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

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Outline

- 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), the whole region can be divided into the near region and the far region to the box.
- For each box (charges inside), the contribution from the boxes (charges) in its near region is calculated directly.
- For each box, its far region is where we can play tricks and gain efficiency!

Strategy of FMM

Tree code, Barnes-Hut

- For any box, its field in its far region can be expressed by a multipole expansion. (box-particle relation, $O(N \log N)$.)
- Multipole expansion in source box can be converted into local expansion in observer box.(box-box relation, $O(N)$.) FMM
- For each box, the field contributed from the far region boxes (charges) can be calculated from the local expansion.
- For each box, the total field is the summation of the near region part and the far region part.

II. Multiple Level Fast Multipole Algorithm in DA framework

Two operations in COSY:

- Automatic Taylor expansion of a function

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

In COSY,

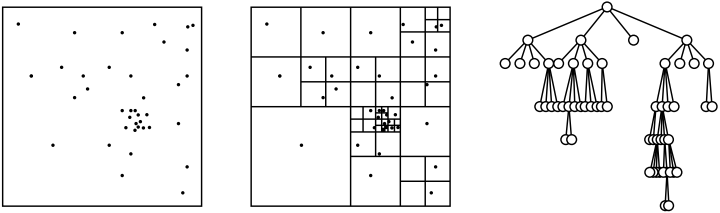
$$f(x+\boxed{da(1)}) = f(x) + f^{'}(x)da(1) + \frac{1}{2!}f^{''}(x)da(1)^2 + \frac{1}{3!}f^{'''}(x)da(1)^3 + \ldots$$

- Composition of two maps

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

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

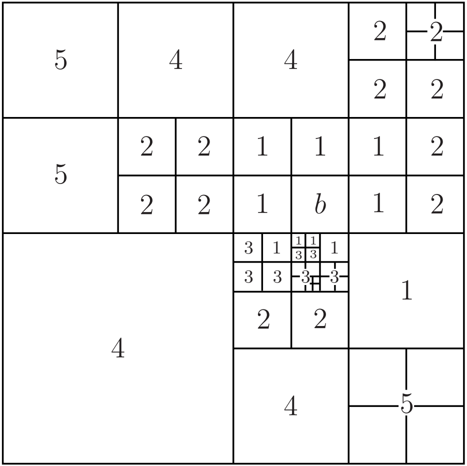
MLFMA



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 descents descendants of b's colleagues that are not adjacent to b.
- List 4, (X_b) All the boxes whose list 3 contains b.

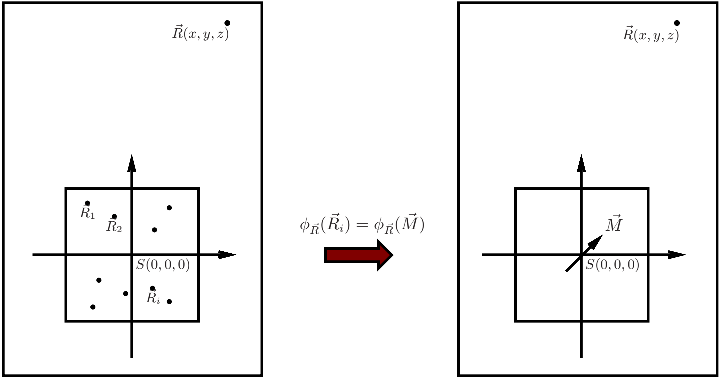


- List 5, (Y_b) All the other boxes. (All the boxes that are well separated from b's parent.)

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

Multipole expansion from charges (for the childless boxes)



MLFMA

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

with

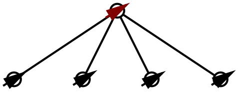
$$d_x = \frac{x}{x^2+y^2+z^2}, \quad d_y = \frac{y}{x^2+y^2+z^2},$$

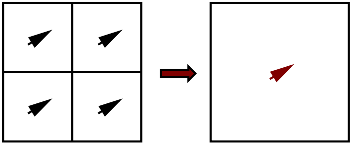
$$d_z = \frac{z}{x^2+y^2+z^2}, \quad d_r = \sqrt{d_x^2+d_y^2+d_z^2},$$

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

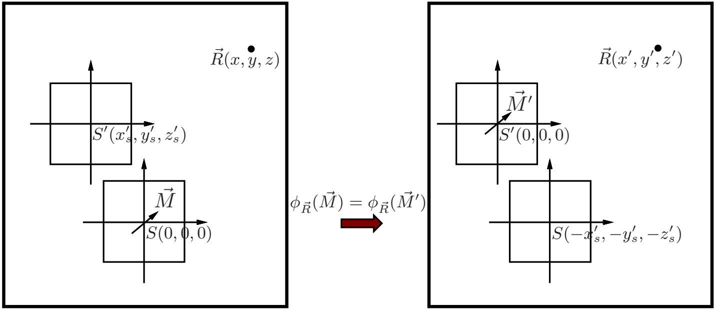
Error $\quad |\epsilon| \leqq C \cdot \left(\frac{a}{r}\right)^{p+1} \cdot \frac{1}{r-a}$, where $C = \sum_{i=1}^{n} |q_i|$ and $r_i \leq a$ for any i.

Multipole expansions for the parent boxes





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.

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

with

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

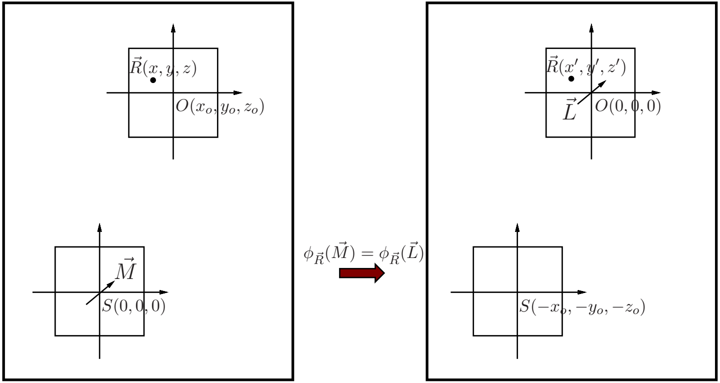
Single Level FMM

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

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

The relation between the new and the old DA variables

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

with

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

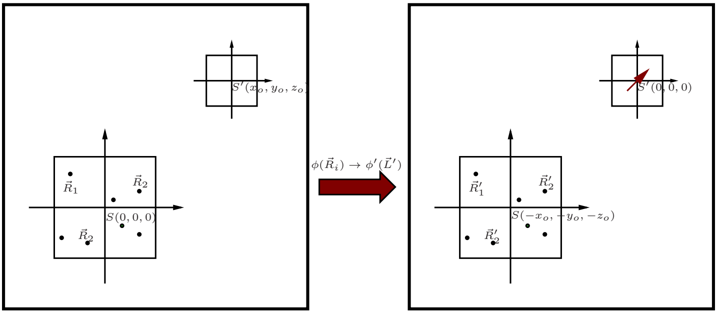
The multipole expansion in the source frame $\phi = \boxed{d_r} \cdot \boxed{\bar{\phi}}$
The local expansion in the observer frame

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

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

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

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

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

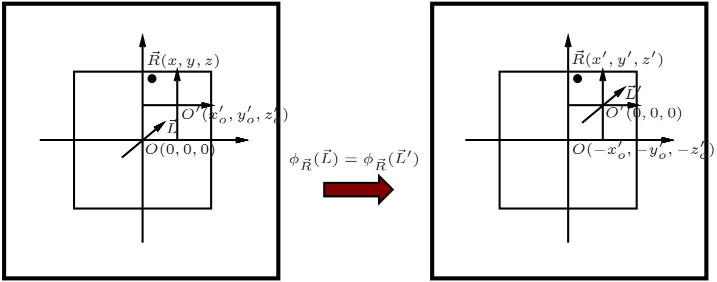
Calculate the field from the multipole expansion.
The multipole expansion is $\phi = d_r \cdot \bar{\phi}$, then

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

with

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

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



DA variables in the child box frame

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

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.

- 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.

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

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

TM representation

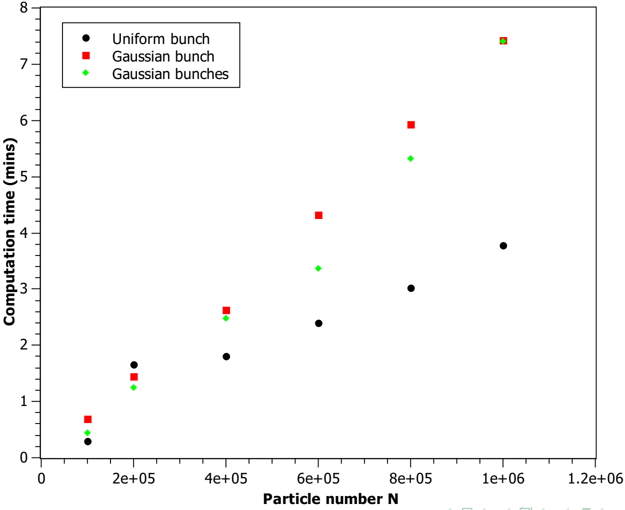
$$\begin{aligned} f(x+\boxed{tm(1)}) &\to (f(x)+f^{'}(x)tm(1)+\frac{1}{2!}f^{''}(x)tm(1)^2+\cdots+\frac{1}{n!}f^{n}(x)tm(1)^n,\boxed{I}) \\ &\to (TM_f, I) \\ \text{with} \quad & f(x)-TM_f(x)\in I \end{aligned}$$

Expansions

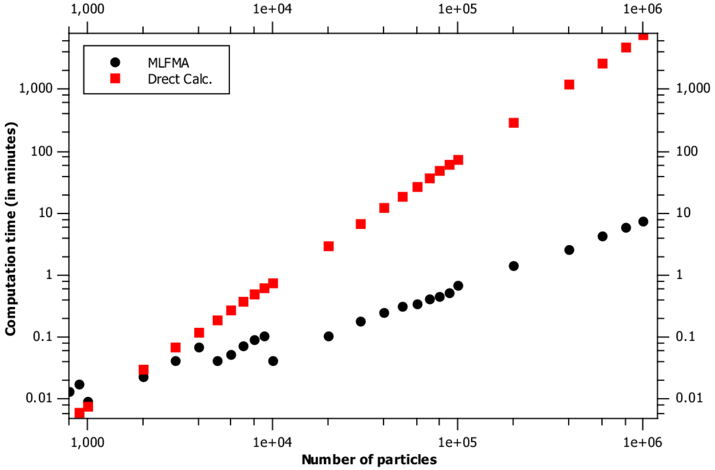
$$\begin{aligned} \vec{M} = d_r\cdot\phi_{\mathrm{da}} &\to \vec{M} = d_r\cdot(\phi_{\mathrm{tm}}, I) \\ \vec{L} = \phi_{\mathrm{da}} &\to \vec{L} = (\phi_{\mathrm{tm}}, I) \end{aligned}$$

III. Numerical experiments

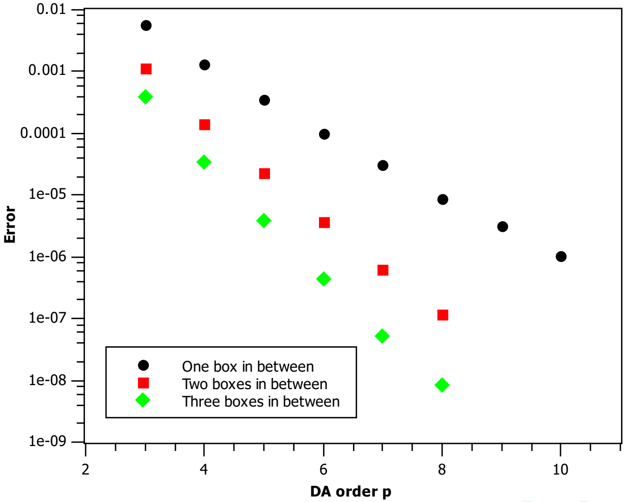
Computation time for different charge distribution



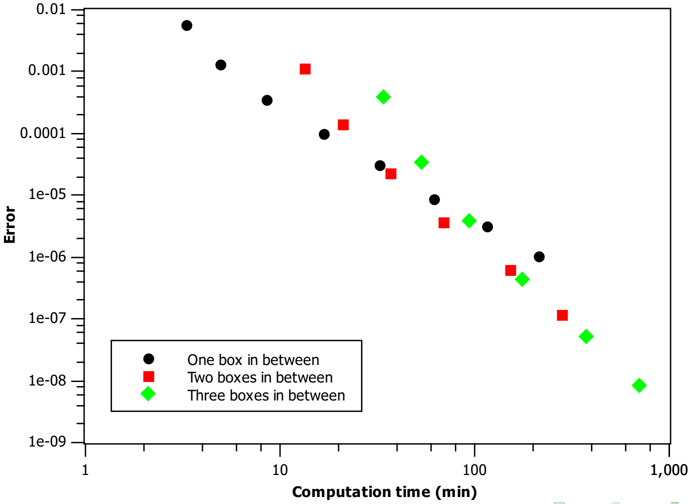
Compare the MLFMA with direct calculation



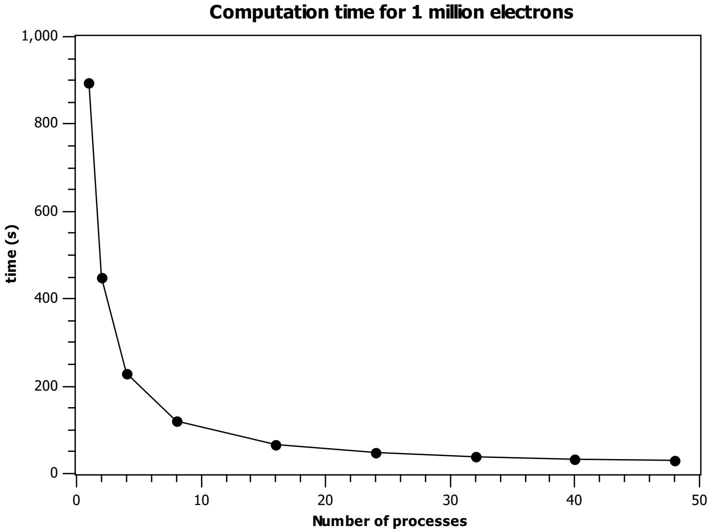
Accuracy increases with DA order



Accuracy and computation time



Numerical experiments



Summary and Future work

Summary

- Combined the FMM with DA for a new algorithm, sacles with $O(N)$.
- MLFMA works for arbitrary charge distribution.
- Parrallel MLFMA, 10 million MSU HPC np=90, p=5, t=167s.

Future work

- Keep polishing the algorithm.
- Boundary conditions.
- TM version for rigorous calculation.
- Map method.
- Simulation.

THANK YOU!