

# The Fast Multipole Method in the Differential Algebra Framework for Space Charge Field Calculation

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- Introduction of the fast multipole method (FMM)
- Multiple level fast multipole algorithm (MLFMA) in the differential algebra framework
- Numerical experiment results

## I. INTRODUCTION

Most algorithm in beam community follows 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

- Include the charged region with a box, then cut the box into small boxes.
- For each box (and the charges inside), different relations with other boxes, result in different treatments.
- For each box (charges inside), the contribution from the boxes **attached** is calculated directly.
- For each box, the contribution for the boxes **separated** can be expressed by multipole expansions or local expansions.  
(**box-box relation**,  $O(N)$ .)

## II. Multiple Level Fast Multipole Algorithm in DA framework

Two operations in COSY:

- Automatic Taylor expansion of a function

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

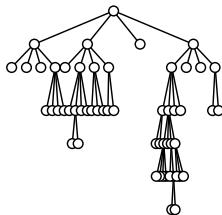
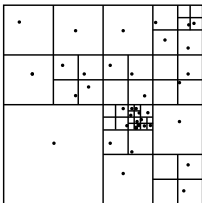
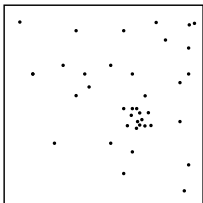
In COSY,

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

- 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.



Define:

parent boxes, child boxes, childless boxes, colleagues



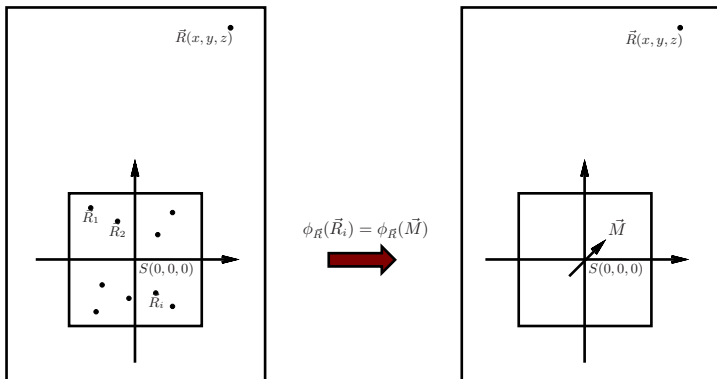
- **List 1**, ( $U_b$ ) Empty if  $b$  is a parent box. All the childless boxes adjacent to  $b$  and  $b$  itself if  $b$  is a childless box.
- **List 2**, ( $V_b$ ) All the child boxes of the colleagues of  $b$ 's parent box that are well separated to  $b$ .
- **List 3**, ( $W_b$ ) Empty if  $b$  is a parent box. All the descents descendants 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.)

5	4		4		2	2	
					2	2	
5	2	2	1	1	1	2	
	2	2	1	$b$	1	2	
4				3	1	1	1
				3	3	3	
				2	2		
				4		5	

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

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

Multipole expansion from charges (for the childless boxes)



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

with

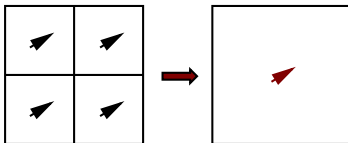
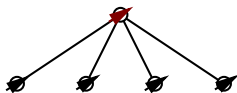
$$d_x = \frac{x}{x^2 + y^2 + z^2}, \quad d_y = \frac{y}{x^2 + y^2 + z^2},$$

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

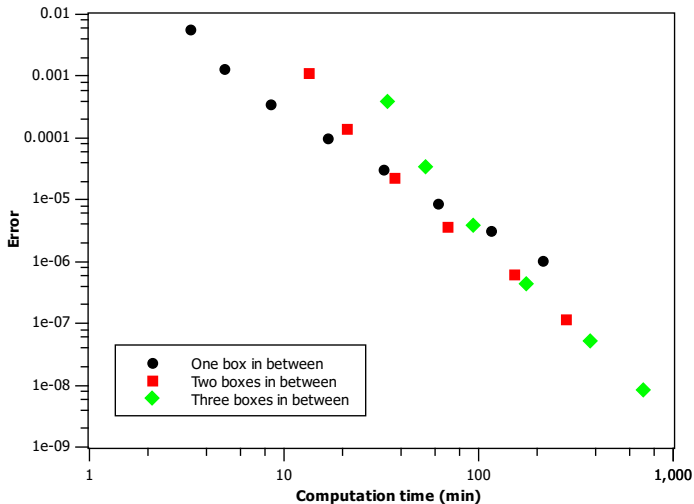
$$\bar{\phi}_{c2m} = \sum_{i=1}^n \left\{ q_i / \sqrt{1 + (x_i^2 + y_i^2 + z_i^2)d_r^2 - 2x_i d_x - 2y_i d_y - 2z_i d_z} \right\}.$$

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

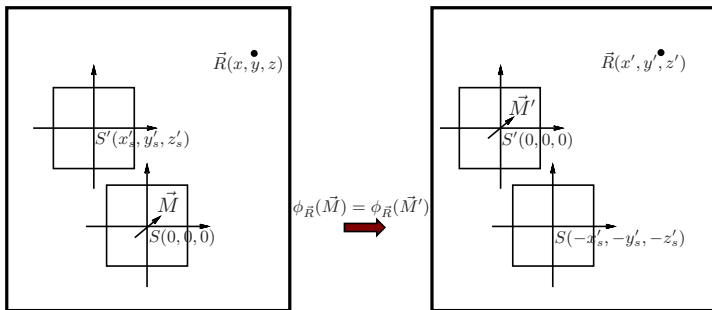
Multipole expansions for the parent boxes



## Accuracy and computation time



Translate the position of a multipole expansion



In parent box frame, new DA variables are chosen as

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

$$d'_z = \frac{z - z'_o}{r'^2} = \frac{z'}{r'^2},$$

Relation between the old and new DA variables.

$$d_x = (d'_x + x'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R,$$

$$d_y = (d'_y + y'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R,$$

$$d_z = (d'_z + z'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R,$$

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  $\phi = \underline{d}_r \cdot \bar{\phi}_{c2m}$

In the parent box frame

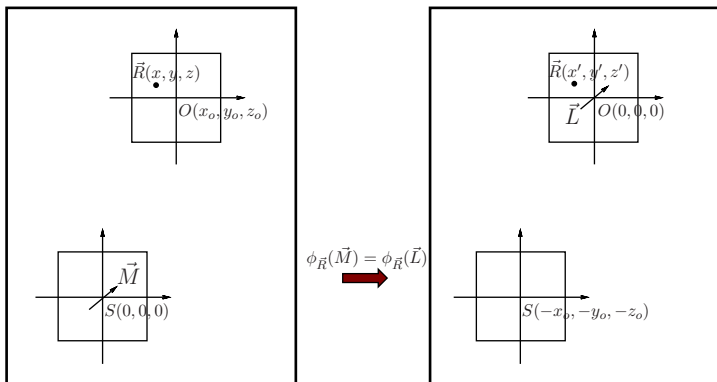
$$\phi' = \underline{d}'_r \cdot \sqrt{R} \cdot \phi_{m2m} = \underline{d}'_r \cdot \bar{\phi}_{m2m}$$

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

Convert a multipole expansion into a local expansion



New DA variables in the observer frame

$$d'_x = x - x'_o = x',$$

$$d'_y = y - y'_o = y',$$

$$d'_z = z - z'_o = z'.$$

The relation between the new and the old DA variables

$$d_x = (x'_o + d'_x) \cdot R,$$

$$d_y = (y'_o + d'_y) \cdot R,$$

$$d_z = (z'_o + d'_z) \cdot R.$$

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

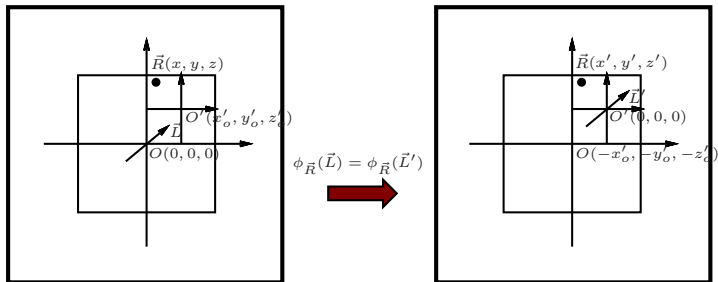
$$\phi = \sqrt{R} \cdot \bar{\phi}_{m2l} = \phi_{m2l}$$

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

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

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



DA variables in the child box frame

$$d_x = x'_o + d'_x,$$

$$d_y = y'_o + d'_y,$$

$$d_z = z'_o + d'_z.$$

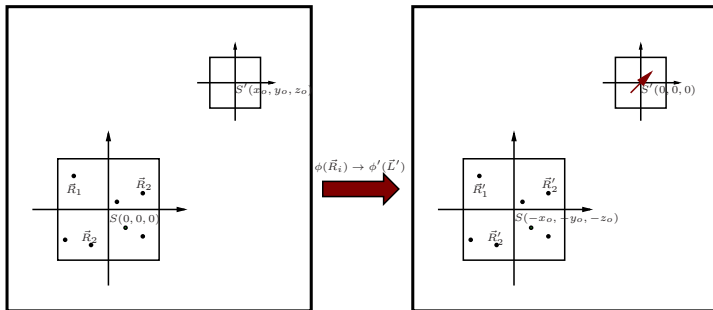
The local expansion in the parent box frame is  $\phi_{m2l}$ .

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

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

Error

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



- 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

$$E_x = \left\{ -\frac{\partial \bar{\phi}}{\partial d_x} \cdot (d_r^2 - 2d_x^2) + 2\frac{\partial \bar{\phi}}{\partial d_y} \cdot d_x d_y + 2\frac{\partial \bar{\phi}}{\partial d_z} \cdot d_x d_z + \bar{\phi} \cdot d_x \right\} \cdot d_r$$

$$E_y = \left\{ 2\frac{\partial \bar{\phi}}{\partial d_x} \cdot d_y d_x - \frac{\partial \bar{\phi}}{\partial d_y} (d_r^2 - 2d_y^2) + 2\frac{\partial \bar{\phi}}{\partial d_z} \cdot d_y d_z + \bar{\phi} \cdot d_y \right\} \cdot d_r$$

$$E_z = \left\{ 2\frac{\partial \bar{\phi}}{\partial d_x} \cdot d_z d_x + 2\frac{\partial \bar{\phi}}{\partial d_y} \cdot d_z d_y - \frac{\partial \bar{\phi}}{\partial d_z} \cdot (d_r^2 - d_z^2) + \bar{\phi} \cdot d_z \right\} \cdot d_r$$

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.

DA representation

$$f(x + da(1)) \rightarrow f(x) + f'(x)da(1) + \frac{1}{2!}f''(x)da(1)^2 + \cdots + \frac{1}{n!}f^n(x)da(1)^n$$

TM representation

$$f(x + tm(1)) \rightarrow (f(x) + f'(x)tm(1) + \frac{1}{2!}f''(x)tm(1)^2 + \cdots + \frac{1}{n!}f^n(x)tm(1)^n, I)$$

$$\rightarrow (TM_f, I)$$

with  $f(x) - TM_f(x) \in I$

Expansions

$$\vec{M} = d_r \cdot \phi_{da} \rightarrow \vec{M} = d_r \cdot (\phi_{tm}, I)$$

$$\vec{L} = \phi_{da} \rightarrow \vec{L} = (\phi_{tm}, I)$$

## III. Numerical experiments

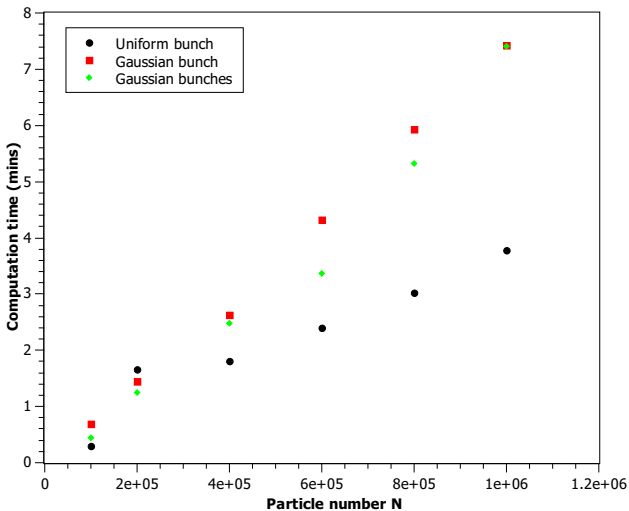




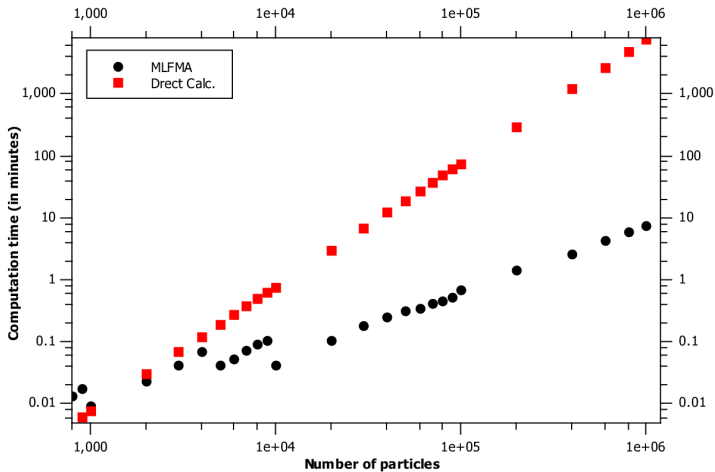




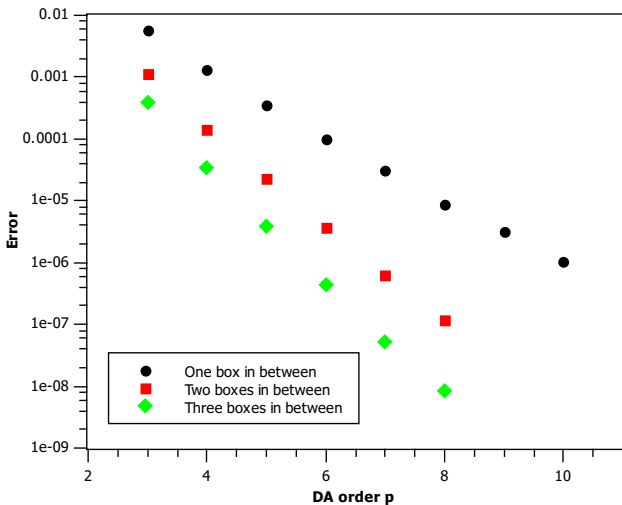
## Computation time for different charge distribution



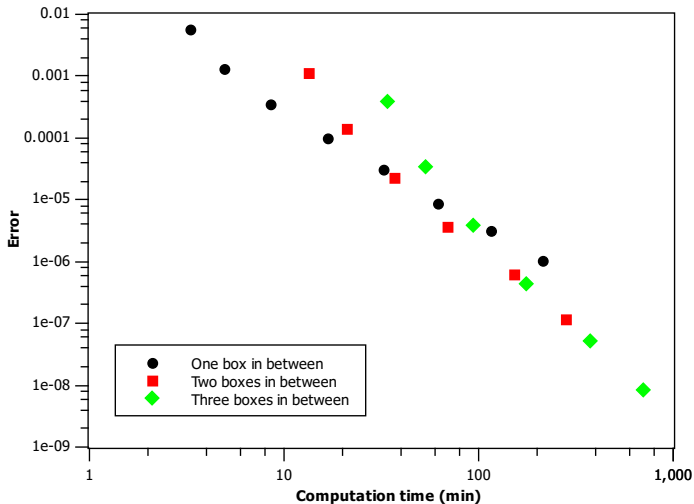
## Compare the MLFMA with direct calculation



Accuracy increases with DA order



## Accuracy and computation time



## Computation time for 1 million electrons

