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

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Dec. 8th, 2011 Jefferson Lab
Introduction of the fast multipole method (FMM)

Single level fast multipole method in the differential algebra (DA) framework

Multiple level fast multipole algorithm (MLFMA) in the differential algebra framework

Parallel multiple level fast multipole algorithm in the differential algebra framework

Numerical experiment results
I. INTRODUCTION
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!
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, $O(N)$.)

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. Single Level FMM in DA framework
Two operations in COSY:

- Automatic Taylor expansion of a function

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

In COSY,

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

- 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.
Hierarchical tree structure
Near region and Far region

First Level

Second Level
- Near region (neighbors)
- Far region
Multipole expansion from charges (for the childless boxes)
Single Level FMM

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

with

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

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

Error

\[
|\epsilon| \leq C \cdot \left( \frac{a}{r} \right)^{p+1} \cdot \frac{1}{r-a}, \quad \text{where} \quad C = \sum_{i=1}^{n} |q_i| \quad \text{and} \quad r_i \leq a \quad \text{for any} \quad i.
\]
Single Level FMM

Multipole expansions for the parent boxes
Translate the position of a multipole expansion

\[ \vec{M}_S(0, 0, 0) \rightarrow \vec{M}'_{S'}(x'_s, y'_s, z'_s) \]

\[ \vec{R}(x, y, z) \rightarrow \vec{R}(x', y', z') \]

\[ \phi_{\vec{R}}(\vec{M}) = \phi_{\vec{R}}(\vec{M}') \]
In parent box frame, new DA variables are chosen as

\[
d'_x = \frac{x - x'_o}{r'^2} = \frac{x'}{r'^2}, \quad d'_y = \frac{y - y'_o}{r'^2} = \frac{y'}{r'^2}, \quad d'_z = \frac{z - z'_o}{r'^2} = \frac{z'}{r'^2},
\]

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

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.
Interaction list

- Single Level FMM
- Interaction list
- Already calculated

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Convert a multipole expansion into a local expansion

\[ \vec{R}(x, y, z) \]
\[ O(x_o, y_o, z_o) \]
\[ \vec{M} \]
\[ S(0, 0, 0) \]

\[ \phi_{\vec{R}}(\vec{M}) = \phi_{\vec{R}}(\vec{L}) \]

\[ \vec{R}(x', y', z') \]
\[ O(0, 0, 0) \]
\[ \vec{L} \]
\[ S(-x_o, -y_o, -z_o) \]
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

\[
dx = (x'_o + d'_x) \cdot R,
\]
\[
dy = (y'_o + d'_y) \cdot R,
\]
\[
dz = (z'_o + d'_z) \cdot R.
\]

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 $\phi = d_r \cdot \vec{\phi}$.

The local expansion in the observer frame

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

where $\sqrt{R}$ is converted from $d_r, \vec{\phi}_{m2l} = \vec{\phi} \circ M_{m2l}$, 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

\[ \phi_{\vec{R}}(\vec{L}) = \phi_{\vec{R}}(\vec{L}') \]

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DA variables in the child box frame

\[
\begin{align*}
  d_x &= x'_o + d'_x, \\
  d_y &= y'_o + d'_y, \\
  d_z &= z'_o + d'_z.
\end{align*}
\]

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.
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 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.
Efficiency scales with $O(N)$
III. MULTIPLE LEVEL FAST MULTIPOLe ALGORITHM
• Single Level FMM works well for uniform charge distribution.
• How about a distribution far away from uniform?
• **Multiple Level Fast Multiple Algorithm** (MLFMA) works for arbitrary charge distribution. J. Carrier, L. Greengard and V. Rokhlin, 1988
• Divide a box into small boxes only when it hold more than $s$ particles.
• Save only the nonempty boxes.
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.

<table>
<thead>
<tr>
<th>Relations</th>
<th>Operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c \in U_b )</td>
<td>( b \in U_c )</td>
</tr>
<tr>
<td>( c \in V_b )</td>
<td>( b \in V_c )</td>
</tr>
<tr>
<td>( c \in W_b )</td>
<td>( b \in X_c )</td>
</tr>
<tr>
<td>( c \in X_b )</td>
<td>( b \in W_c )</td>
</tr>
<tr>
<td>( c \in Y_b )</td>
<td>( b \in Y_c )</td>
</tr>
</tbody>
</table>
Calculate the local expansion from charges.

\[ \vec{R}_1, \vec{R}_2, \vec{R}_2' \]

\[ S(0, 0, 0) \quad S'(x_o, y_o, z_o) \]

\[ \phi(\vec{R}_i) \rightarrow \phi'(\vec{L}') \]
In the observer (small box) frame, the new DA variables are

\[
\begin{align*}
    d'_x & = x - x'_o = x', \\
    d'_y & = y - y'_o = y', \\
    d'_z & = z - z'_o = z'.
\end{align*}
\]

Then the local expansion is

\[
\phi_L = \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2}}
\]

\[
= \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x'_o - x_i + d'_x)^2 + (y'_o - y_i + d'_y)^2 + (z'_o - z_i + d'_z)^2}}
\]

Error

\[
|\epsilon| \leq C \cdot \left( \frac{r'}{b} \right)^{p+1} \cdot \frac{1}{b - r'}
\]
Calculate the field from the multipole expansion.

The multipole expansion is \( \phi = d_r \cdot \bar{\phi} \), then

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

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

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

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.
Numerical results for the uniform distribution bunches

<table>
<thead>
<tr>
<th>$n$</th>
<th>$s$</th>
<th>$p$</th>
<th>$t_M$ (min)</th>
<th>$t_d$ (min)</th>
<th>$Err_1$ ($\times 10^{-4}$)</th>
<th>$Err_2$ ($\times 10^{-4}$)</th>
<th>$Err_3$ ($\times 10^{-4}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e5</td>
<td>400</td>
<td>5</td>
<td>0.292</td>
<td>75.315</td>
<td>1.241</td>
<td>1.388</td>
<td>1.271</td>
</tr>
<tr>
<td>2e5</td>
<td>400</td>
<td>5</td>
<td>1.655</td>
<td>300.030</td>
<td>1.498</td>
<td>1.504</td>
<td>1.498</td>
</tr>
<tr>
<td>4e5</td>
<td>400</td>
<td>5</td>
<td>1.801</td>
<td>$1.205 \times 10^3$</td>
<td>1.482</td>
<td>1.519</td>
<td>1.554</td>
</tr>
<tr>
<td>6e5</td>
<td>400</td>
<td>5</td>
<td>2.395</td>
<td>$2.711 \times 10^3$</td>
<td>1.538</td>
<td>1.550</td>
<td>1.524</td>
</tr>
<tr>
<td>8e5</td>
<td>400</td>
<td>5</td>
<td>3.026</td>
<td>$4.820 \times 10^3$</td>
<td>1.522</td>
<td>1.497</td>
<td>1.537</td>
</tr>
<tr>
<td>1e6</td>
<td>400</td>
<td>5</td>
<td>3.785</td>
<td>$7.532 \times 10^3$</td>
<td>1.520</td>
<td>1.402</td>
<td>1.526</td>
</tr>
</tbody>
</table>
Numerical results for the Gaussian distribution bunches

<table>
<thead>
<tr>
<th>$n$</th>
<th>$s$</th>
<th>$p$</th>
<th>$t_M$ (min)</th>
<th>$t_d$ (min)</th>
<th>$Err_1$ ($\times 10^{-4}$)</th>
<th>$Err_2$ ($\times 10^{-4}$)</th>
<th>$Err_3$ ($\times 10^{-4}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e5</td>
<td>400</td>
<td>5</td>
<td>0.693</td>
<td>75.315</td>
<td>4.074</td>
<td>3.181</td>
<td>3.509</td>
</tr>
<tr>
<td>2e5</td>
<td>400</td>
<td>5</td>
<td>1.448</td>
<td>300.030</td>
<td>4.174</td>
<td>3.260</td>
<td>3.370</td>
</tr>
<tr>
<td>4e5</td>
<td>400</td>
<td>5</td>
<td>2.624</td>
<td>$1.205 \times 10^3$</td>
<td>4.051</td>
<td>3.281</td>
<td>3.509</td>
</tr>
<tr>
<td>6e5</td>
<td>400</td>
<td>5</td>
<td>4.325</td>
<td>$2.711 \times 10^3$</td>
<td>4.189</td>
<td>3.268</td>
<td>3.501</td>
</tr>
<tr>
<td>8e5</td>
<td>400</td>
<td>5</td>
<td>5.932</td>
<td>$4.820 \times 10^3$</td>
<td>4.122</td>
<td>3.307</td>
<td>3.668</td>
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<tr>
<td>1e6</td>
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<td>5</td>
<td>7.420</td>
<td>$7.532 \times 10^3$</td>
<td>3.995</td>
<td>3.200</td>
<td>3.464</td>
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</tbody>
</table>
Numerical results for the Gaussian distribution bunch groups

<table>
<thead>
<tr>
<th>$n$</th>
<th>$s$</th>
<th>$p$</th>
<th>$t_M$ (min)</th>
<th>$t_d$ (min)</th>
<th>$Err_1 \times 10^{-4}$</th>
<th>$Err_2 \times 10^{-4}$</th>
<th>$Err_3 \times 10^{-4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e5</td>
<td>400</td>
<td>5</td>
<td>0.449</td>
<td>75.315</td>
<td>2.864</td>
<td>4.257</td>
<td>3.262</td>
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<tr>
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<td>400</td>
<td>5</td>
<td>1.256</td>
<td>300.030</td>
<td>5.276</td>
<td>4.954</td>
<td>4.040</td>
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<tr>
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<td>2.475</td>
<td>$1.205 \times 10^3$</td>
<td>1.505</td>
<td>3.852</td>
<td>3.124</td>
</tr>
<tr>
<td>6e5</td>
<td>400</td>
<td>5</td>
<td>3.374</td>
<td>$2.711 \times 10^3$</td>
<td>7.115</td>
<td>3.332</td>
<td>3.765</td>
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<tr>
<td>8e5</td>
<td>400</td>
<td>5</td>
<td>5.321</td>
<td>$4.820 \times 10^3$</td>
<td>7.693</td>
<td>4.574</td>
<td>4.163</td>
</tr>
<tr>
<td>1e6</td>
<td>400</td>
<td>5</td>
<td>7.412</td>
<td>$7.532 \times 10^3$</td>
<td>2.972</td>
<td>6.436</td>
<td>3.652</td>
</tr>
</tbody>
</table>
Computation time for different charge distribution

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Compare the MLFMA with direct calculation
Accuracy increases with DA order
Accuracy and computation time

![Graph showing error against computation time with different box configurations.]
IV. PARALLEL MULTIPLE LEVEL FAST MULTIPOLe ALGORITHM
COSY’s MPI support: PLOOP and ALL-to-ALL communication:

\[
PLOOP \ 1 \ NP; \\
STATEMENTS;
\]

\[
ENDPLOOP PMAP; \\
\]

where NP is the number of processes and PMAP is an array whose last dimension is equal to or greater than NP.
Compressed tree, S. Aluru
Build the tree in parallel

- Hold particles
- Find the root box
- Cut the box
- Parent boxes?
- Gather all particles and save them
- Hold particles
- Find the root box
- Cut the box
- Parent boxes?
- Gather all particles and save them

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Distribute the tree

- Processor 1
- Processor 2
- Processor 3
- Processor 4
Calculate the multipole expansions in parallel. Distribute the tree

- \( \vec{M} \) for childless boxes
- UPWARDS \( \vec{M} \) for parent boxes
- Save all \( \vec{M} \) in local MEM

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Calculate the local expansion and potential/field in parallel.

- Action lists for all boxes
  - DOWNWARDS $\vec{L}$ for all boxes
  - Field/Potential Calculation
  - Field/Potential Distribution

- Action lists for all boxes
  - DOWNWARDS $\vec{L}$ for all boxes
  - Field/Potential Calculation
  - Field/Potential Distribution
Description of PMLFMA

- **Construct** the compressed tree structure in parallel.
- **Upward**: Calculate the multipole expansion in parallel.
- **Downward**: Calculate the local expansion in parallel.
- **Calculate the potential/field** in parallel.
- **Distribute the potential/field** to the corresponding process.
Parallel Efficiency

\[ E(N, P) = \frac{1}{P} \frac{T_{\text{seq}}(N)}{T(N, P)}, \quad N = 1,000,000. \]
Bottleneck of the current parallel algorithm: Memory usage!

- Calculate at most 10 million particles now.
- COSY Infinity 9.1 is 32bit program, Fortran 77/90
- Intel Fortran compiler has 2GB memory limit for 32 bit program
- Each process has no more than 2GB memory
- Number of particles and multipole expansions saved in the local memory is limited.

MSU HPC
np=90 p=5
167s
V. NUMERICAL EXAMPLES IN BEAM DYNAMIC SIMULATION
Numerical Examples

Single current loop

1e6 electrons pass through a single current loop

1e6 electrons go through a single current loop
Numerical Examples

Single current loop

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Numerical Examples

Single current loop
Hard edge model of the accelerating field
Numerical Examples

Hard edge model of the accelerating field
Summary

- Combined the FMM with DA for a new algorithm, scales with $O(N)$.
- Single Level FMM works for uniform distribution.
- MLFMA works for arbitrary charge distribution.
- Parallel MLFMA, 10 million.

Future work

- Keep polishing the algorithm.
- Boundary conditions.
- Map method.
- Simulation.
THANK YOU!