The Multiple Level Fast Multipole Method in the Differential Algebra Framework for Space Charge Field Calculation and Simulations on femtosecond electron imaging and spectroscopy

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Outline

- Multiple level fast multipole algorithm (MLFMA) in the differential algebra framework
- Simulation results on femetosecond electron imaging and spectroscopy

I. Multiple Level Fast Multipole Algorithm in DA framework

MLFMA

- Space charge effect is an important effect in the photo-emission process that generates the femtosecond electron bunch
- To simulate space charge effect, one needs an algorithm that has good efficiency and good accuracy.
- The MLFMA is a good choice, because it
  - scales linearly with the number of particles for any arbitrary charge distribution (grid free)
  - does NOT artificially smooth the field
- Using DA, one can
  - calculate not only the field, but also its high order derivatives
  - represent the multipole/local expansions in Cartesian coordinates naturally
  - considerably simply the math

MLFMA

- The DA based MLFMA is developed as a package for COSY Infinity
- COSY is a scientific computing system
  - DA and TM data types (ODE, flows, PDE, automatic differentiation, range bounding, etc.)
  - beam physics package
- More information on

  http://www.cosyinfinity.org

Two operations in COSY:

- Automatic Taylor expansion of a function

$$f(x+\boxed{\delta x}) = f(x) + f^{'}(x)\delta x + \frac{1}{2!}f^{''}(x)\delta x^2 + \frac{1}{3!}f^{'''}(x)\delta x^3 + ...$$

In COSY,

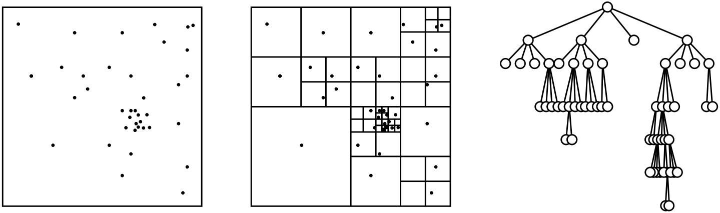
$$f(x+\boxed{da(1)}) = f(x) + f^{'}(x)da(1) + \frac{1}{2!}f^{''}(x)da(1)^2 + \frac{1}{3!}f^{'''}(x)da(1)^3 + ...$$

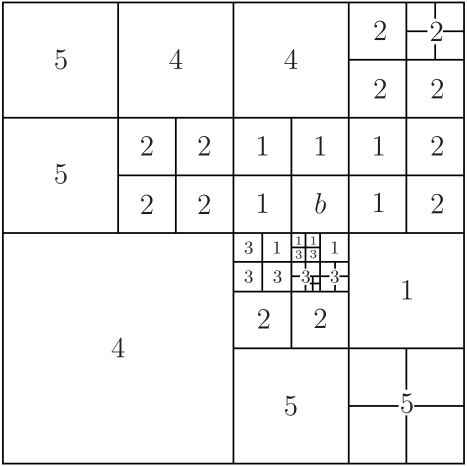
- Composition of two maps

$$G(x) = G(F) \circ F(x), \text{ or } G(x) = G(F(x))$$

In COSY, it can be done by the command POLVAL.

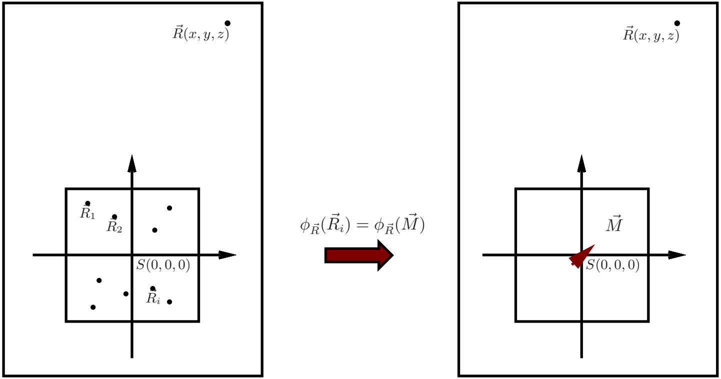
- Fast Multipole Method (FMM), L.Greengard and V.Rokhlin, 1987
- Cut the whole region into boxes of hierarchical tree structure.
- Multipole expansions and local expansions.
- For any arbitrary distribution, scales linearly with the number of particles.





Relations		Operations
$c \in 1_b$	$b \in 1_c$	$C_c \to C_b,\ C_b \to C_c$
$c \in 2_b$	$b \in 2_c$	$M_c \to L_b,\ M_b \to L_c$
$c \in 3_b$	$b \in 4_c$	$M_c \to C_b,\ C_b \to L_c$
$c \in 4_b$	$b \in 3_c$	$C_c \to L_b,\ M_b \to C_c$
$c \in 5_b$	$b \in 5_c$	Do nothing

Multipole expansion from charges (for the childless boxes)



$$
\begin{aligned}
\phi &= \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x-x_i)^2+(y-y_i)^2+(z-z_i)^2}} \\
&= \sum_{i=1}^{n} \frac{d_r \cdot q_i}{\sqrt{1+(x_i^2+y_i^2+z_i^2)d_r^2-2x_i d_x-2y_i d_y-2z_i d_z}} \\
&= d_r \cdot \bar{\phi}_{\mathrm{c2m}}
\end{aligned}
$$

with

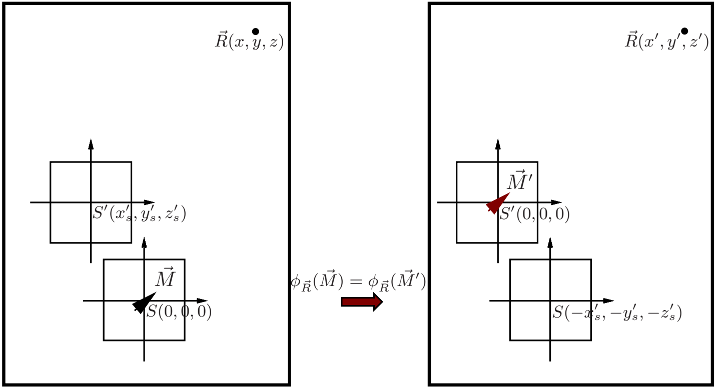
$$
d_x = \frac{x}{x^2+y^2+z^2}, \quad d_y = \frac{y}{x^2+y^2+z^2},
$$

$$
d_z = \frac{z}{x^2+y^2+z^2}, \quad d_r = \sqrt{d_x^2+d_y^2+d_z^2},
$$

$$
\bar{\phi}_{\mathrm{c2m}} = \sum_{i=1}^{n} \left\{ q_i \Big/ \sqrt{1+(x_i^2+y_i^2+z_i^2)d_r^2-2x_i d_x-2y_i d_y-2z_i d_z} \right\}.
$$

Error $\quad |\epsilon| \leqq C \cdot \left(\frac{a}{r}\right)^{p+1} \cdot \frac{1}{r-a}$, where $C = \sum_{i=1}^{n} |q_i|$ and $r_i \leq a$ for any i.

Translate the position of a multipole expansion



In parent box frame, new DA variables are chosen as

$$d'_x = \frac{x - x'_o}{r'^2} = \frac{x'}{r'^2}, \qquad d'_y = \frac{y - y'_o}{r'^2} = \frac{y'}{r'^2}$$
$$d'_z = \frac{z - z'_o}{r'^2} = \frac{z'}{r'^2},$$

Relation between the old and new DA variables.

$$\boxed{\begin{aligned} d_x &= (d'_x + x'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R, \\ d_y &= (d'_y + y'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R, \\ d_z &= (d'_z + z'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R, \end{aligned}}$$

M_{m2m}

with

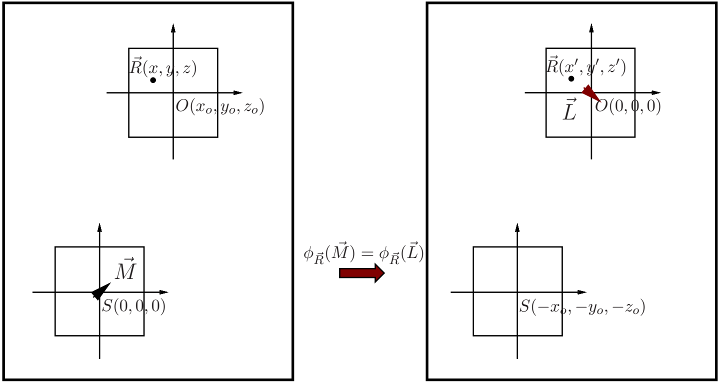
$$R = \frac{1}{1 + (x'^2_o + y'^2_o + z'^2_o)(d'^2_x + d'^2_y + d'^2_z) + 2x'_o d'_x + 2y'_o d'_y + 2z'_o d'_z}.$$

In child box frame $\phi = \boxed{d_r} \cdot \boxed{\bar{\phi}_{c2m}}$.
In the parent box frame

$$\phi' = \boxed{d'_r \cdot \sqrt{R}} \cdot \boxed{\phi_{m2m}} = d'_r \cdot \bar{\phi}_{m2m}$$

with $d'_r = \sqrt{d'^2_x + d'^2_y + d'^2_z}$,
and $\phi_{m2m} = \bar{\phi}_{c2m} \circ M_{m2m}$,
where M_{m2m} is the map from the old DA variables into the new DA variables

Convert a multipole expansion into a local expansion



New DA variables in the observer frame

$$\begin{aligned} d'_x &= x - x'_o = x', \\ d'_y &= y - y'_o = y', \\ d'_z &= z - z'_o = z'. \end{aligned}$$

The relation between the new and the old DA variables

$$\boxed{\begin{aligned} d_x &= (x'_o + d'_x) \cdot R, \\ d_y &= (y'_o + d'_y) \cdot R, \\ d_z &= (z'_o + d'_z) \cdot R. \end{aligned}} \qquad M_{m2l}$$

with

$$R = \frac{1}{(x'_o + d'_x)^2 + (y'_o + d'_y)^2 + (z'_o + d'_z)^2}.$$

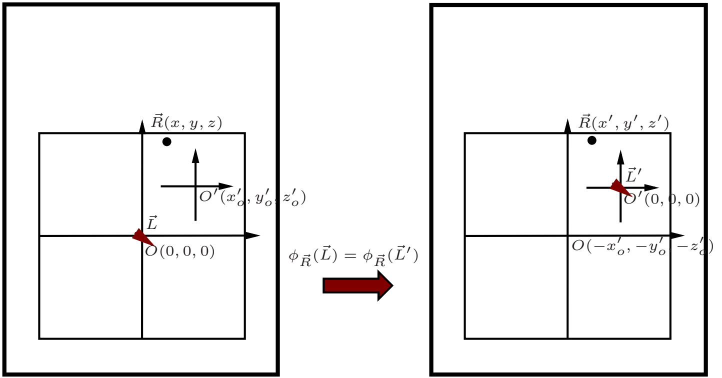
The multipole expansion in the source frame $\phi = \boxed{d_r} \cdot \boxed{\bar{\phi}}$
The local expansion in the observer frame

$$\phi = \boxed{\sqrt{R}} \cdot \boxed{\bar{\phi}_{m2l}} = \phi_{m2l}$$

where $\sqrt{R}$ is converted from d_r, $\bar{\phi}_{m2l} = \bar{\phi} \circ M_{m2l}$,
and M_{m2l} is the map between the DA variables.
Error

$$|\epsilon| \leq C \cdot \left(\frac{a}{r'_o}\right)^{p+1} \cdot \frac{1}{r'_o - a} + C \cdot \left(\frac{r'}{b}\right)^{p+1} \cdot \frac{1}{b - r'}.$$

Translate a local expansion from a parent box to its child boxes



DA variables in the child box frame

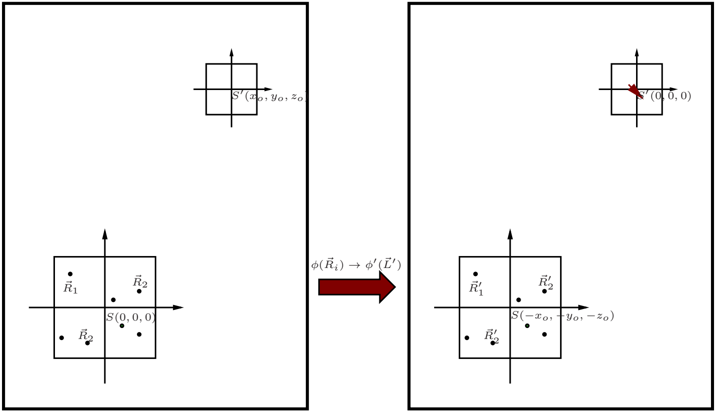
$$\boxed{\begin{aligned} d_x &= x'_o + d'_x, \\ d_y &= y'_o + d'_y, \\ d_z &= z'_o + d'_z. \end{aligned}} \qquad M_{l2l}$$

The local expasion in the parent box frame is ϕ_{m2l}.
The local expansion in the child box frame is

$$\phi = \phi_{m2l} \circ M_{l2l} = \phi_{l2l},$$

where M_{l2l} is the map between the old and the new DA variables.

Calculate the local expansion from charges.



In the observer (small box) frame, the new DA variables are

$$\begin{aligned} d'_x &= x - x'_o = x', \\ d'_y &= y - y'_o = y', \\ d'_z &= z - z'_o = z'. \end{aligned}$$

Then the local expansion is

$$\begin{aligned} \phi_{\mathrm{L}} &= \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}} \\ &= \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x'_o - x_i + d'_x)^2 + (y'_o - y_i + d'_y)^2 + (z'_o - z_i + d'_z)^2}} \end{aligned}$$

Error

$$|\epsilon| \leqq C \cdot \left(\frac{r'}{b}\right)^{p+1} \cdot \frac{1}{b - r'}$$

- Now we have the potential expressed as a polynomial of coordinates up to order p.
- Take the derivative of a coordinates to get the field expression in a polynomial of coordinates up to order $p-1$.
- Submit the charge positions into the expression to calculate the potential/field.

Calculate the field from the multipole expansion.
The multipole expansion is $\phi = d_r \cdot \bar{\phi}$, then

$$
\begin{aligned}
E_x &= \{-\frac{\partial\bar{\phi}}{\partial d_x} \cdot (d_r^2 - 2d_x^2) + 2\frac{\partial\bar{\phi}}{\partial d_y} \cdot d_x d_y + 2\frac{\partial\bar{\phi}}{\partial d_z} \cdot d_x d_z + \bar{\phi} \cdot d_x\} \cdot d_r \\
E_y &= \{2\frac{\partial\bar{\phi}}{\partial d_x} \cdot d_y d_x - \frac{\partial\bar{\phi}}{\partial d_y}(d_r^2 - 2d_y^2) + 2\frac{\partial\bar{\phi}}{\partial d_z} \cdot d_y d_z + \bar{\phi} \cdot d_y\} \cdot d_r \\
E_z &= \{2\frac{\partial\bar{\phi}}{\partial d_x} \cdot d_z d_x + 2\frac{\partial\bar{\phi}}{\partial d_y} \cdot d_z d_y - \frac{\partial\bar{\phi}}{\partial d_z} \cdot (d_r^2 - d_z^2) + \bar{\phi} \cdot d_z\} \cdot d_r
\end{aligned}
$$

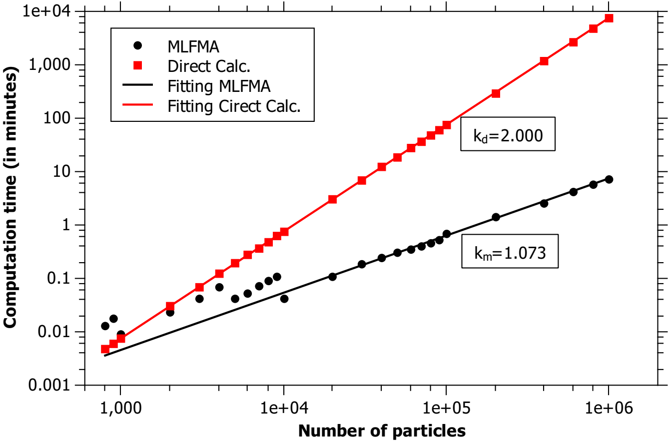
with

$$
d_r = \sqrt{d_x^2 + d_y^2 + d_z^2}.
$$

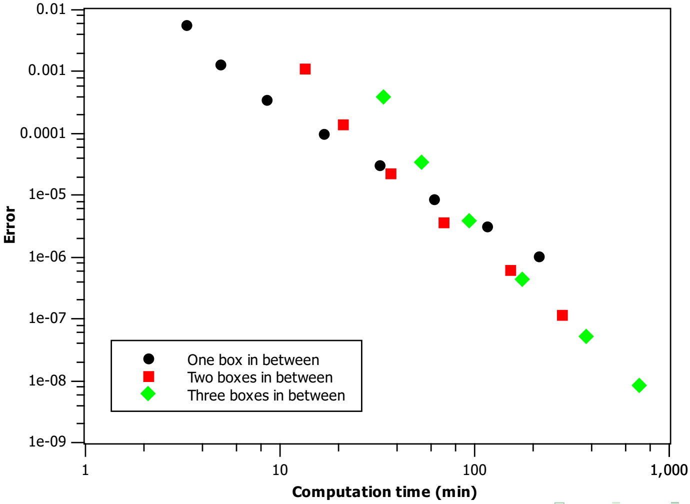
Description of the MLFMA

- Construct the hierarchical box structure (partial tree).
- Upwards: Calculate the multipole expansions for all the boxes.
- Downwards: For each box, check its the relation with other boxes and operate according to the above table. Then translate the local expansion from parent boxes to the child boxes.
- Calculate the potential/field, which comes from direct calculation and multipole or local expansions.

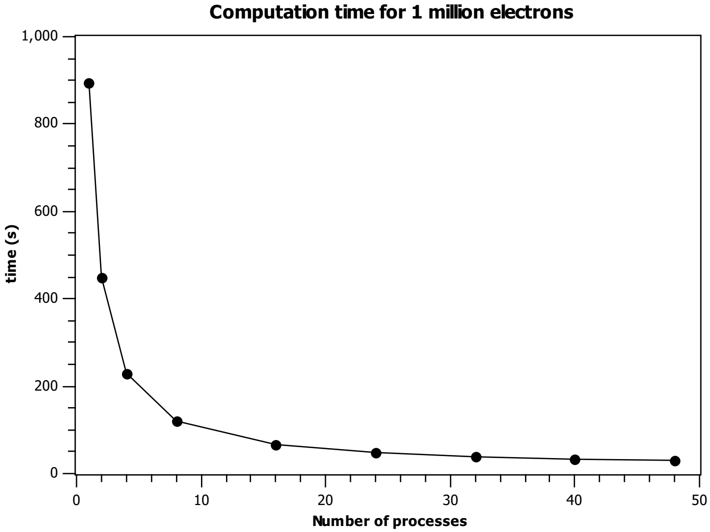
Compare the MLFMA with direct calculation



Accuracy and computation time

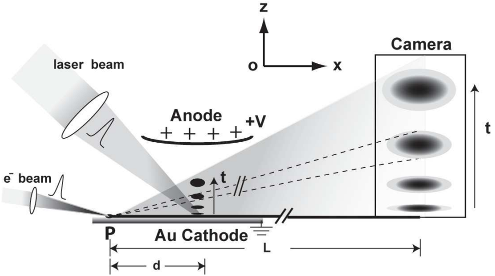


Numerical experiments



II. Simulation results on femetosecond imaging and spectroscopy

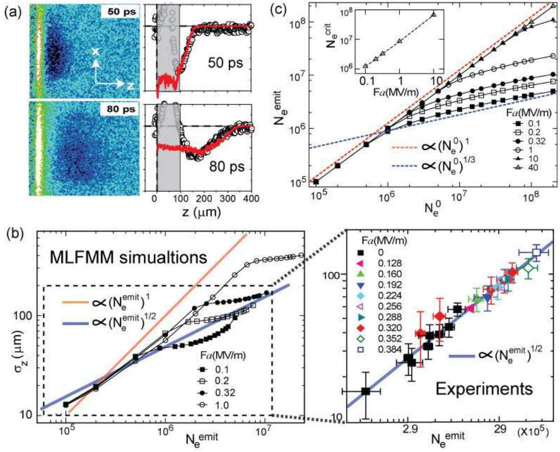
Experiment setup:



Simulation model:

- Three-step model of photoemission
- Extraction field F_a, space charge field, surface image charges
- Up to several millions of macro-particles in simulation

Simulation

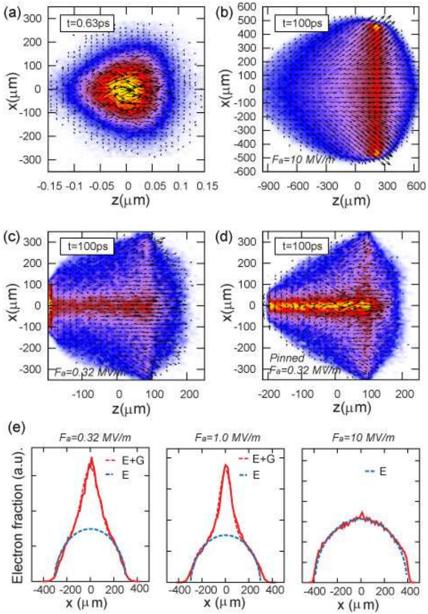


(a) Electron bunch profiles (b) Bunch length vs. N_e^{emit}
(c) N_e^{emit} vs. N_e^0 showing virtual cathode effect

1 .Z. Tao, H. Zhang, P. M. Duxbury, M. Berz, C.-Y. Ruan, Journal of Applied Physics 111 (2012) 044316

2. J. Portman, H. Zhang, Z. Tao, etc., Applied Physics Letter, in press, 2013

Simulation



(a) Initial electron bunch profiles in x-z plane

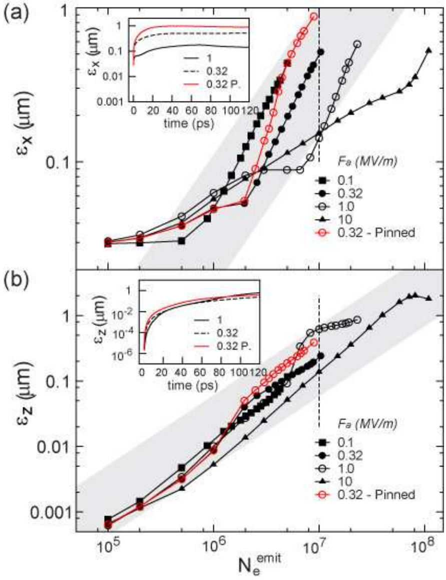
(b) Electron bunch profiles in x-z plane at 100ps under strong F_a (10 MV/m)

(c) Electron bunch profiles in x-z plane at 100ps under weak F_a (0.32 MV/m)

(d) Electron bunch profiles in x-z plane at 100ps under weak F_a (0.32 MV/m) with a pinned image field

(e) Electron charge distributions under different fields

Simulation

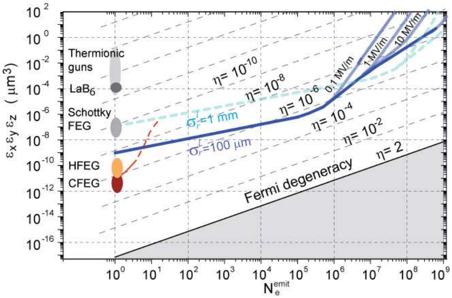


(a) ε_x for different field and different $N_\mathrm{e}^\mathrm{emit}$. Affected by the virtual cathode effect.

(b) ε_y for different field and different $N_\mathrm{e}^\mathrm{emit}$. Not affected by the virtual cathode effect. Driven by internal field and nonlinearities.

Simulation

Figure: 6D emittance $\varepsilon_x \varepsilon_y \varepsilon_z$ versus $N_{\mathrm{e}}^{\mathrm{emit}}$ for the extended electron sources with sizes σ_r^I (100 μm, 1mm), thermionic guns, Schottky, cold (CFEG) and heated (HFEG) field-emission guns[1]



1 Science of Microscopy, Eds. P.W. Hawkes, and J.C.H. Spence (Springer, New York, 2008)

- Degeneracy ($\eta = B_{6D}\varepsilon_0$, $B_{6D} = N_{\mathrm{e}}/(\varepsilon_x^2 \varepsilon_z)$) can improved with flat photoemission cathode until the virtual cathode threshold.
- Increasing extraction field is helpful, because it defers the onset of virtual cathode effect.
- Large emitting area increases the $N_{\mathrm{e}}^{\mathrm{emit}}$, but not necessary degeneracy (brightness).
- No gain by using sharp emitters (FEGs or atom-sized emitters) due to their poor emittance scaling with N_{e}.

Summary

1.The multiple Level Fast Multipole Algorithm

- Grid-free, works for any arbitrary charge distribution with an efficiency $O(N)$.
- Calculate both the potential/field and its derivatives

2. Studied the virtual cathode effect quantitatively in femtosecond electron generation

- $N_{\mathrm{e}}^{\mathrm{emit}}$, ε_x, η
- Increase F_a can defer the onset of virtual cathod effect

3. Transition into virtual cathode regime might be described by two fluids

4. η is affected by different factors.

THANK YOU!