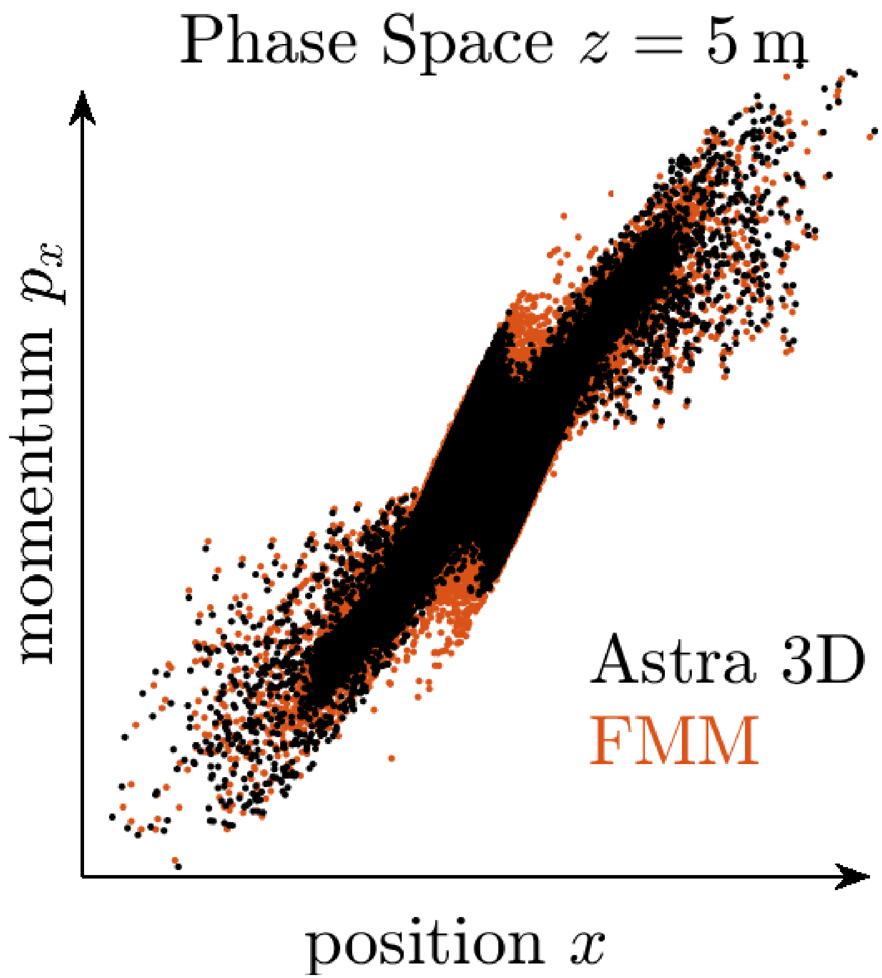
$t_{Astra}/t_{PPM} \sim 9$

<u>FMM:</u>
(OMP)

$t_{FMM}/t_{PPM} \sim 27$

(Emission with Astra 2D - 3D tracking started at $z = 10$ cm)

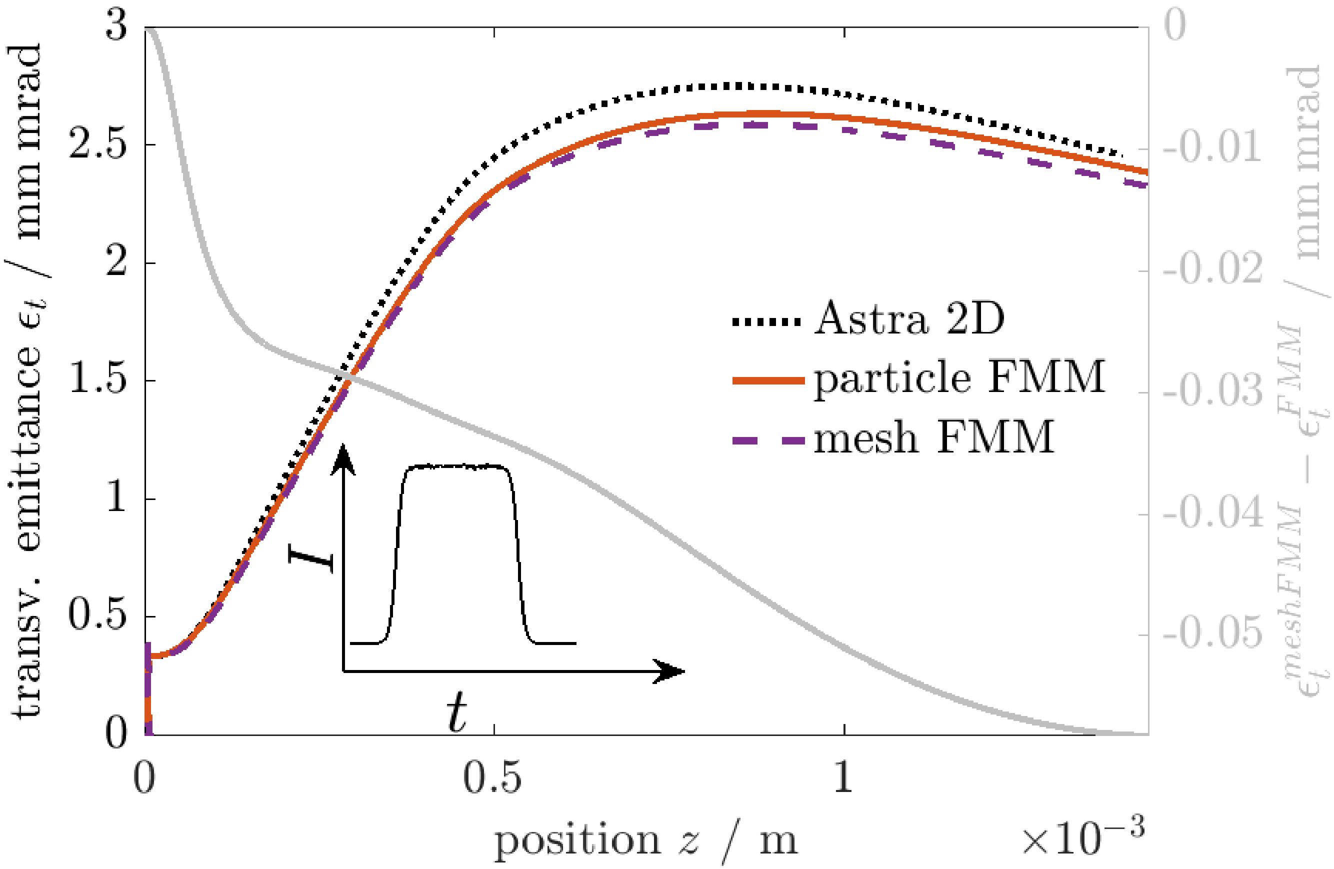
Simulation of the PITZ Injector
3D Space Charge Particle Tracking



Single particle noise increases ϵ_t of FMM/PPM w.r.t. Astra3D

<u>Ongoing work:</u>
Investigate smoothening using mesh

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



Astra 2D:
(single core)

$t_{FMM}/t_{Astra} \sim 11$

$\delta_\epsilon \sim 10^{-1}$ mm mrad

Mesh FMM:
(OMP, $\Delta_{\vec{x}} \sim 10^{-5}$ m)

$t_{FMM}/t_{meshFMM} \sim 6$

$\delta_\epsilon \sim 10^{-2}$ mm mrad

Red. Mesh FMM:

$t_{FMM}/t_{red.FMM} \sim 12$

Simulation PITZ Injector:

$Q_b = 1\ \mathrm{nC}$, $\sigma_{transv} = 0.4\ \mathrm{mm}$, $\tau_{pulse} = 22\ \mathrm{ps}$, $E_{RF} \sim 60\,\frac{\mathrm{MV}}{\mathrm{m}}$, #particles $\sim 5 \times 10^6$

Outlook
Agenda for the REPTIL FMM Code

Status Quo:

\+ Satisfactory performance results for REPTIL FMM simulations

\- Non-optimized code segments slow down computation

Ongoing and Future Code Development:

- Optimization of REPTIL
  Parallelized 3D space charge tracking code for accelerator applications

- Step by step towards self consistent photo emission models
  Simulation of high current particle injectors