Multiple Level Fast Multipole Algorithm in Differential Algebra Frame and Its Prospective Usage in Photoemission Simulation

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- Part 1. The Multiple Level Fast Multipole Algorithm (MLFMA)
- Part 2. Photoemission Model
Basic idea of the Fast Multipole Method

- As to the sources, their effects on the far away observers can be expressed by multipole expansions.
- As to the observers, all the multipole expansions can be converted into the local expansions in the near region of them. The total local expansion includes the effects of all the sources that are far away enough.
- As to the observers, the effects of the nearby sources are calculated directly.
- Both the multipole expansions and the local expansions can be translated and grouped.
- The computation complex is $O(N)$, $N$ is the particle number.
To be more specific ...
The hierarchical structure and the tree.
A few definitions.

- A box is a *parent box* if the algorithm has split it into smaller boxes. Otherwise it is a *childless box*.
- A *child box* is a nonempty box resulting from the direct division of a parent box.
- *Colleagues* are adjacent boxes of the same size (at the same level).
- If two boxes do NOT touch each other, they are *well separated*. 
MLFMA: Relations between the boxes

Five kinds of relations between the boxes.

![Diagram showing five kinds of relations between boxes](image-url)
Five kinds of relations between the 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.)
The algorithm can be described as follows. (Note: The algorithm is described in a way that is easier to understand. The real coding algorithm is different.)

- Selected a number $s$. Any childless box cannot contain more than $s$ particles. Setup the hierarchical structure.

- **Upwards**: From finest level to the coarsest level, for each box $b$ calculate its multipole expansion. If $b$ is childless, calculate the multipole expansion from the charges inside. If $b$ is a parent box, calculate the multipole expansion by shifting the multipole expansions of its children to the center of $b$ and sum up.
**Downwords**: From the coarsest level to the finest level, for each box \( b \) do the following.

1. **\( U_b \)**: Calculate the potential/field from the charges inside the boxes in \( U_b \) directly.
2. **\( V_b \)**: Convert the multipole expansions in \( V_b \) the into local expansions inside \( b \) and sum up.
3. **\( W_b \)**: Calculate the potential/field from the multipole expansions in \( W_b \).
4. **\( X_b \)**: Calculate the local expansion inside \( b \) from the charges inside the boxes in \( X_b \).
5. If possible shift the local expansion of \( b \)'s parent to \( b \) and add it up to the local expansion of \( b \).
6. Calculate the potential/field from the local expansion and add it up to the potential/field on the charges inside \( b \).
Multipole expansion from the charges

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

\[ = \sum_{i=1}^{n} \frac{d_r \cdot q_i}{\sqrt{1 + (x_i^2 + y_i^2 + z_i^2)}d_r^2 - 2x_i d_x - 2y_i d_y - 2z_i d_z} \]

\[ = d_r \cdot \bar{\phi}_M \]

with

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

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

- Map between the old and new DA variables ($M_1$).

  New frame centered at $(x'_o, y'_o, z'_o)$ and the new DA variables are

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

  The map $M_1$ is

  \[
  d_x = (d'_x + x'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R, \\
  d_y = (d'_y + y'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R, \\
  d_z = (d'_z + z'_o \cdot (d'^2_x + d'^2_y + d'^2_z)) \cdot R,
  \]

  with

  \[
  R = \frac{1}{1 + (x'^2 + y'^2 + z'^2)(d'^2_x + d'^2_y + d'^2_z) + 2x'_o d'_x + 2y'_o d'_y + 2z'_o d'_z}.
  \]
Multipole expansion in the new frame

\[ \tilde{\phi}_M = \tilde{\phi}_M \circ M_1, \]

\[
d_r = \frac{1}{\sqrt{(x - x'_o + x'_o)^2 + (y - y'_o + y'_o)^2 + (z - z'_o + z'_o)^2}} \]

\[
d'_r = \frac{d_r'}{\sqrt{1 + (x'_o^2 + y'_o^2 + z'_o^2)d''_r^2 + 2x'_od'_x + 2y'_od'_y + 2z'_od'_z}} \]

\[
d'_r = d'_r \cdot \sqrt{R}, \]

\[
d'_r = \sqrt{d''_x^2 + d''_y^2 + d''_z^2}. \]

then

\[
\phi' = \tilde{\phi}_M \cdot d'_r \cdot \sqrt{R} = d'_r \cdot \tilde{\phi}'_M. \]
Convert a multipole expansion into a local expansion.

- Map between the old and new DA variables ($M_2$).

New frame centered at $(x'_o, y'_o, z'_o)$, and the new DA variables are

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

The map $M_2$ is

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

with $R = \frac{1}{(x'_o+d'_x)^2+(y'_o+d'_y)^2+(z'_o+d'_z)^2}$.
Local expansion in the new frame.

\[ \tilde{\phi}_L = \tilde{\phi}_M \circ M_2, \]

\[ d'_r = \sqrt{R}, \]

then

\[ \phi_L = \tilde{\phi}_M \cdot \sqrt{R}. \]
Local Expansion from the charges

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

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

with

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

- The map between the old and the new DA variables

\[
d_x = x'_o + d'_x, \\
d_y = y'_o + d'_y, \\
d_z = z'_o + d'_z.
\]

- The local expansion in the new frame

\[
\phi'_L = \phi_L \circ M_3.
\]
Calculate the field from the multipole expansion

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

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

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

with

\[
d_r = \sqrt{d_x^2 + d_y^2 + d_z^2}.
\]
MLFMA: Numerical Results

\[ Error = \sqrt{\frac{\sum_i (\phi_{\text{num}}(\vec{r}_i) - \phi_{\text{exact}}(\vec{r}_i))^2}{\sum_i \phi_{\text{exact}}^2(\vec{r}_i)}} \]

Table: Relative error for 1 million particle calculation

<table>
<thead>
<tr>
<th>order</th>
<th>1 Gaussian Bunch</th>
<th>N Gaussian Bunches</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( E_x )</td>
<td>( E_y )</td>
</tr>
<tr>
<td>5</td>
<td>0.417E-3</td>
<td>0.330E-3</td>
</tr>
<tr>
<td>6</td>
<td>0.122E-3</td>
<td>0.900E-4</td>
</tr>
<tr>
<td>7</td>
<td>0.475E-4</td>
<td>0.353E-4</td>
</tr>
</tbody>
</table>
1 million particles, $s = 200$, Asterix, 4 Core (8 Hyperthreaded) Intel Xeon Processor X5677, 3.5GHz

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (mins)</td>
<td>9.449</td>
<td>5.578</td>
<td>3.571</td>
<td>2.759</td>
</tr>
</tbody>
</table>

1 million particles, $s = 200$, Obelix, 4 of the 12 Core Magny Cours AMD Opteron Processors 6174, 2.2GHz

<table>
<thead>
<tr>
<th>$N_p$</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>24</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time (mins)</td>
<td>18.877</td>
<td>10.339</td>
<td>5.515</td>
<td>3.216</td>
<td>2.133</td>
<td>1.950</td>
</tr>
</tbody>
</table>
MLFMA: Conclusions and Further Work

Conclusions

1. Works for $1/r^\nu$ with any real $\nu$.
2. Works for basic functions of $1/r$.
3. Works for $e^{-r}$.
4. Polynomial of $r$ can be calculated term by term.

Future work

1. Polishing the algorithm: error estimation, compressed tree, TM version ...
2. Map method
3. More elegant parallel version, 10 million particles
Assume the electrons have a uniform distribution within the energy band of $[E_f - E_{ph} + W, E_f]$. After collision, electron energy $E_e \in [E_f + W, E_f + E_{ph}]$.

To overcome the workfunction, $v_{zmin} = \sqrt{\frac{2(E_f+W)}{m}}$.

For a given energy, only the electrons whose velocities are inside an incident cone of the angle $\theta_{max}$ with respect to the $z$ direction can escape. And

$$\cos \theta_{max} = \frac{v_{zmin}}{\nu} = \sqrt{\frac{E_f + W}{E_e}}. \quad (1)$$
Assume the electron moves to a random direction after the collision, for a given energy, the possibility to escape is in proportion to the solid angle of the cone.

\[ P_{\text{esc.}} = \frac{2\pi(1 - \cos \theta_{\text{max}})}{4\pi} = 0.5 \cdot (1 - \cos \theta_{\text{max}}). \]

Given another angle \( \phi \in [0, 2\pi] \),
\[ v_z = v \cdot \cos \theta, \quad v_x = v \cdot \sin \theta \cdot \cos \phi, \quad \text{and} \quad v_y = v \cdot \sin \theta \cdot \sin \phi. \]

Assume the work function is abrupt at the surface, the initial velocities of the electrons in the air side are

\[ v_{xi} = v_x, \quad v_{yi} = v_y, \quad \text{and} \quad v_{zi} = \sqrt{v_z^2 - 2(E_f + W)/m}. \quad (2) \]
Photonemission Model: Algorithm

Algorithm

- Assume the laser pulse has a Gaussian distribution with standard deviation $\sigma$ in the time domain.
  
  1. Cut $[-3\sigma, +3\sigma]$ into $N$ even parts.
  
  2. Energy in the $i^{\text{th}}$ part is $dE_i = E_l \cdot (\text{erf}(t_2/\sigma) - \text{erf}(t_1/\sigma))$, with $t_1 = -3\sigma + (i - 1) \cdot dt$, $t_2 = -3\sigma + i \cdot dt$ and $dt = 6\sigma/N$.

- The number of outgoing electrons are $R \cdot dE_l/E_{ph}$.

- Initial velocities and positions for the outgoing electrons.
  
  1. Random number $E_e \in [E_f + W, E_f + E_{ph}]$, calculate $\cos\theta_{\text{max}}$ by Eq. (1). Another random number $c \in [0, 1]$.

  2. If $c > 1 - \cos\theta$, discard $E_e$ and repeat step (1). Otherwise accept $E_e$ and continue.

  3. Random number $\theta \in [0, \theta_{\text{max}}]$ and another random number $\phi \in [0, 2\pi]$, calculate the initial velocities by Eq. (2).

  4. $x_i$ and $y_i$ are random numbers of the Gaussian distributions with the standard deviations $\sigma_x$ and $\sigma_y$, $z_i = 0$. 
The positive hole: same $x_i$ and $y_i$, and $z_{−i} ∈ [−L, 0)$ with uniform distribution, where $L$ is the thickness of the gold film. (Is it reasonable?)

Solve the dynamic equations for the outgoing electrons, considering the space charge effect. External field can be included. Once the $z$ coordinate of an electron is less than zero, remove it and the respective positive hole from our calculation.
Questions

- Can we expect valuable results from the simulation?
- Is the model reasonable?