The Fast Multipole Method in the Differential Algebra Framework for the Computation of 3D Space Charge Fields and Transfer Maps

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ICAP 2012

Outline

- Introduction of the fast multipole method (FMM)
- Details of the differential algebra (DA) based fast multipole method
  - Single level fast multipole algorithm for uniform charge distribution
  - Multiple level fast multipole algorithm (MLFMA) for any charge distribution
- Simulation example

Introduction

Most algorithms in beam community fall into two categories:

- Particle Particle Interaction (PPI): MAPRO2, SC3DELP, TOPKARK, SCHERM, Improved SCHERM,
- Particle in Cell (PIC): SCHEFF, PICNIC, GPT, IMPACT Z, WARP

We want to bring a new algorithm into the beam community:

- Fast Multipole Method (FMM), L.Greengard and V.Rokhlin, 1987

Strategy of FMM

- Enclose the charged region with a box, then cut the box into small boxes.
- For each box, the whole region can be divided into the near region and the far region to the box.
- Near region interaction is calculated directly.
- Far region interaction is approximately calculated by the multipole expansions and the local expansions. Efficiency is $O(N)$.

Single Level FMM

Two operations in COSY:

- Automatic Taylor expansion of a function

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

In COSY,

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

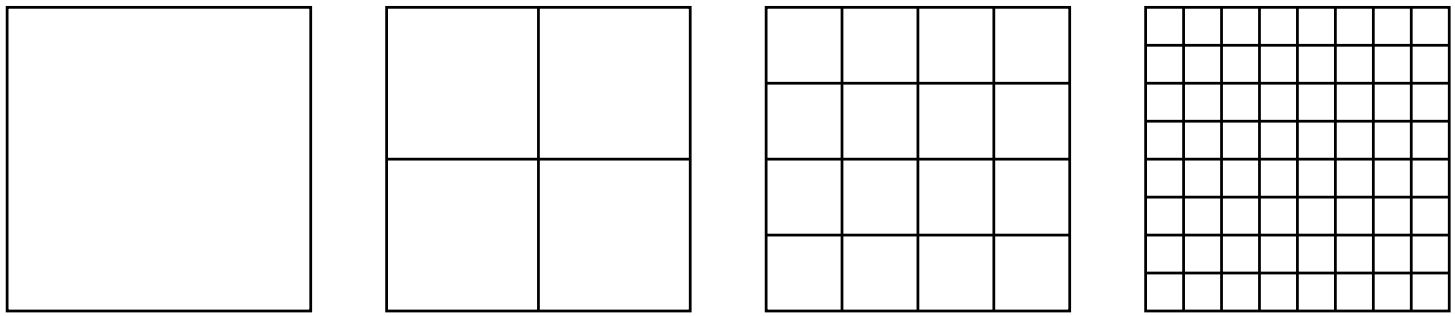
- Composition of two maps

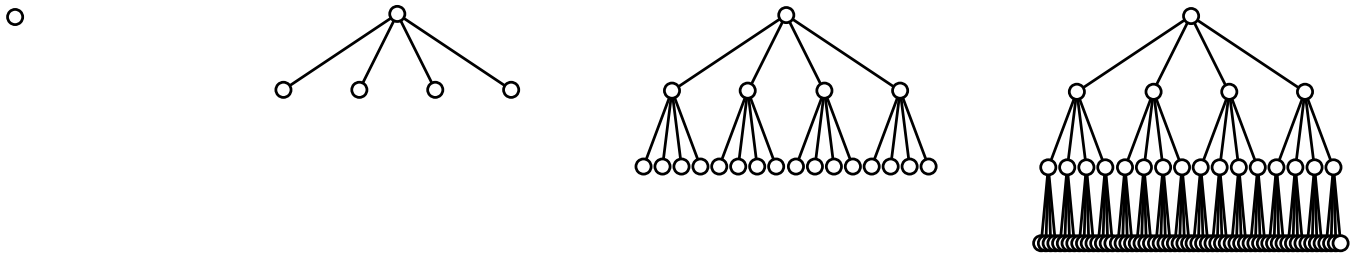
$$G(x) = G(F) \circ F(x), \text{ or } G(x) = G(F(x))$$

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

Single Level FMM

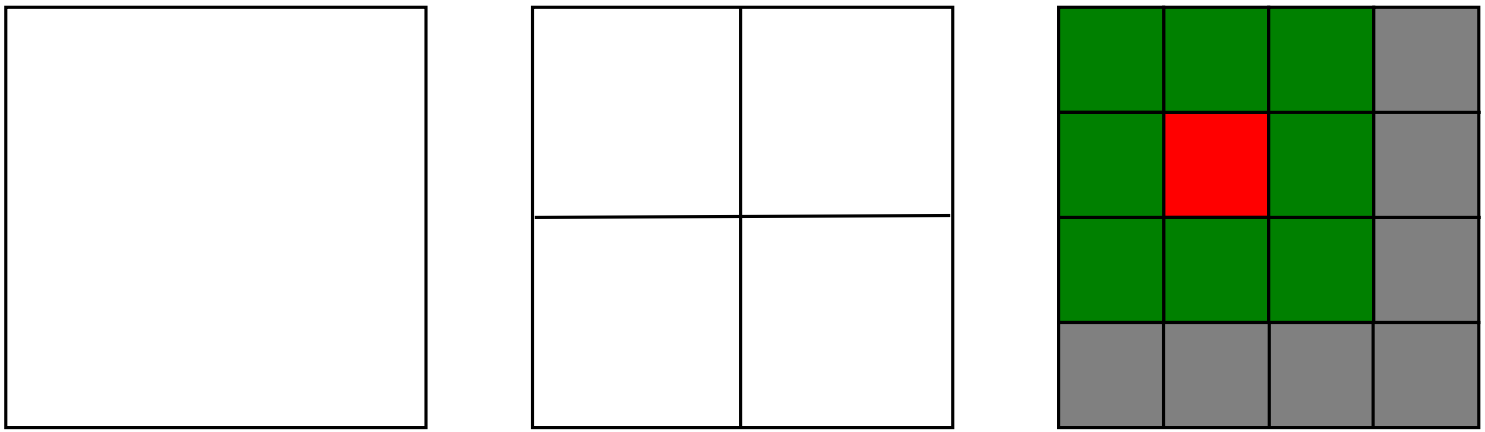
Hierarchical tree structure



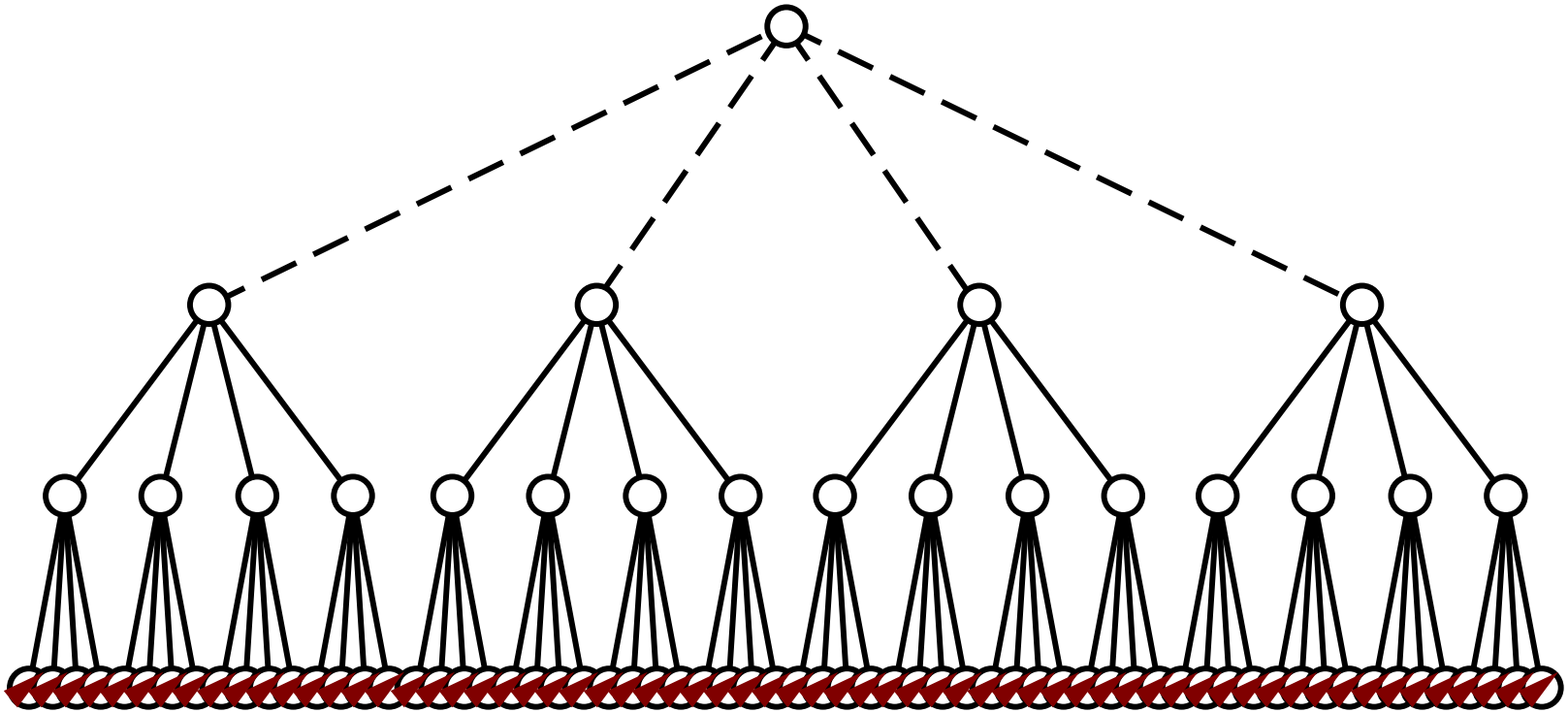


Single Level FMM

Near region and Far region

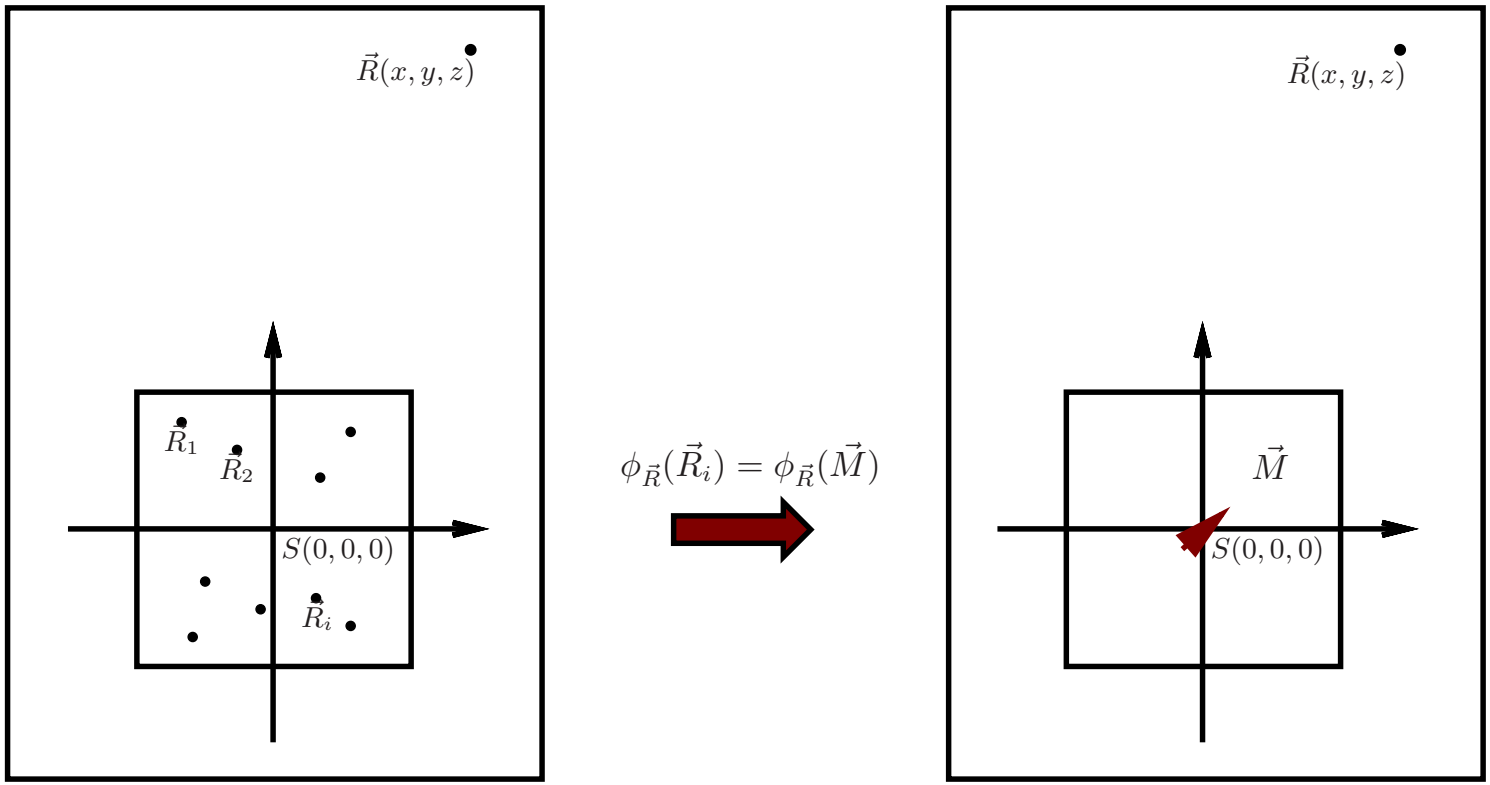


Single Level FMM



Single Level FMM

Multipole expansion from charges (for the childless boxes)



Single Level FMM

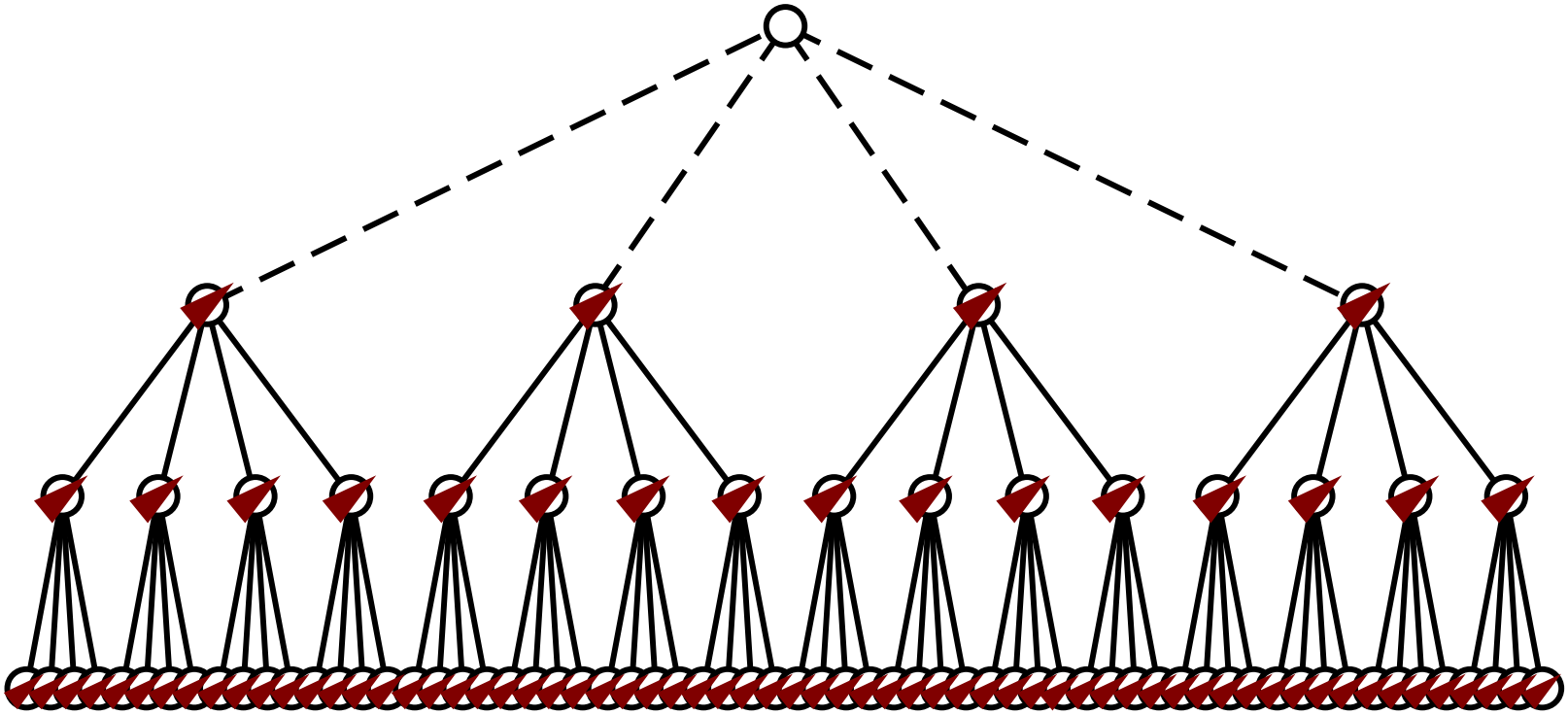
$$
\begin{aligned}
\phi &= \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x-x_i)^2+(y-y_i)^2+(z-z_i)^2}} \\
&= \sum_{i=1}^{n} \frac{d_r \cdot q_i}{\sqrt{1+(x_i^2+y_i^2+z_i^2)d_r^2-2x_i d_x-2y_i d_y-2z_i d_z}} \\
&= d_r \cdot \bar{\phi}_{\mathrm{c2m}}
\end{aligned}
$$

with

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

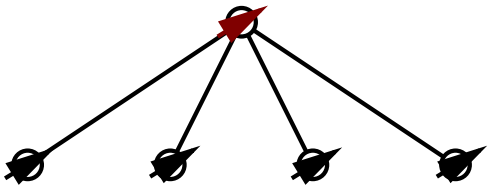
Error $|\epsilon| \leqq C \cdot \left(\frac{a}{r}\right)^{p+1} \cdot \frac{1}{r-a}$, where $C = \sum_{i=1}^{n} |q_i|$ and $r_i \leq a$ for any i.

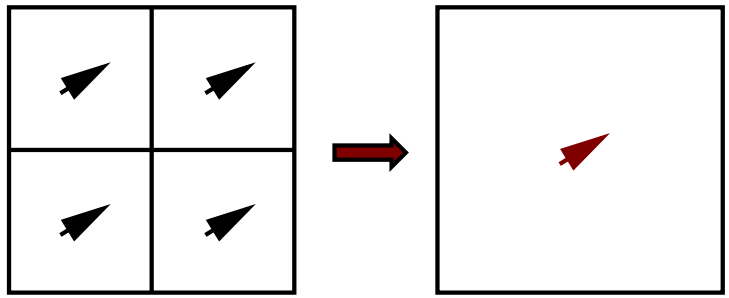
Single Level FMM



Single Level FMM

Multipole expansions for the parent boxes





Single Level FMM

In the 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 the new DA variables.

$$\begin{aligned} d_x &= (d_x' + x_o' \cdot (d_x'^2 + d_y'^2 + d_z'^2)) \cdot R, \\ d_y &= (d_y' + y_o' \cdot (d_x'^2 + d_y'^2 + d_z'^2)) \cdot R, \\ d_z &= (d_z' + z_o' \cdot (d_x'^2 + d_y'^2 + d_z'^2)) \cdot R, \end{aligned}$$

M_{m2m}

with

$$R = \frac{1}{1 + (x_o'^2 + y_o'^2 + z_o'^2)(d_x'^2 + d_y'^2 + d_z'^2) + 2x_o'd_x' + 2y_o'd_y' + 2z_o'd_z'}.$$

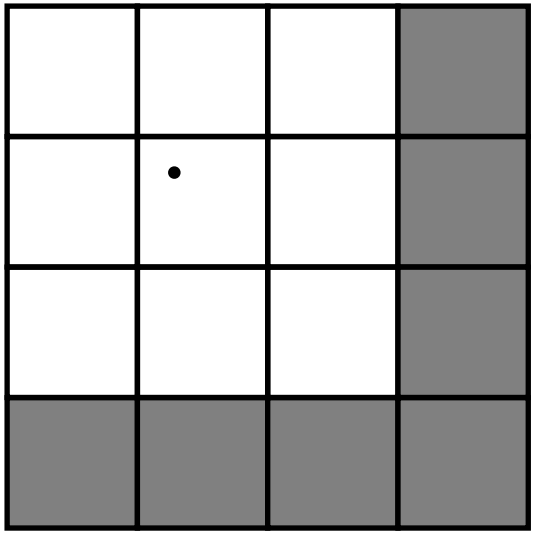
Single Level FMM

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

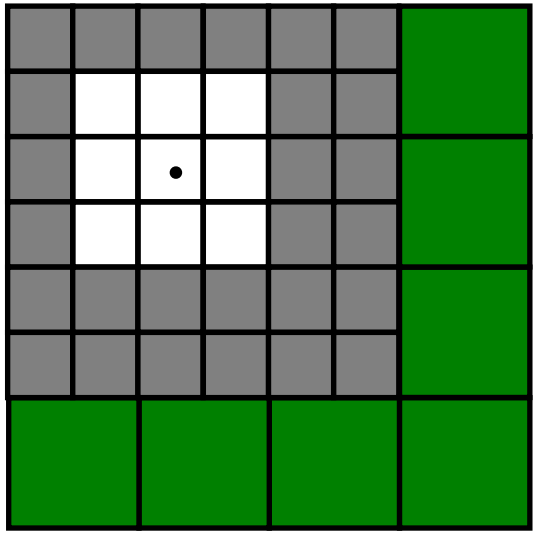
$$\phi' = d_r' \cdot \sqrt{R} \cdot \phi_{m2m} = d_r' \cdot \bar{\phi}_{m2m}$$

with $d_r' = \sqrt{d_x'^2 + d_y'^2 + d_z'^2}$,
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

Single Level FMM

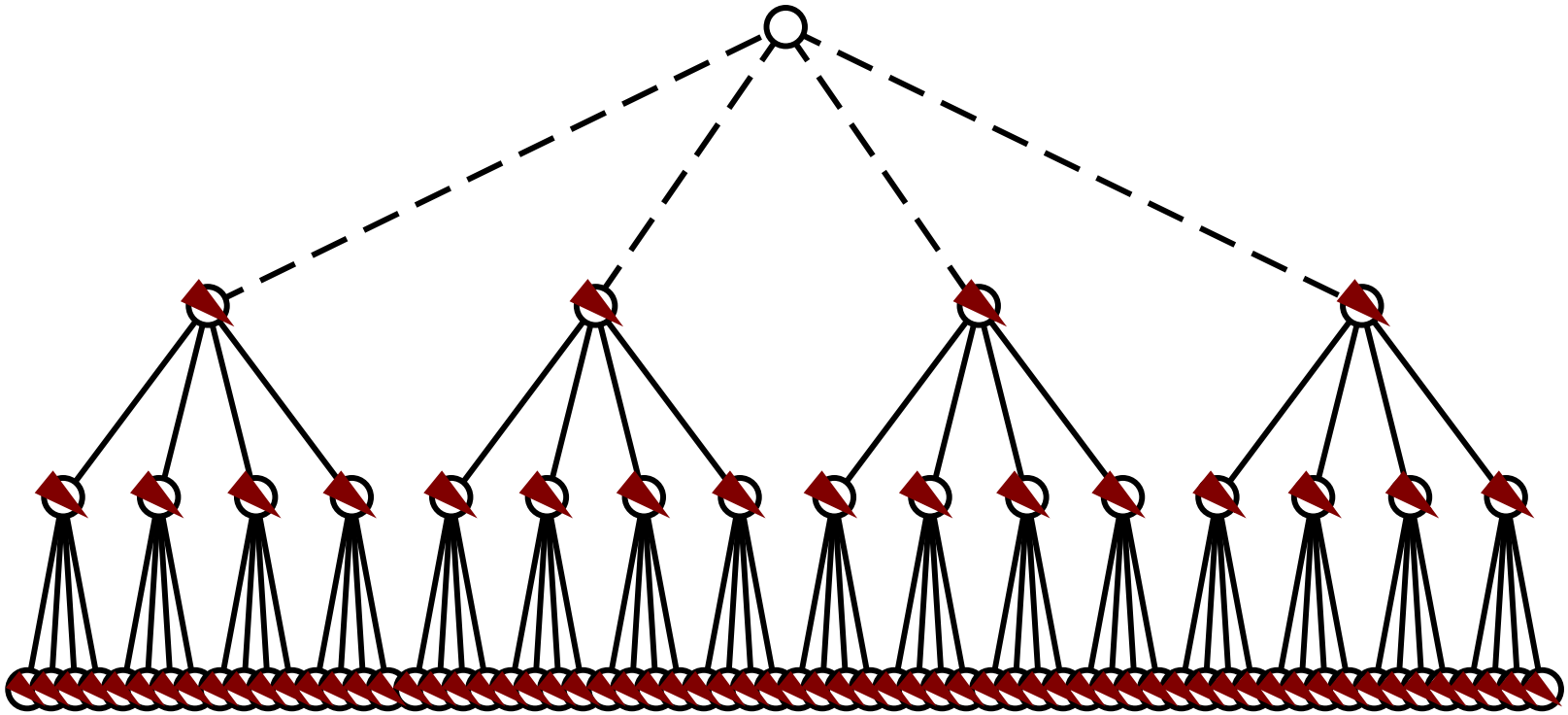


Near region
Far region



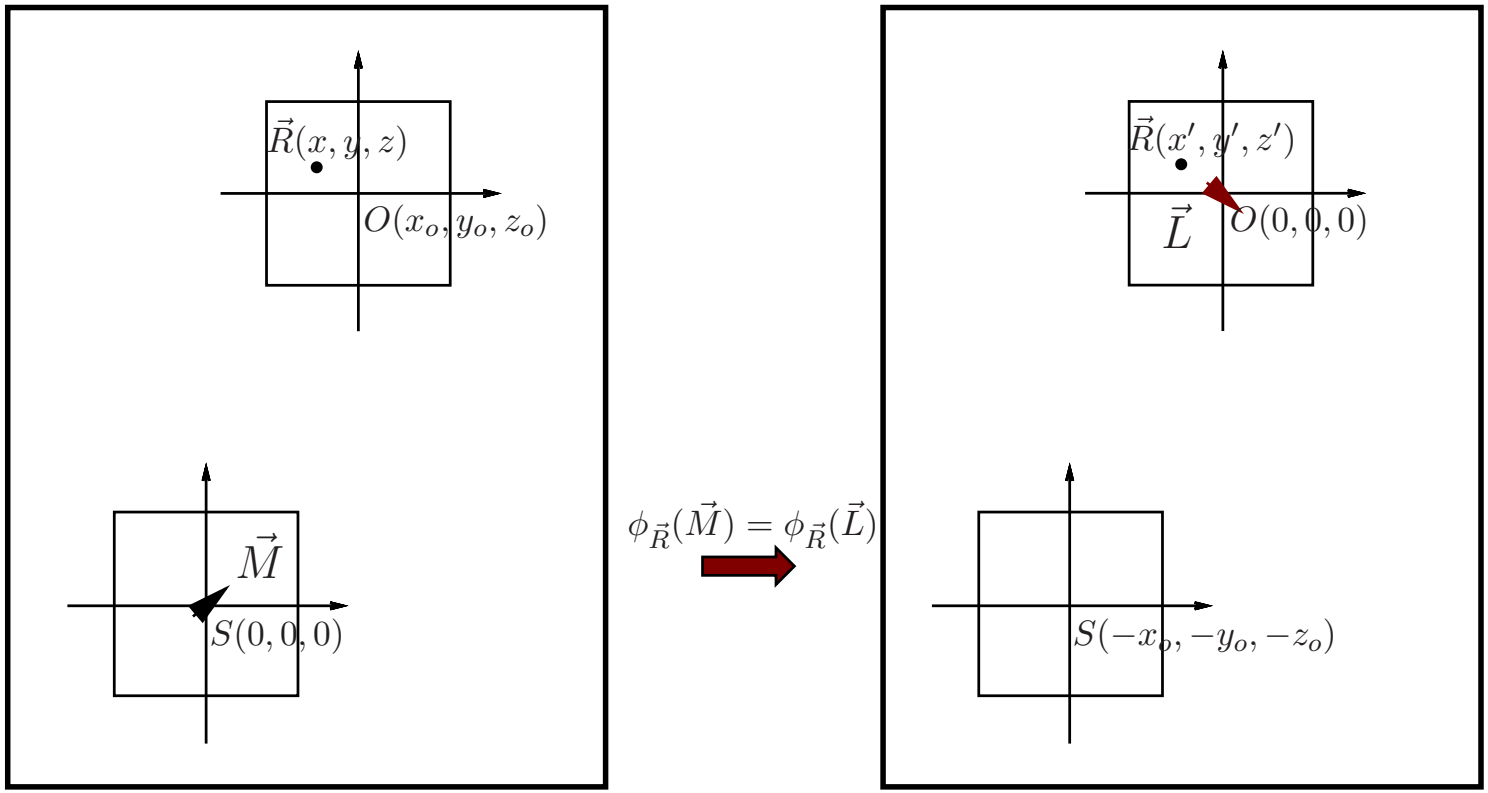
Near region
Far region

Single Level FMM



Single Level FMM

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

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

with

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

Single Level FMM

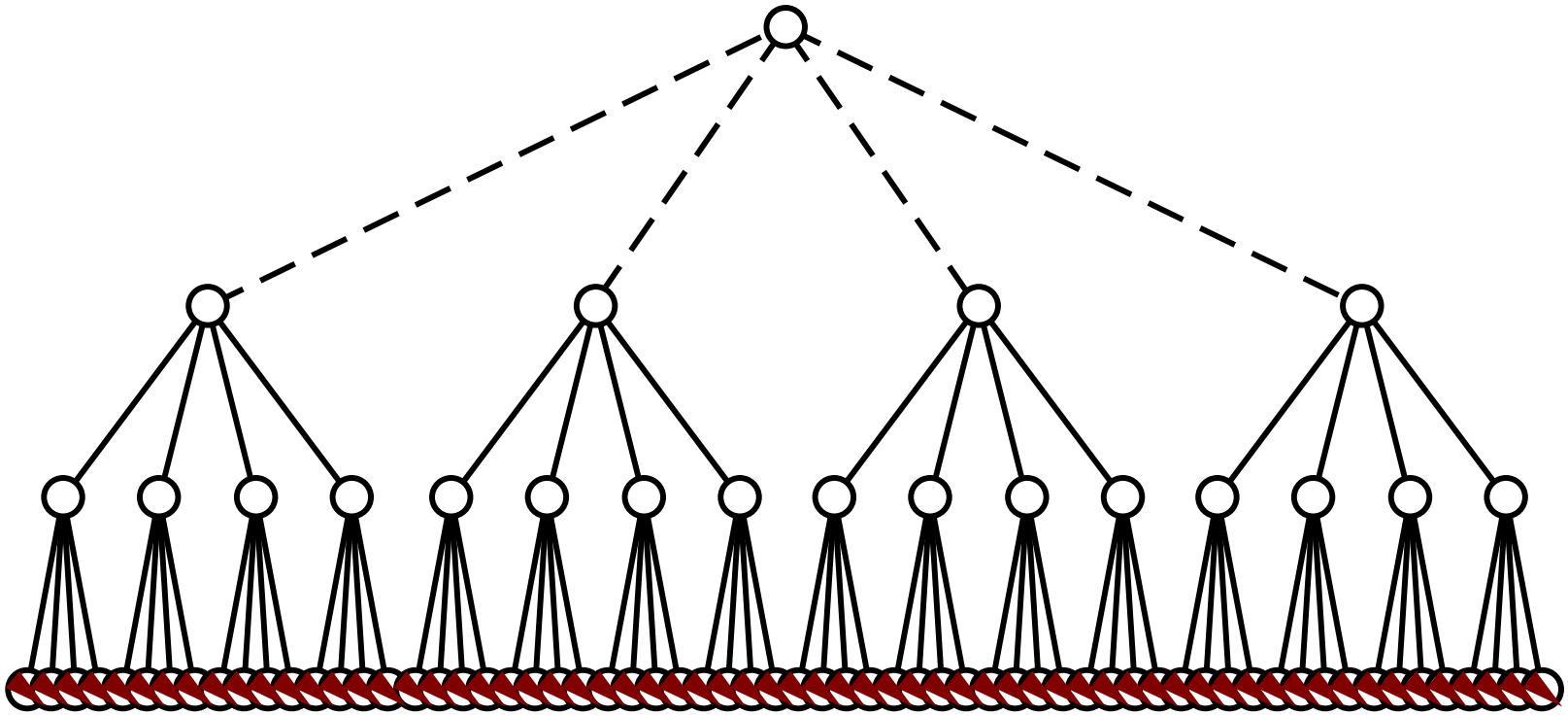
The multipole expansion in the source frame $\phi = d_r \cdot \bar{\phi}$
The local expansion in the observer frame

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

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

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

Single Level FMM



DA variables in the child box frame

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

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.

Single Level FMM

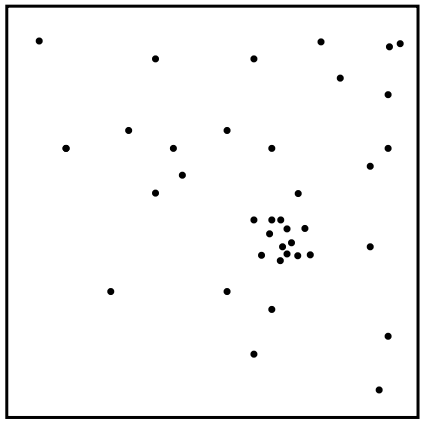
- Now we have the potential expressed as a polynomial of coordinates up to order p.
- Take the derivative of the coordinates to get the field expression in a polynomial of coordinates up to order $p-1$.
- Submit the charge positions into the expression to calculate the potential/field.

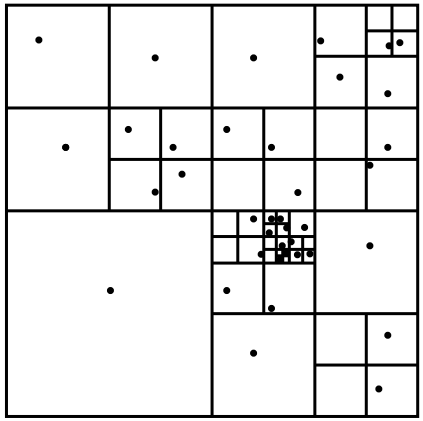
Single Level FMM

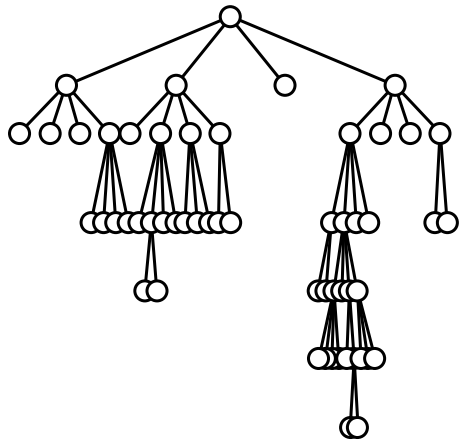
Description of the single level FMM

- Tree construction. Include all the charges in a box, then cut the box into small boxes until each childless box includes less than s charged particles. Thus we get a hierarchical tree structure of boxes.
- Upwards. Calculate the multipole expansion of childless boxes from charges, and then calculate the multipole expansion of parent boxes from child boxes.
- Downwards. For each box, calculate the local expansion from the multipole expansions in the interaction list. Then translate the local expansion of parent boxes into child boxes.
- Potential/Field calculation. For each childless boxes, calculate the far region field from the local expansion, and calculate the near region field directly by Coulomb theorem. Take the summation.

MLFMA



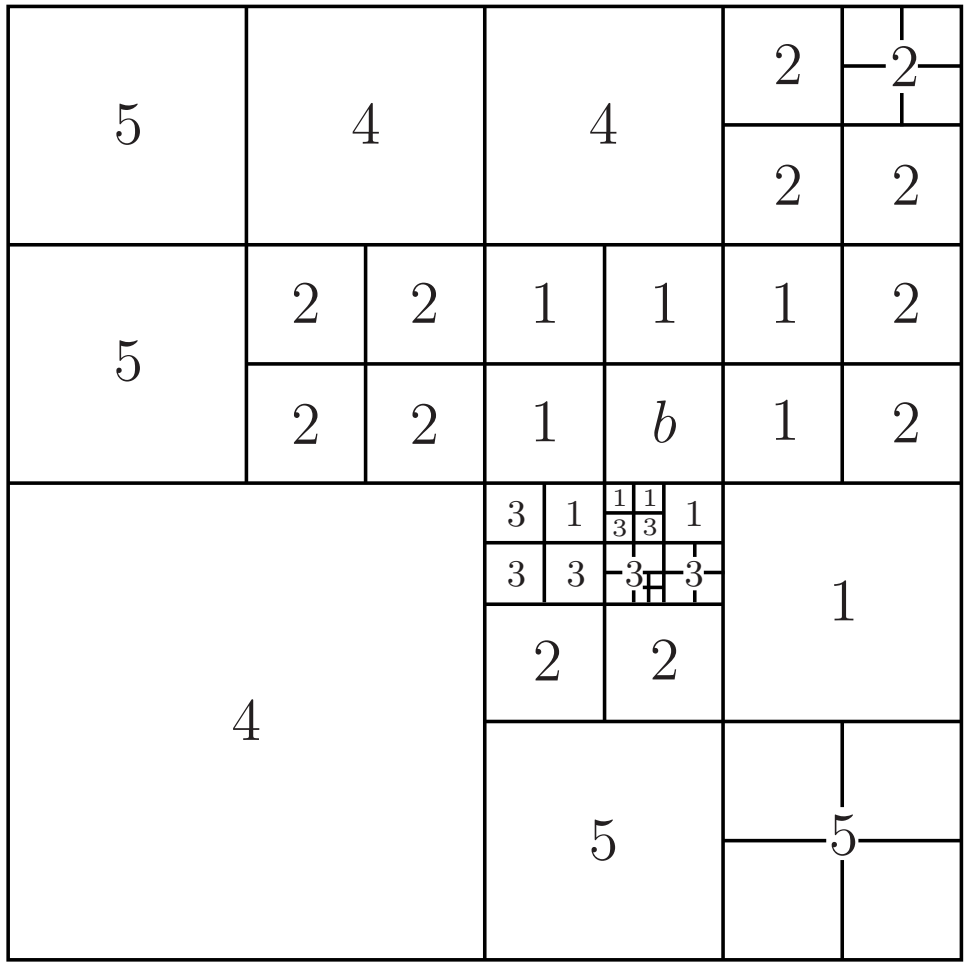




Define:

parent boxes, child boxes, childless boxes, colleagues

- List 1, (U_b) Empty if b is a parent box. All the childless boxes adjacent to b and b itself if b is a childless box.
- List 2, (V_b) All the child boxes of the colleagues of b's parent box that are well separated to b.
- List 3, (W_b) Empty if b is a parent box. All the descent of b's colleagues that are not adjacent to b.
- List 4, (X_b) All the boxes whose list 3 contains b.



- List 5, (Y_b) All the other boxes. (All the boxes that are well separated from b's parent.)

Considering two boxes b and c, operations according to their relations.

Relations		Operations
$c \in U_b$	$b \in U_c$	$C_c \to C_b$, $C_b \to C_c$
$c \in V_b$	$b \in V_c$	$M_c \to L_b$, $M_b \to L_c$
$c \in W_b$	$b \in X_c$	$M_c \to C_b$, $C_b \to L_c$
$c \in X_b$	$b \in W_c$	$C_c \to L_b$, $M_b \to C_c$
$c \in Y_b$	$b \in Y_c$	Do nothing

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

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

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

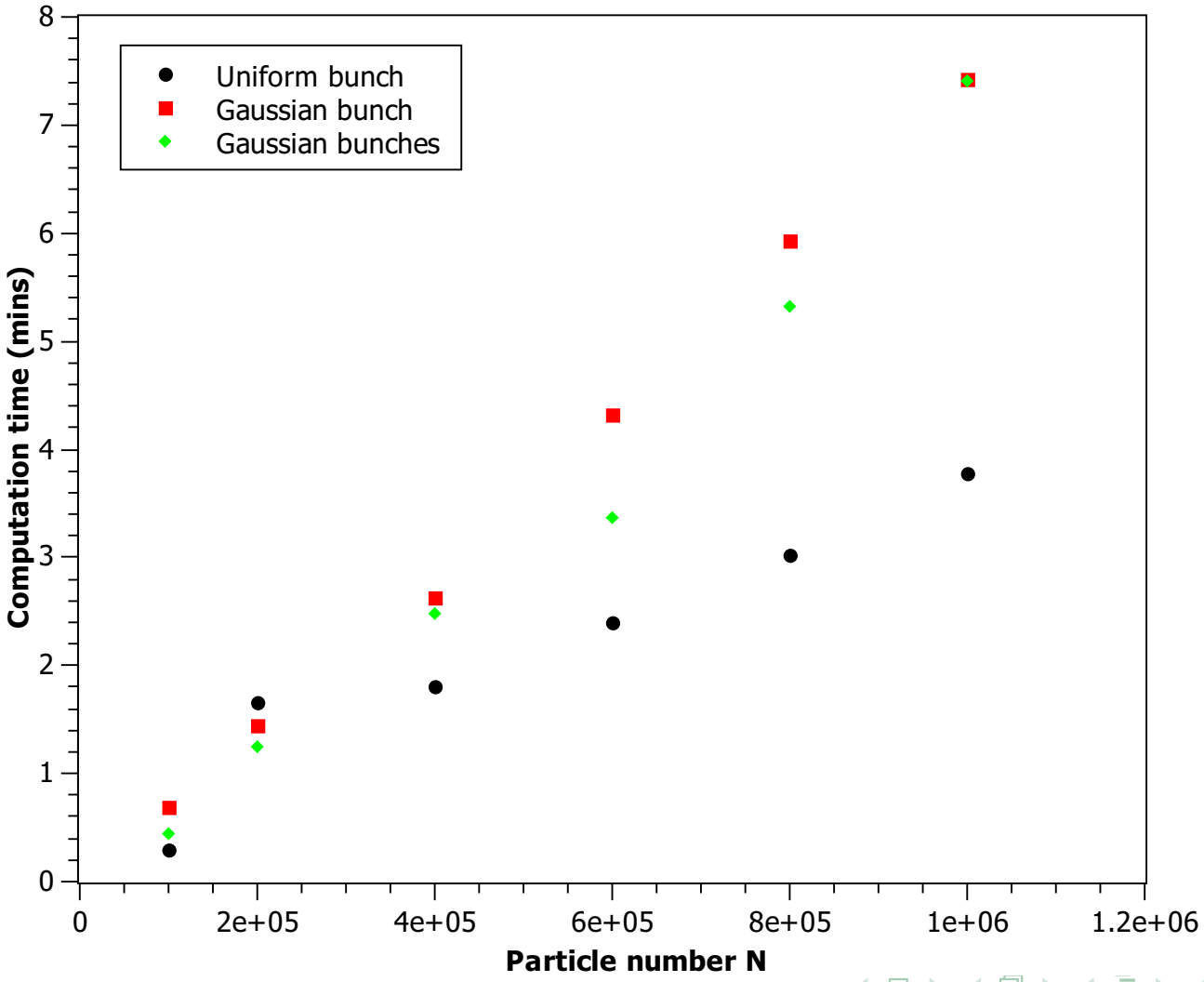
$$
\begin{aligned}
E_x &= \{-\frac{\partial\bar{\phi}}{\partial d_x}\cdot(d_r^2 - 2d_x^2) + 2\frac{\partial\bar{\phi}}{\partial d_y}\cdot d_x d_y + 2\frac{\partial\bar{\phi}}{\partial d_z}\cdot d_x d_z + \bar{\phi}\cdot d_x\}\cdot d_r \\
E_y &= \{2\frac{\partial\bar{\phi}}{\partial d_x}\cdot d_y d_x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

with

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

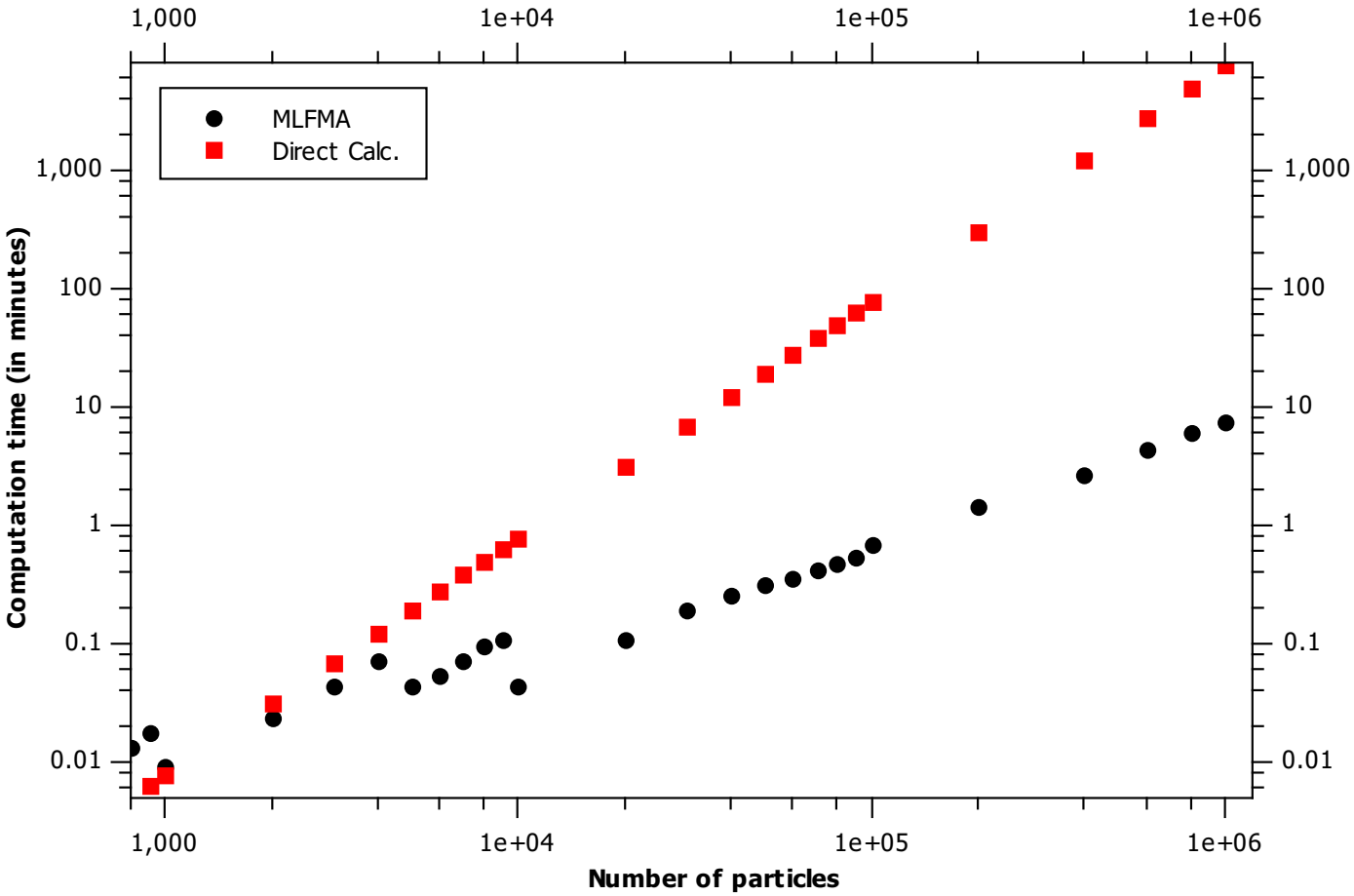
Numerical experiments

Computation time for different charge distribution



Numerical experiments

Compare the MLFMA with direct calculation



Numerical experiments

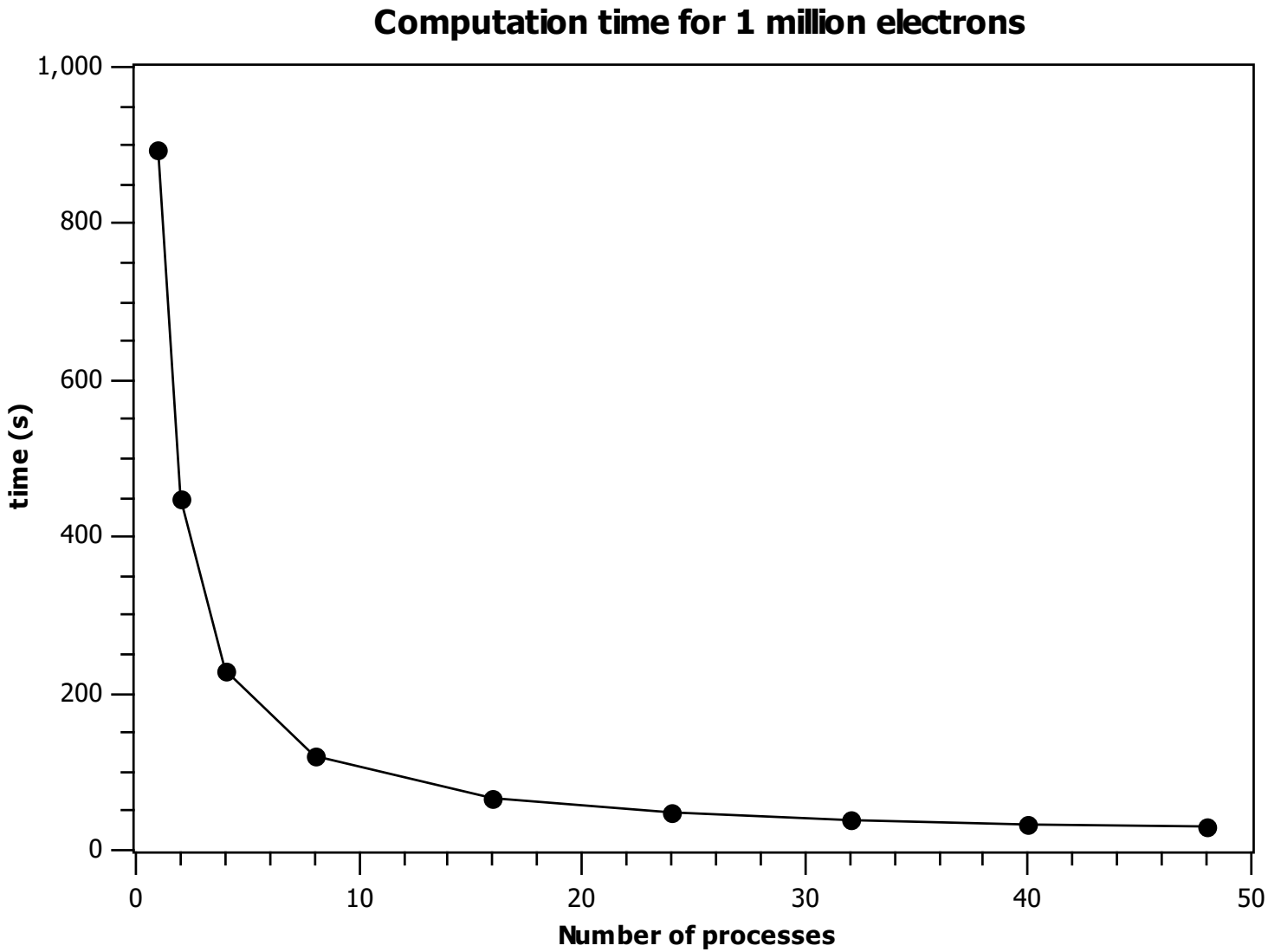


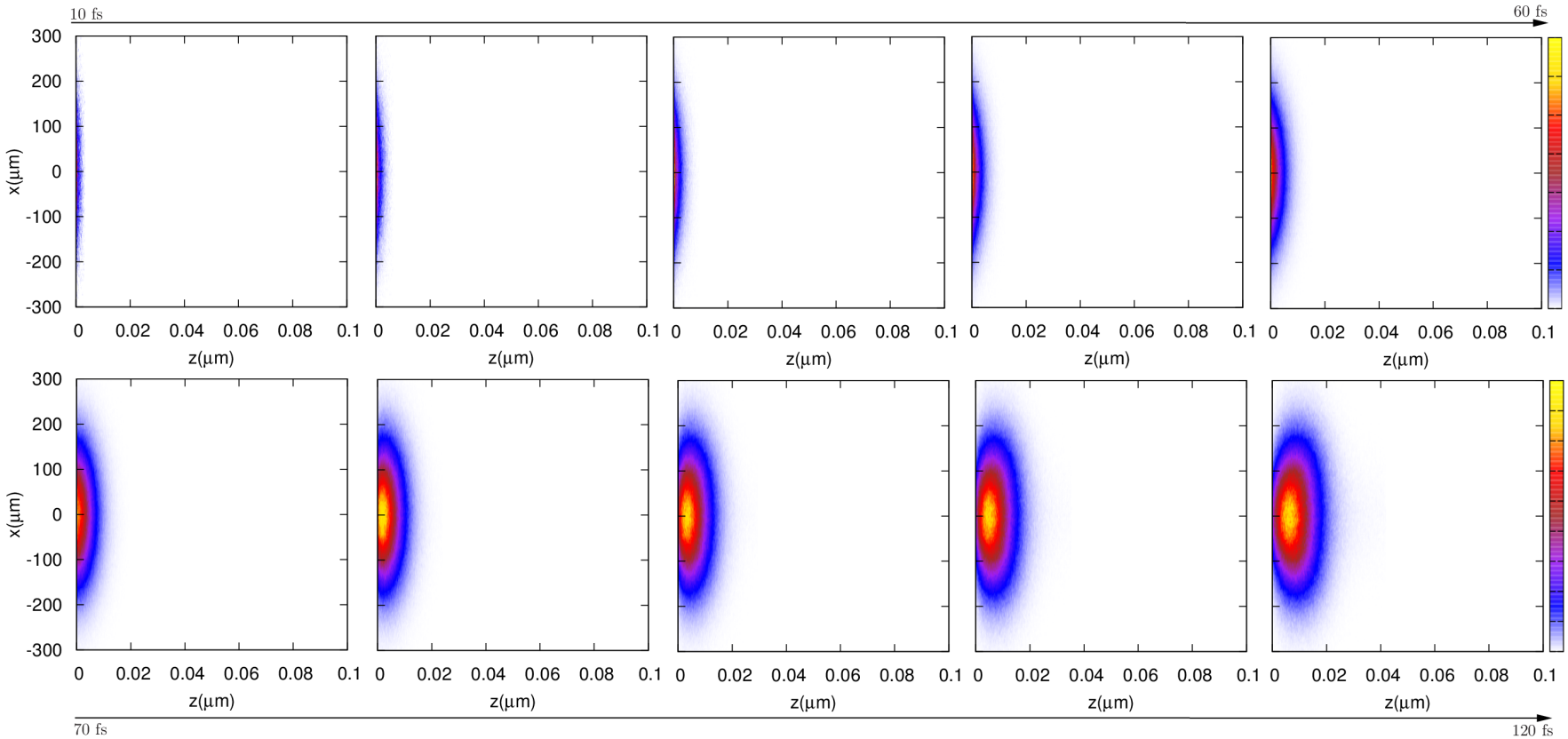
Photo emission process

Assumptions

- Gaussian (FWHM = 50 fs) profile laser pulse applied on a surface, $E_{ph} = 4.65$ eV
- Originally electrons have Fermi energy ($E_f = 5$ eV), and they starts to move after getting energy from photons
- To overcome the work function ($W = 4.45$ eV), only those electrons inside a velocity cone can come out of the surface
- 200 million electrons come out, represented by 2 million macro-particles

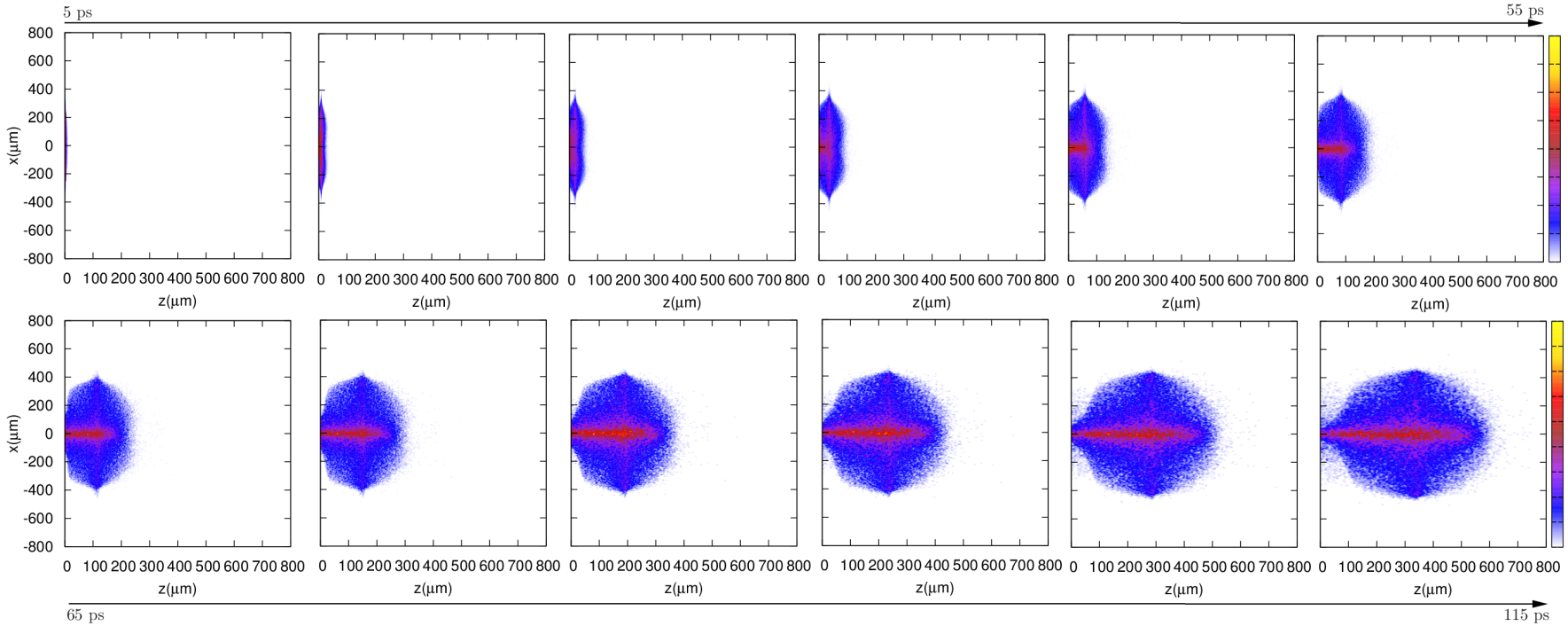
Simulation

During the first 120 fs, a Gaussian laser pulse is applied on the surface.
A constant extracting field of 2kV/m helps the electrons to go out.
Electrons are generated and accumulated, and the bunch is formed.



Simulation

The electron bunch evolves in the following 115 ps.
Some electrons go back into the surface due to the space charge field and the image charge field.
Finally the bunch starts to leave the surface.



Conlusion

The Multiple Level Fast Multipole Algorithm

- Works for any arbitrary charge distribution
- Calculate both the potential/field and its derivatives
- Scales linearly with the number of particles
- Grid-free, good for complicated geometry

Future work

- Include the space charge effect inside a transfer map
- Include boundary conditions
- Apply it in beam dynamic simulations

THANK YOU!