# Advanced space charge tracking methods for high brilliance electron sources

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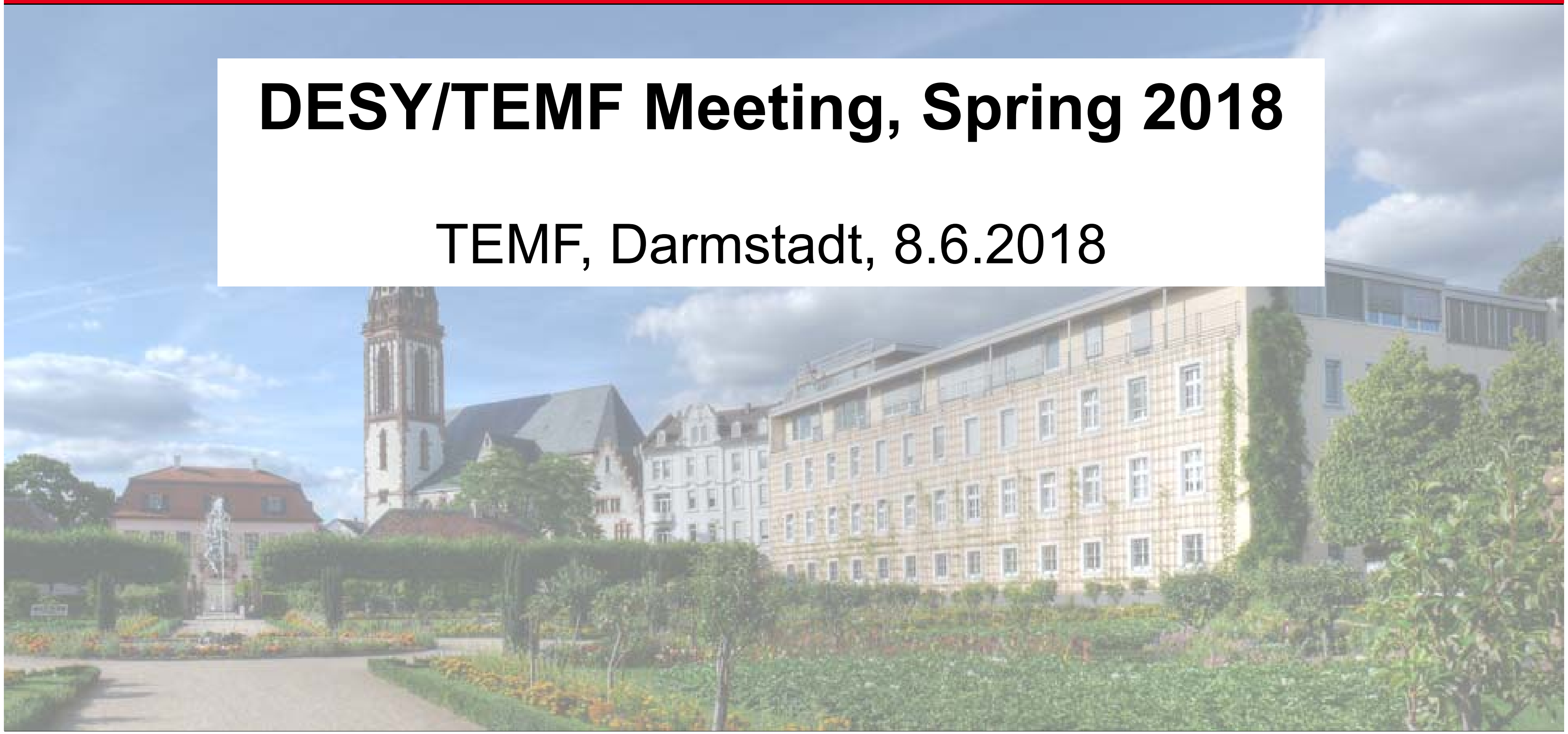


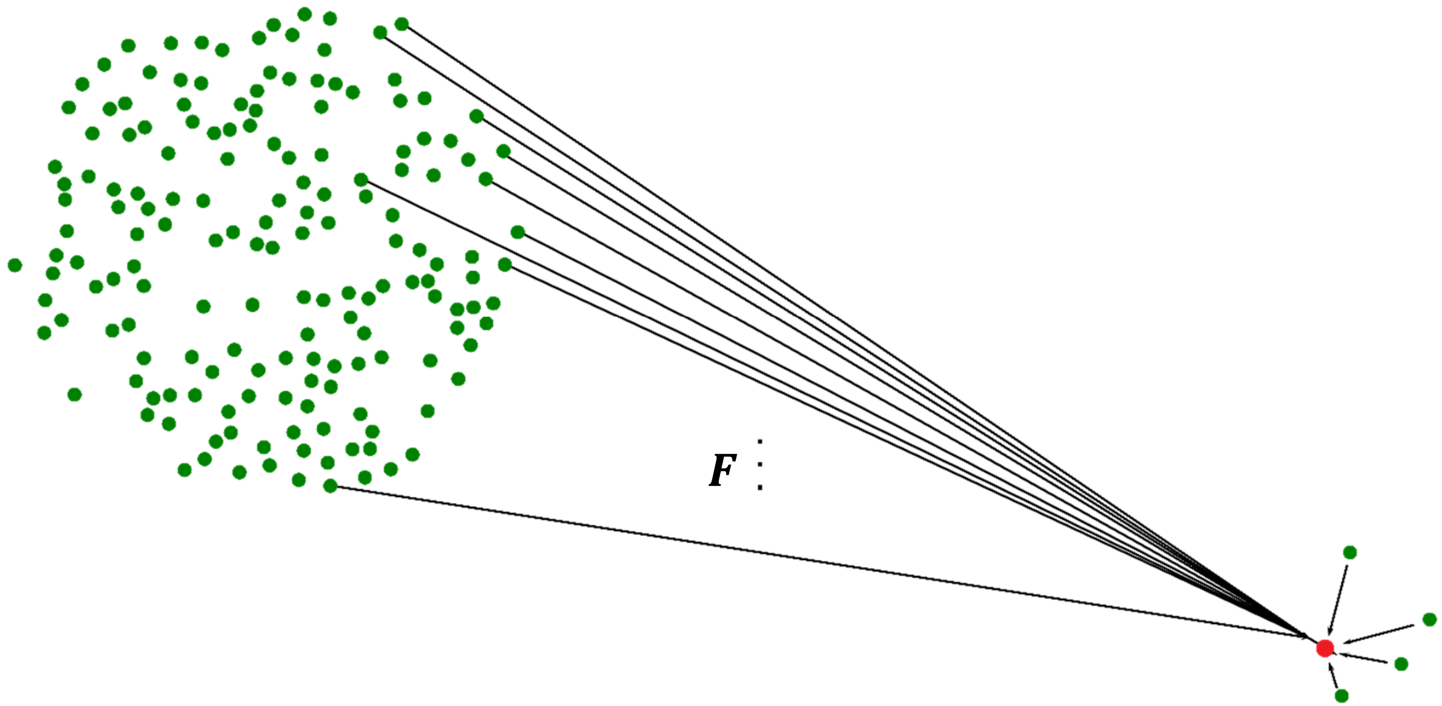
# Structure

- Reminder On Fast Multipole Methods (FMM)
- Simulation of the PITZ Injector
- Convergence of Particle Emission
- Outlook

# Reminder On Fast Multipole Methods
## The Concept

**Problem:**

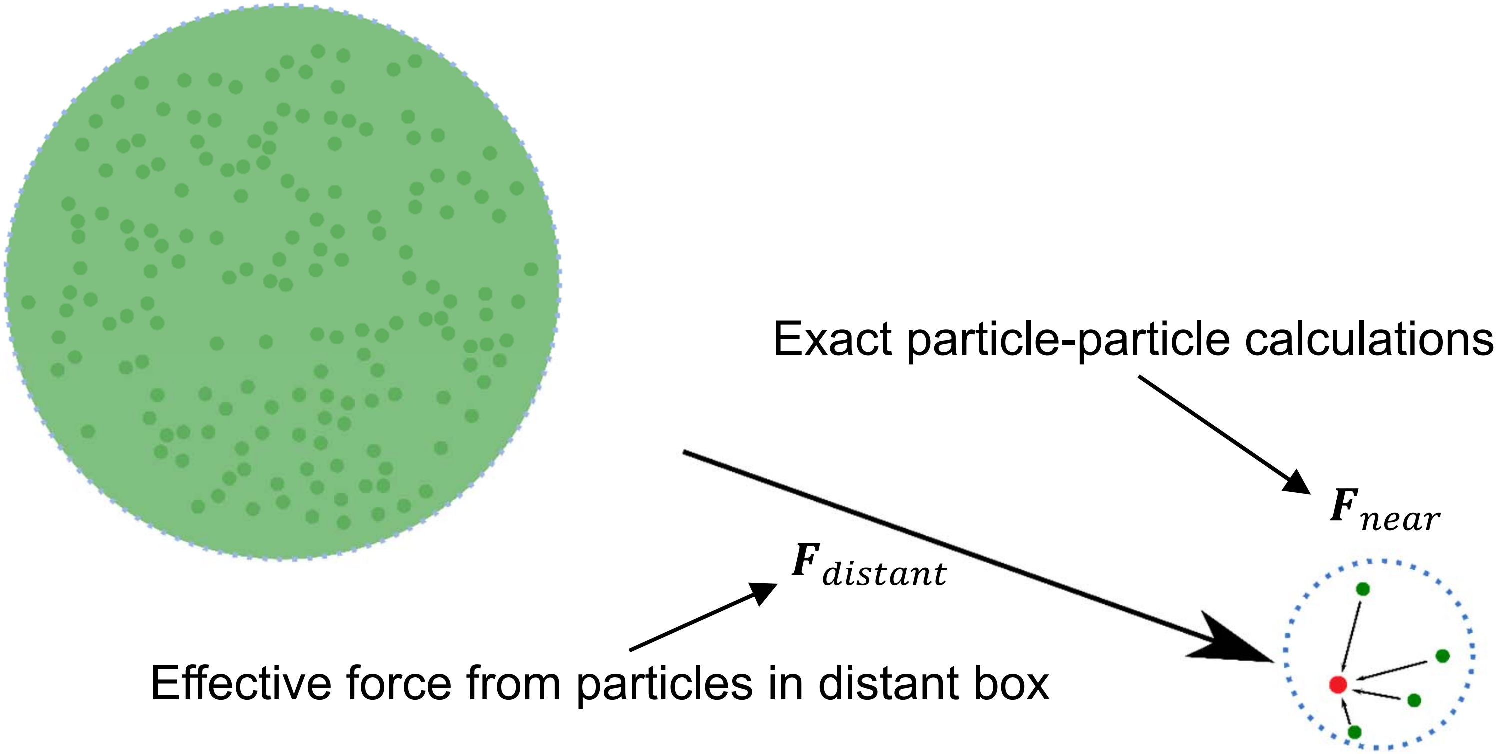
Efficient way to compute many-body interaction needed
→ Reduce complexity to less than $\mathrm{O}(N^2)$



# Reminder On Fast Multipole Methods
## The Concept

**Solution:**

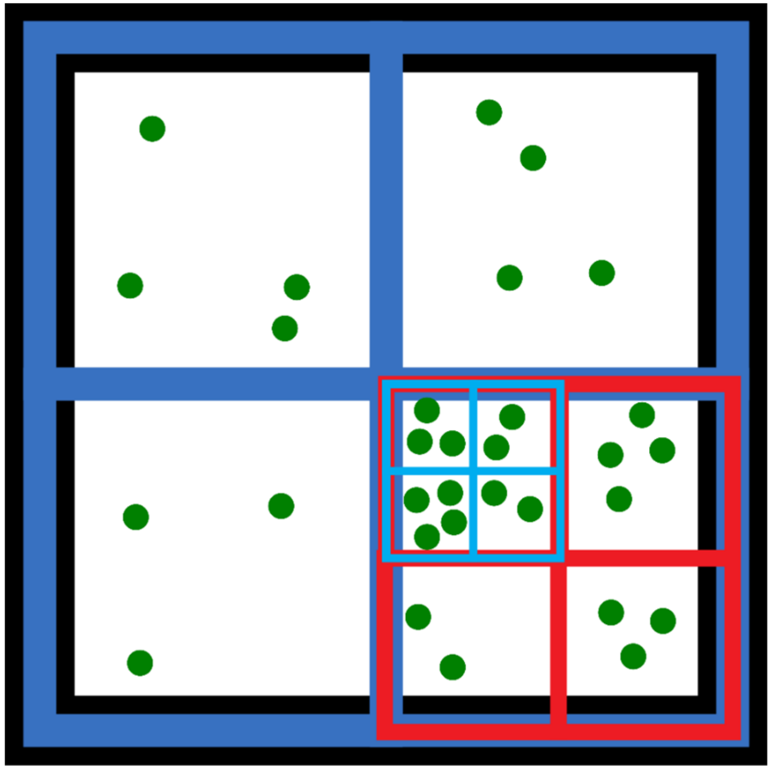
Approx. forces of distant particles, resolve forces of near particles
$\rightarrow \boldsymbol{F}_{tot} = \boldsymbol{F}_{distant} + \boldsymbol{F}_{near}$

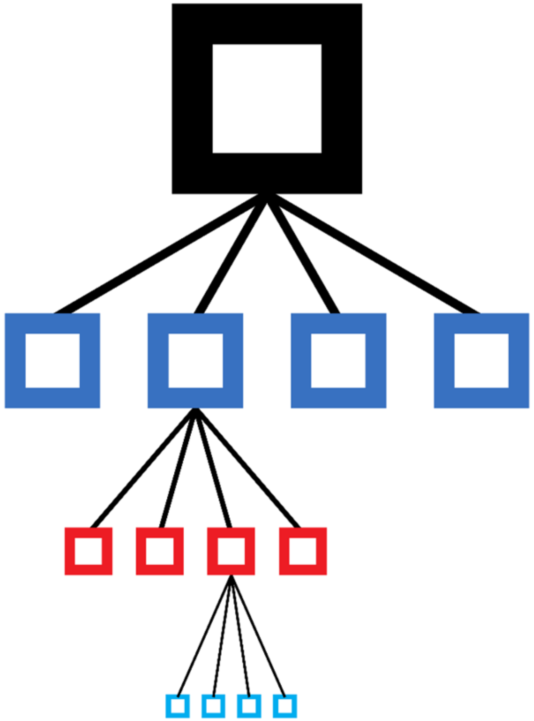


# Reminder On Fast Multipole Methods
## Tree Structure

**Analyze Distribution:**

Use Oct-Tree to identify distant regions of a particle bunch





# Reminder On Fast Multipole Methods
## FMM Interaction Computation

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**Compute Interaction Forces:**

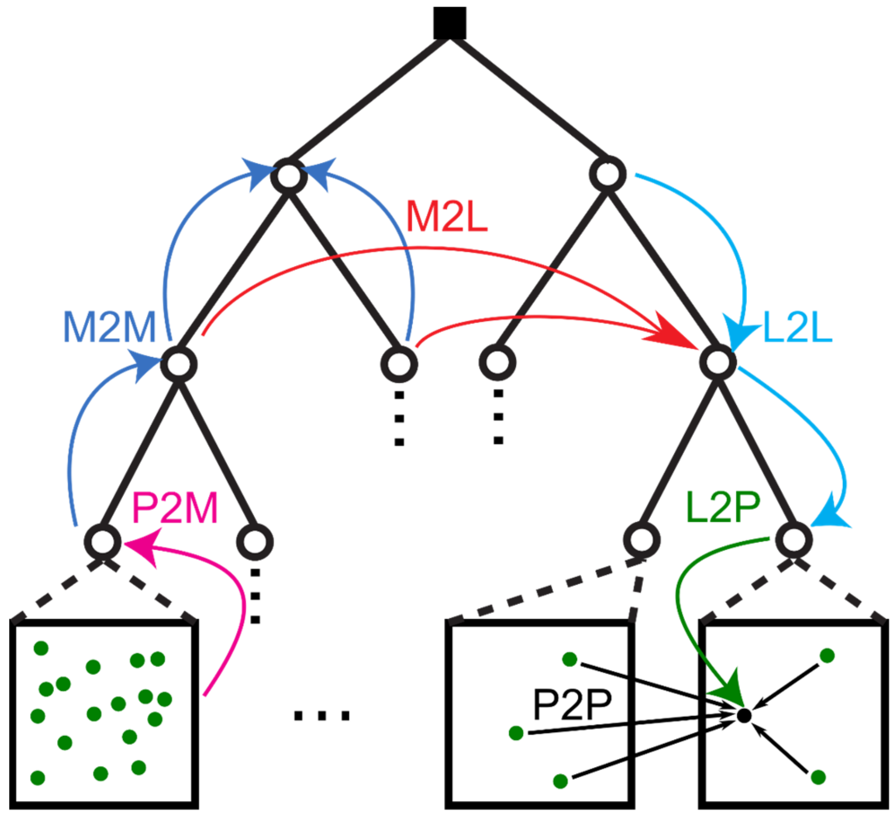
1. Compute multipole expansion of particles contained in each leaf box.

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.

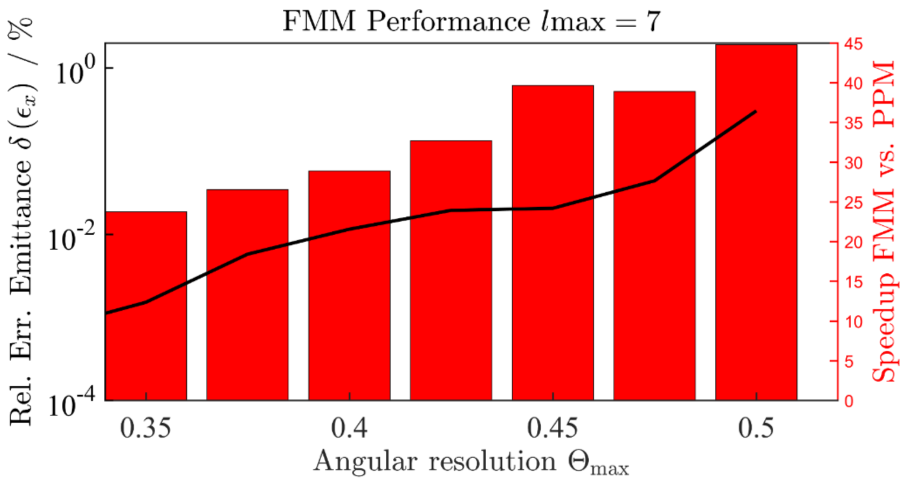
5. Evaluate $F_{distant}$ and $F_{near}$ for each particle in the leaf.
   $\rightarrow \boldsymbol{O}(\boldsymbol{N})$ scaling

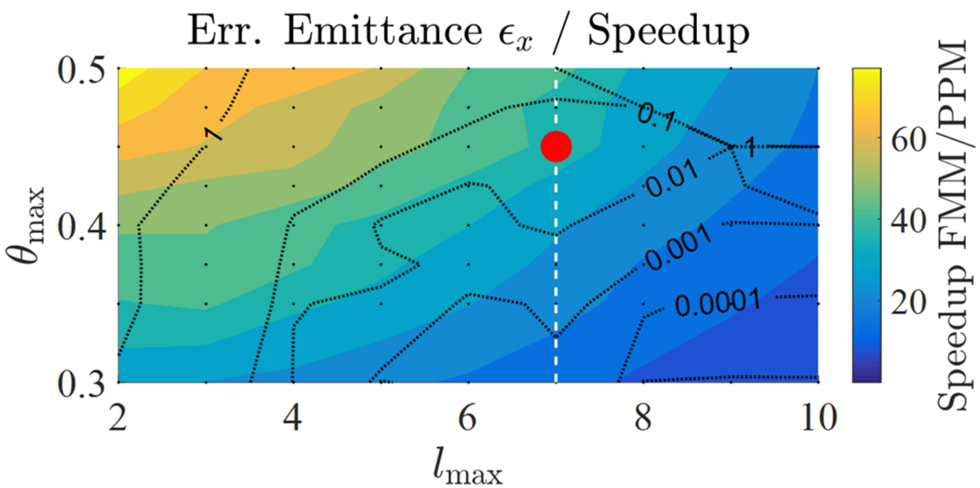



(Plot based on: R. Yokota, ExaFMM User's Manual, 2011)

# Simulation of the PITZ Injector
## FMM Parameter Study





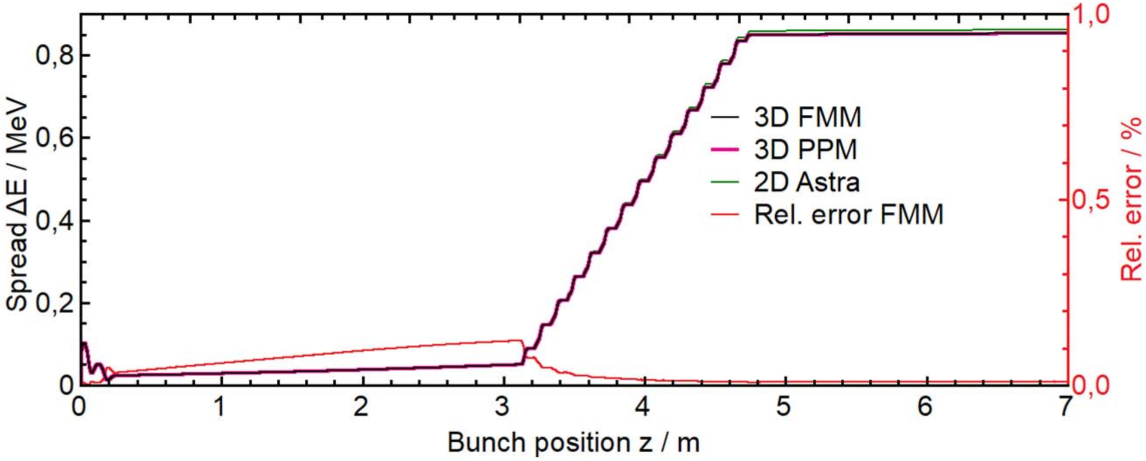

**Parameter Study: $\Theta_{max}$ & $l_{max}$**

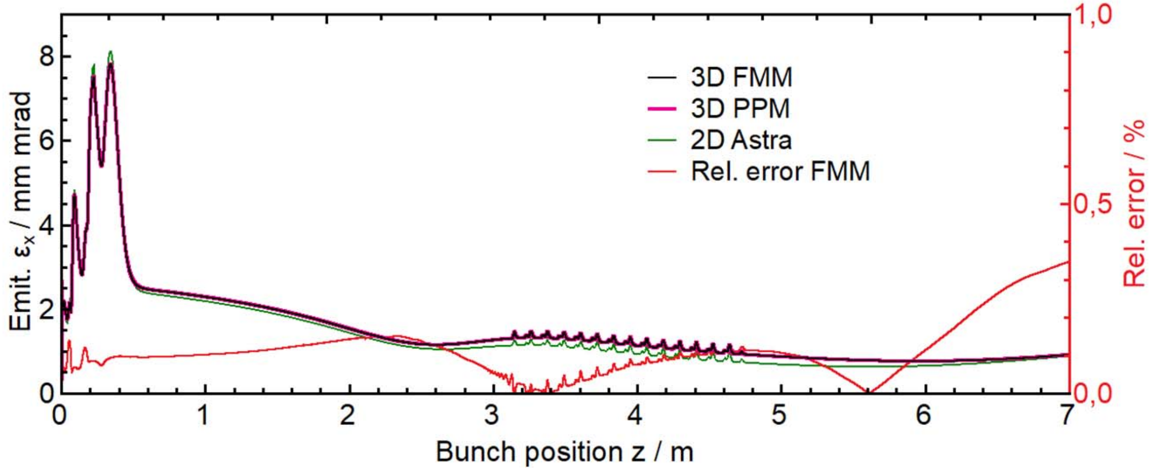
Bunch:
Charge: 1.0 nC
Size: 500k particles
Pulse length: 21.5 ps
Diameter: 0.4 mm

Sample Setup:
Particle emission, 1000 time steps
PPM: 234 processes on HPC cluster
FMM: 14 processes on MC-CPU

⇒ Color: Speedup FMM / PPM
⇒ Contour: Error FMM in %

# Simulation of the PITZ Injector
## FMM Simulation Results




FMM Parameters:

$\Theta_{max} = 0.45,\ l_{max} = 7$

Simulation Setup:

#Particles: 500k

SC-model: Fully 3D UMAF

PPM on HPC Cluster:

#Processes: 400

Time: 56 h 6 min

FMM on Workstation:

#Processes: 48

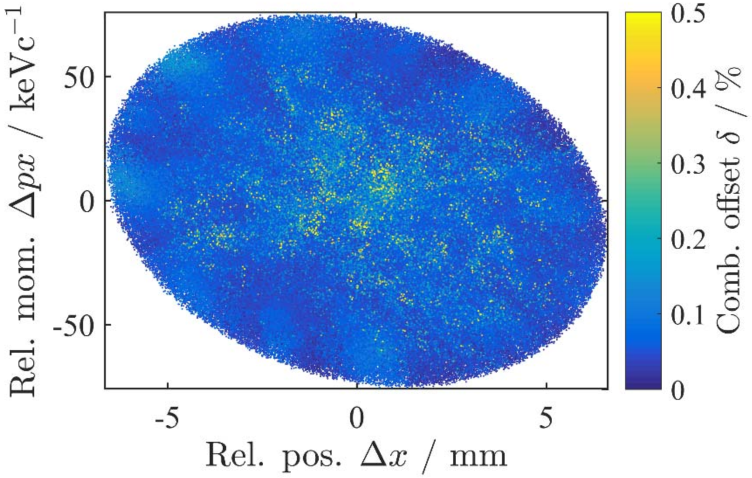
Time: 9 h 24 min

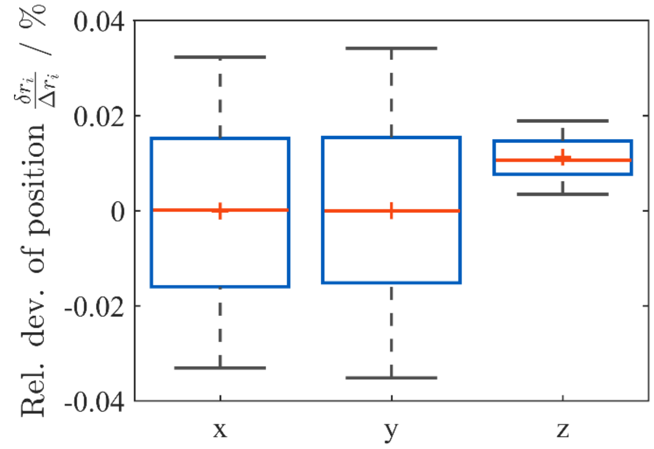
⇒ **FMM 6 times faster**

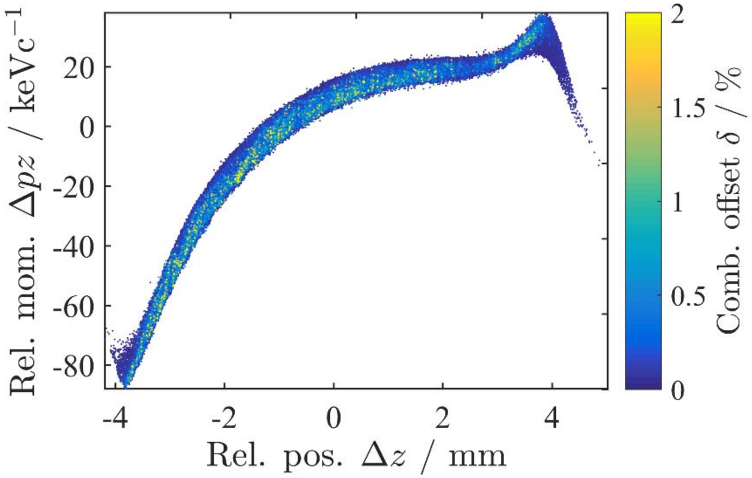
⇒ **FMM error < 0.5%**

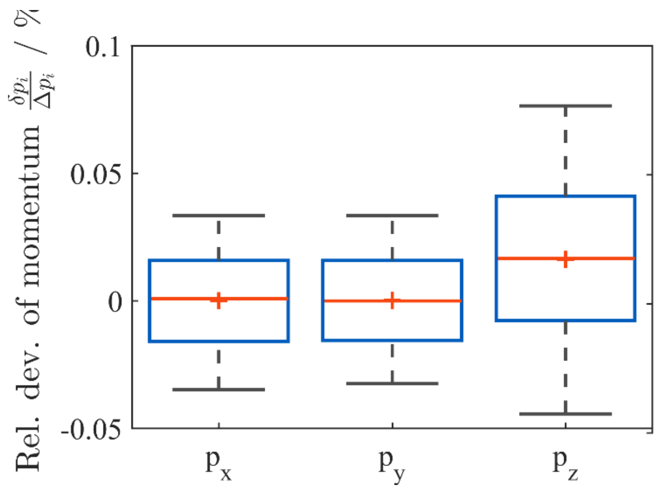
# Simulation of the PITZ Injector

## Phase Space Errors After Gun $(z \approx 40cm)$

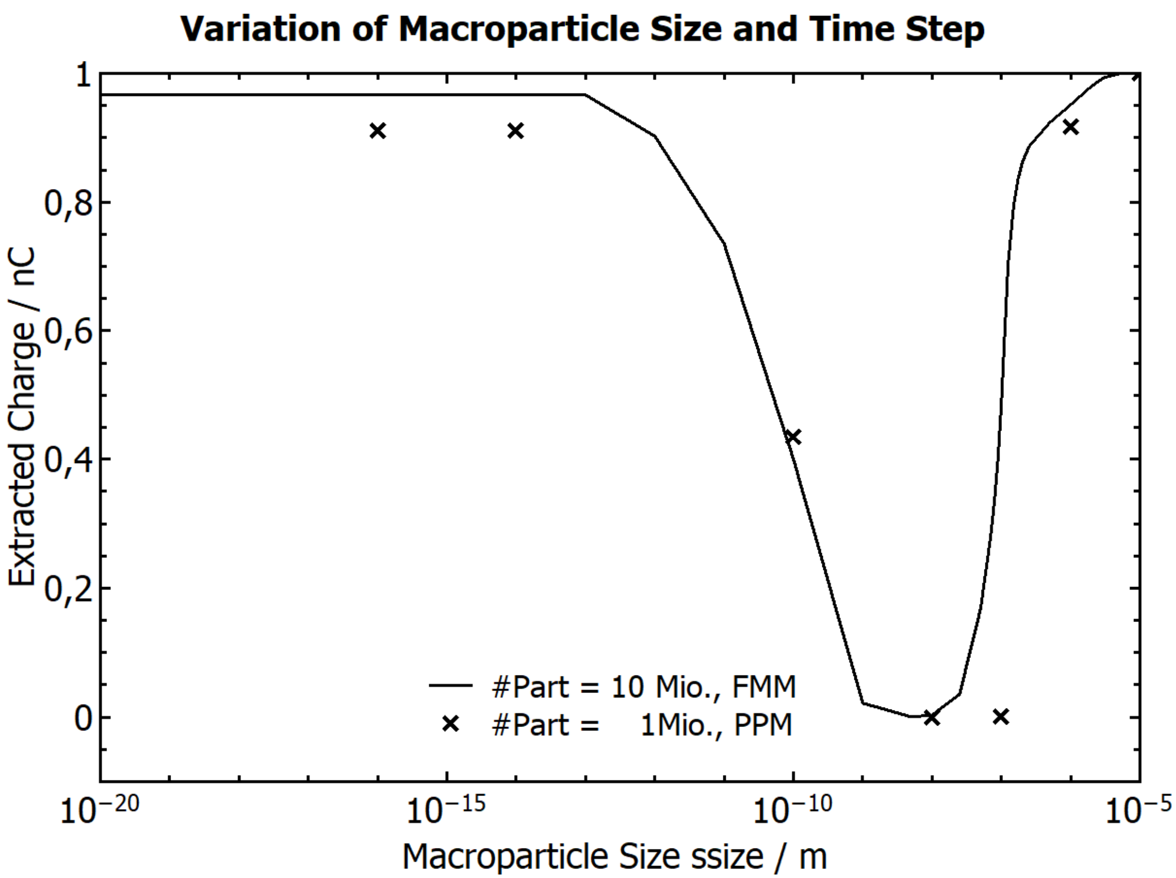


# Convergence of Particle Emission
## Particle Size *ssize*




Bunch:

| | |
|---|---|
| Inp. Charge $Q_{in}$: | 1.0 nC |
| Pulse length: | 21.5 ps |
| Diameter: | 0.3 mm |

Parameters:

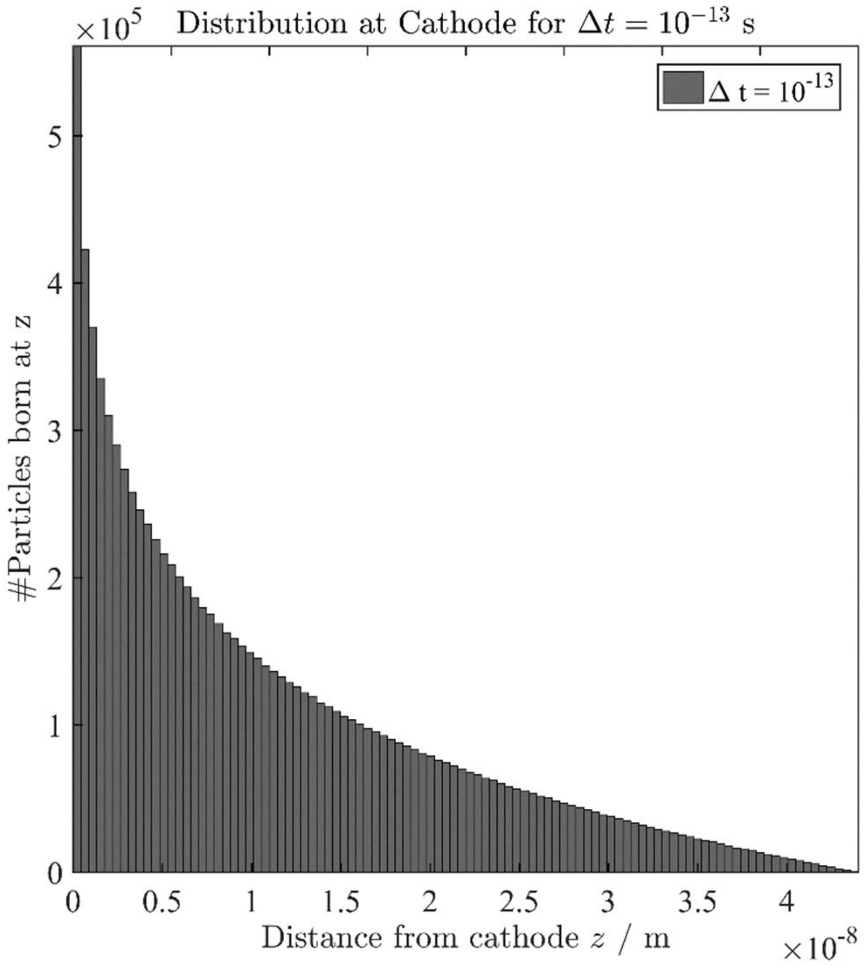
| | |
|---|---|
| Particle Radius: | $ssize$ |
| Time Step: | Δt |
| #Particles: | $N$ |

**Findings:**

⇒ FMM & PPM consistent

⇒ $Q_{out}$ depends on $ssize$

# Convergence of Particle Emission
## Ballistic Emission of Charges



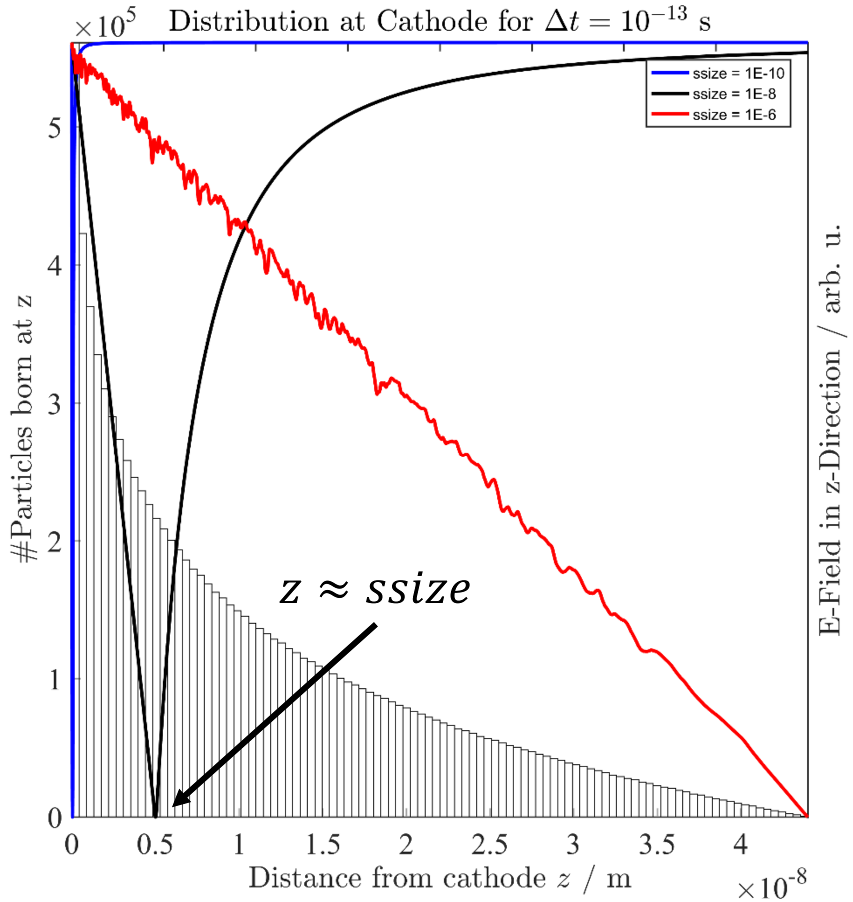

**Ballistic Emission Model:**

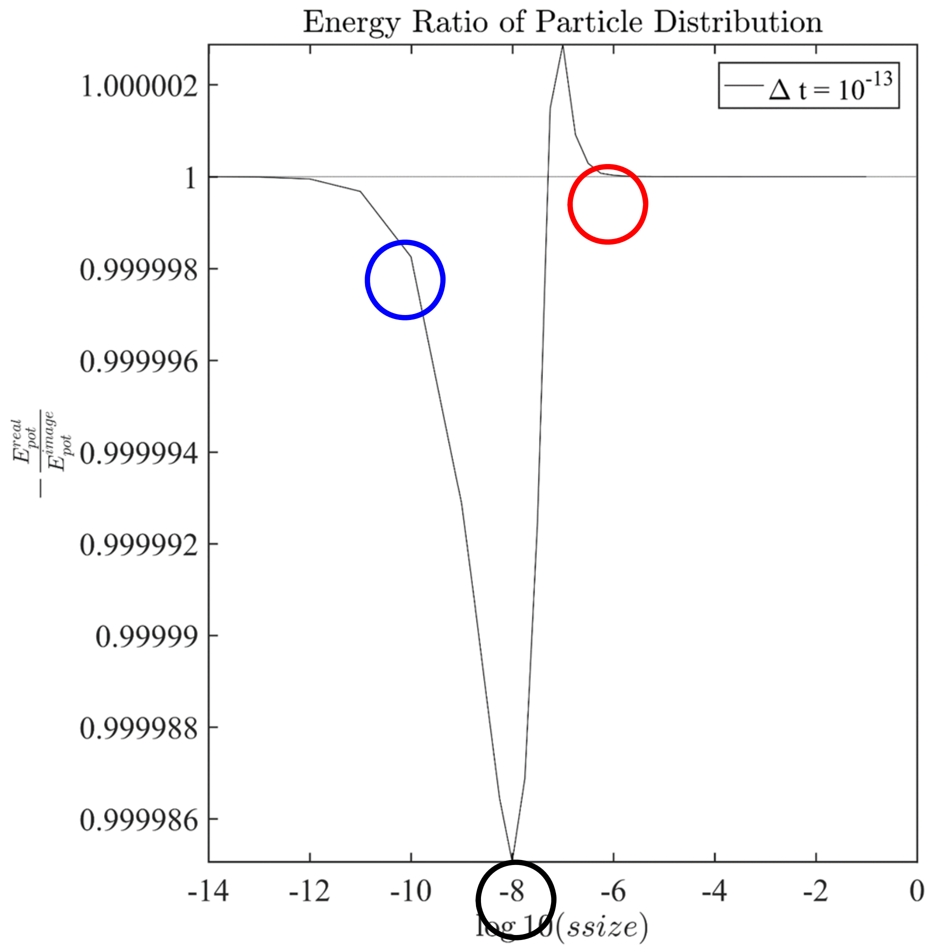
- Initial Particle Position:
  Partial time step, no forces
- Initial Particle Velocity:
  Temperature of cathode,
  $0 \leq v \leq v_{max}^{0} \sim 5 \cdot 10^{5}\,\frac{m}{s}$

⇒ Physics for $z \leq v_{max}^{0} \cdot \Delta t$ not modeled

⇒ Search for numerical convergence

# Convergence of Particle Emission
## Influence of Particle Size Parameter *ssize*

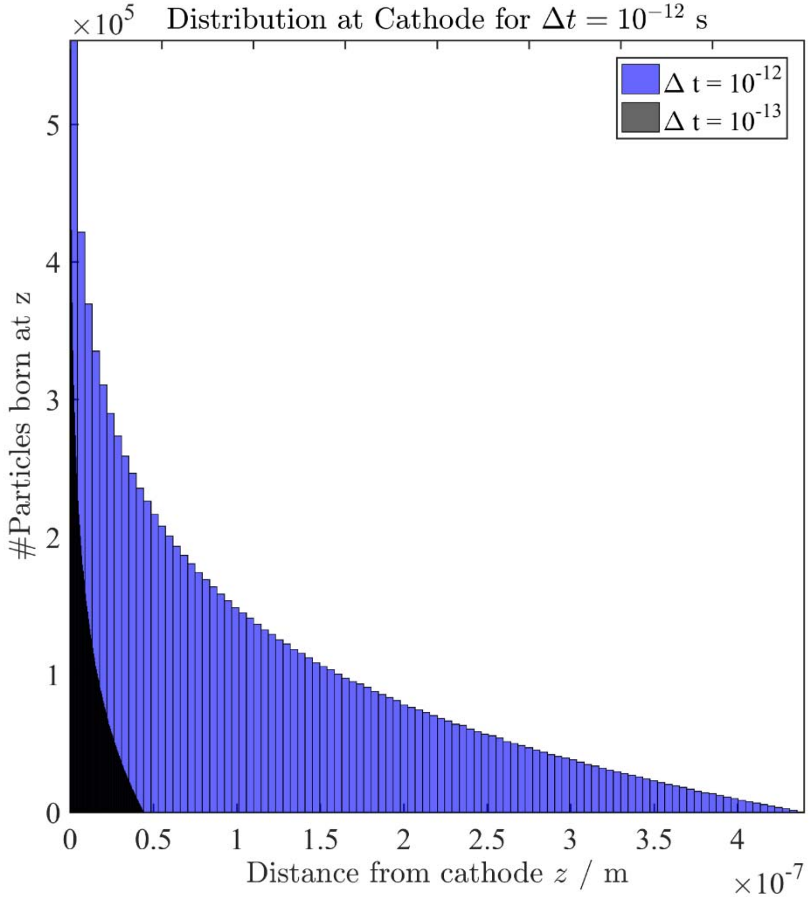


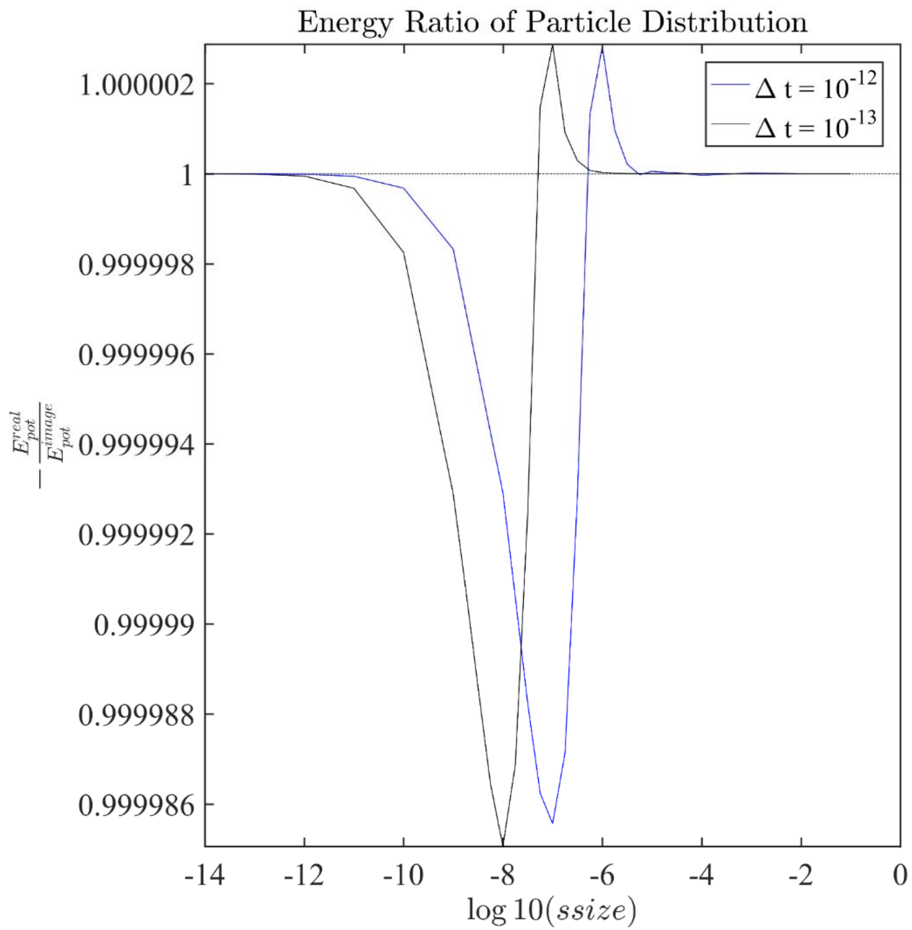




Self-interaction $\vec{E}$-field of particle distribution and corresponding image charges

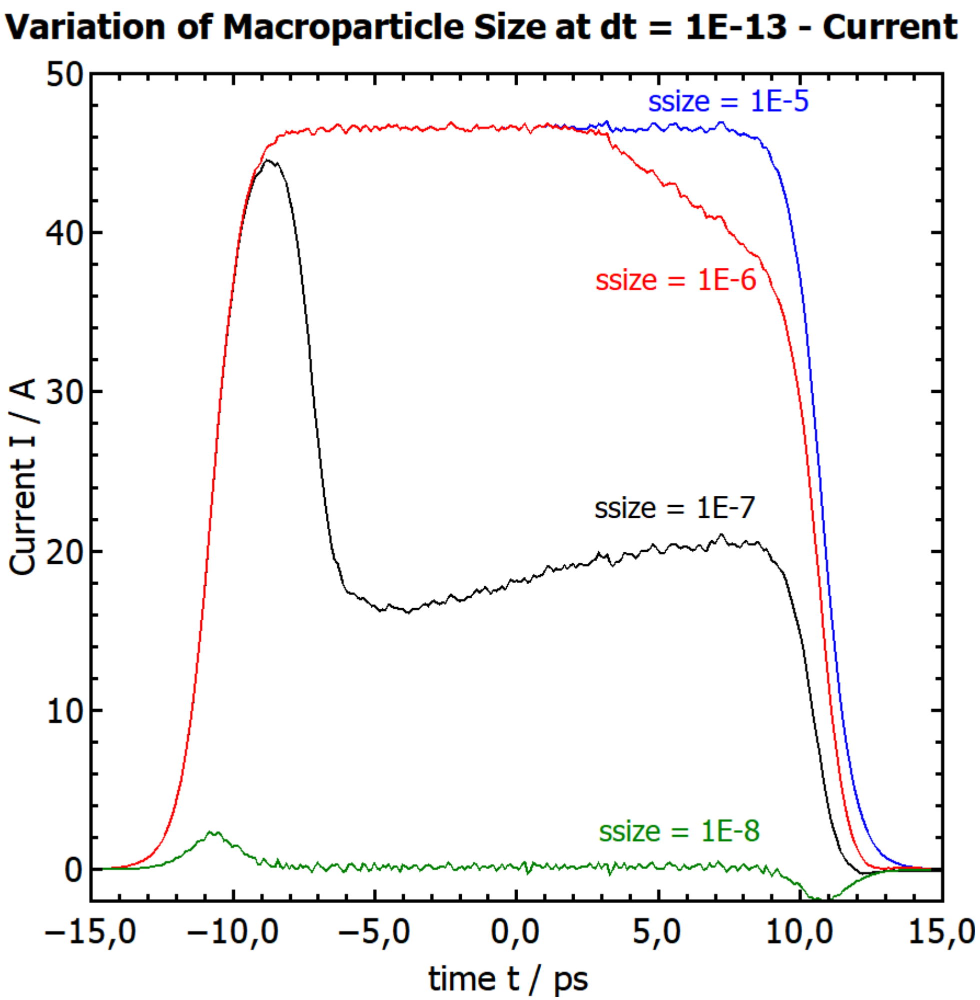
# Convergence of Particle Emission

## Influence of Time Step Δt



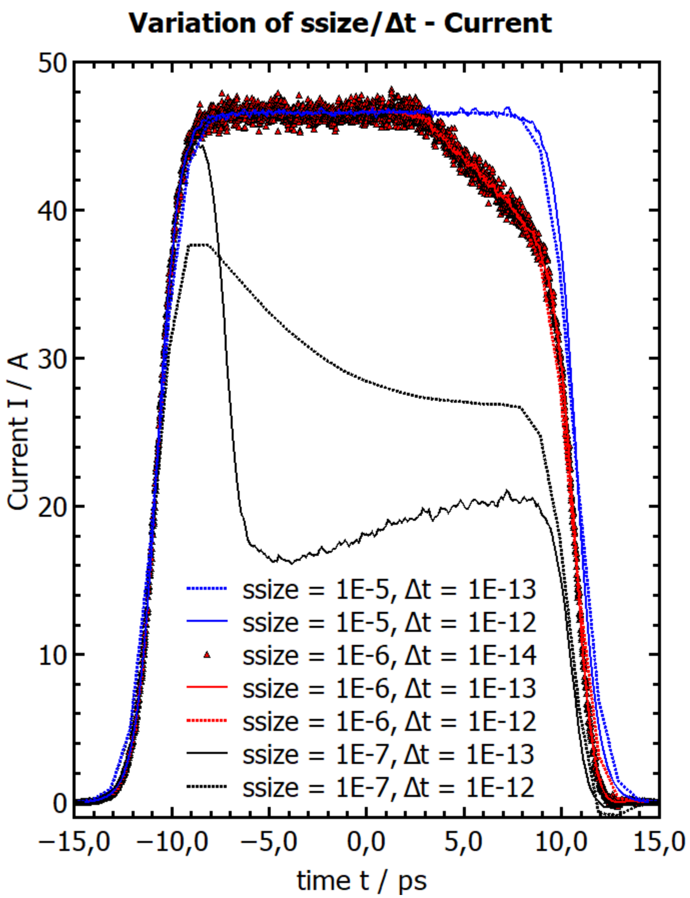
# Convergence of Particle Emission
## FMM Simulation Results



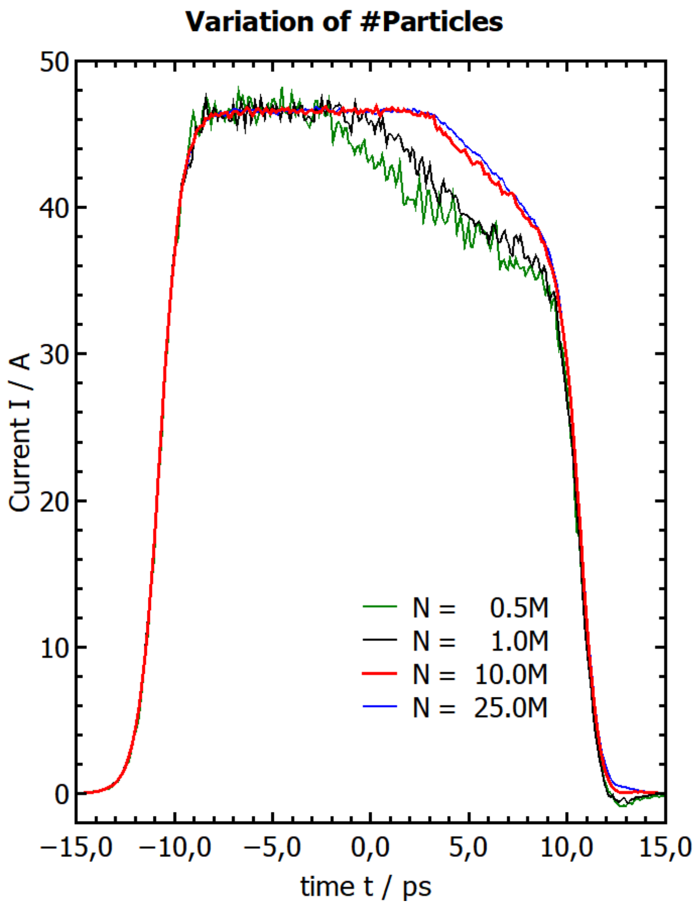

**Fixed:** $N = 10^7, \Delta t = 10^{-13}$
**Varied:** $ssize$

- $\frac{ssize}{\Delta t} \leq 10^6$
  ⇒ Particle loss during emission
- $\frac{ssize}{\Delta t} \geq 10^8$
  ⇒ No space charge limit
- $\frac{ssize}{\Delta t} \approx 10^7$
  ⇒ Try smaller $\Delta t$

# Convergence of Particle Emission
## FMM Simulation Results




**Fixed:** $N = 10^7$
**Varied:** $ssize/\Delta t$




**Fixed:** $\Delta t = 10^{-13}$, $ssize = 10^{-6}$
**Varied:** $N$

# Outlook
## Agenda for the FMM Code

**Status quo:**

+ Satisfactory results for FMM simulations of the PITZ injector

o Detailed large $N$ investigation of the ballistic emission model

- ExaFMM-MPI library is buggy, ExaFMM-GPU library does not work at all

**Ongoing and Future Code Development:**

- Full reimplementation of the FMM ⇒ **REPTIL**
  I. Reliable, clean, OpenMP parallelized C-implementation of FMM-Solver (90% finished)
  II. Further interaction models: Energy binning, UMLF
  III. GPU-accelerated and MPI parallelized FMM functionality

  Parallelized 3D space charge tracking code for applications at XFEL / PITZ

- Step by step towards self consistent emission models
  I. Emission time step including interaction forces (90% finished)
  II. Consider single particle dynamics at cathode
  III. Iterative self-consistent emission models

  Photoemission simulations for the PITZ gun

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