The Multiple Level Fast Multipole Method in the Differential Algebra Framework for Space Charge Field Calculation and Simulations on femtosecond electron imaging and spectroscopy

He Zhang (now Jefferson Lab), Zhensheng Tao, Jenni Portman, Phillip Duxbury, Chong-Yu Ruan, Kyoko Makino, Martin Berz

Michigan State University

FEIS13, Key West, FL
Multiple level fast multipole algorithm (MLFMA) in the differential algebra framework
Simulation results on femtosecond electron imaging and spectroscopy
I. Multiple Level Fast Multipole Algorithm in DA framework
Space charge effect is an important effect in the photo-emission process that generates the femtosecond electron bunch.

To simulate space charge effect, one needs an algorithm that has **good efficiency** and **good accuracy**.

The MLFMA is a good choice, because it

- scales **linearly** with the number of particles for any arbitrary charge distribution (grid free)
- does NOT artificially smooth the field

Using DA, one can

- calculate not only the field, but also its high order derivatives
- represent the multipole/local expansions in Cartesian coordinates naturally
- considerably simplify the math
The DA based MLFMA is developed as a package for COSY Infinity.

COSY is a scientific computing system with:
- DA and TM data types (ODE, flows, PDE, automatic differentiation, range bounding, etc.)
- beam physics package

More information on http://bt.pa.msu.edu/index_cosy.htm
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 be done by the command POLVAL.
- **Fast Multipole Method (FMM)**, L.Greengard and V.Rokhlin, 1987

- Cut the whole region into boxes of **hierarchical tree structure**.

- **Multipole expansions** and **local expansions**.

- For any arbitrary distribution, **scales linearly** with the number of particles.
The Fast Multipole Algorithm in the Differential Algebra Framework to Calculate 3D Self-field between Charged Particles
Multipole expansion from charges (for the childless boxes)

\[ \vec{R}_i(\vec{R}_1, \vec{R}_2, \vec{R}_i) = \phi(\vec{R}_i(\vec{M})) \]

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\[
\phi = \sum_{i=1}^{n} \frac{q_i}{\sqrt{(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2}} \\
= \sum_{i=1}^{n} \frac{d_r \cdot q_i}{\sqrt{1 + (x_i^2 + y_i^2 + z_i^2)}d_r^2 - 2x_id_x - 2y_id_y - 2z_id_z} \\
= d_r \cdot \phi_{c2m}
\]

with

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

\[
\phi_{c2m} = \sum_{i=1}^{n} \left\{ \frac{q_i}{\sqrt{1 + (x_i^2 + y_i^2 + z_i^2)}d_r^2 - 2x_id_x - 2y_id_y - 2z_id_z} \right\}.
\]

Error \[|\epsilon| \leq C \cdot \left( \frac{a}{r} \right)^{p+1} \cdot \frac{1}{r - a}, \text{ where } C = \sum_{i=1}^{n} |q_i| \text{ and } r_i \leq a \text{ for any } i.\]
Translate the position of a multipole expansion

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

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

\[
R = \frac{1}{1 + (x_o'^2 + y_o'^2 + z_o'^2)(d_x'^2 + d_y'^2 + d_z'^2) + 2x_o'd_x' + 2y_o'd_y' + 2z_o'd_z'}.
\]
In 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.
Convert a multipole expansion into a local expansion

\[ \vec{M} \quad (0, 0, 0) \quad \vec{R} (x, y, z) \quad \vec{R} (x', y', z') \]

\[ \vec{L} \quad O(0, 0, 0) \quad \vec{O} (x_o, y_o, z_o) \]

\[ S (-x_o, -y_o, -z_o) \]

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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

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

with

\[
    R = \frac{1}{(x'_o + d'_x)^2 + (y'_o + d'_y)^2 + (z'_o + d'_z)^2}.
\]
The multipole expansion in the source frame \( \phi = d_r \cdot \vec{\phi} \)

The local expansion in the observer frame

\[
\phi = \sqrt{R} \cdot \phi_{m2l} = \phi_{m2l}
\]

where \(\sqrt{R}\) is converted from \(d_r, \phi_{m2l} = \phi \circ M_{m2l}\),

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

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

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.
Calculate the local expansion from charges.

\[ \vec{R}_1 \quad \vec{R}_2 \quad \vec{R}_{2}' \quad \text{S}(0, 0, 0) \quad \text{S}'(x_0, y_0, z_0) \quad \vec{R}_{1}' \quad \vec{R}_{2}' \quad \text{S}'(0, 0, 0) \quad \vec{R}_{2}' \quad \text{S}(-x_0, -y_0, -z_0) \]

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

\[ d'_x = x - x'_o = x', \]
\[ d'_y = y - y'_o = y', \]
\[ d'_z = z - z'_o = z'. \]

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

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

Compare the MLFMA with direct calculation

![Graph comparing MLFMA and direct calculation](chart.png)

- MLFMA
- Direct Calc.
- Fitting MLFMA
- Fitting Direct Calc.

- $k_d = 2.000$
- $k_m = 1.073$

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Numerical experiments

Accuracy and computation time

![Graph showing accuracy and computation time relationship](image-url)
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Numerical experiments

Computation time for 1 million electrons

![Graph showing the computation time for 1 million electrons as a function of the number of processes. The time decreases exponentially as the number of processes increases.]
II. Simulation results on femtosecond imaging and spectroscopy
Experiment setup:

Simulation model:
- Three-step model of photoemission
- Extraction field $F_a$, space charge field, surface image charges
- Up to several millions of macro-particles in simulation
(a) Electron bunch profiles (b) Bunch length vs. $N_e^{\text{emit}}$
(c) $N_e^{\text{emit}}$ vs. $N_e^0$ showing virtual cathode effect

Simulation

(a) Initial electron bunch profiles in x-z plane
(b) Electron bunch profiles in x-z plane at 100ps under strong $F_a$ (10 MV/m)
(c) Electron bunch profiles in x-z plane at 100ps under weak $F_a$ (0.32 MV/m)
(d) Electron bunch profiles in x-z plane at 100ps under weak $F_a$ (0.32 MV/m) with a pinned image field
(e) Electron charge distributions under different fields
(a) $\varepsilon_x$ for different field and different $N_{e}^{\text{emit}}$. Affected by the virtual cathode effect.

(b) $\varepsilon_y$ for different field and different $N_{e}^{\text{emit}}$. Not affected by the virtual cathode effect. Driven by internal field and nonlinearities.
Simulation

Figure: 6D emittance $\varepsilon_x\varepsilon_y\varepsilon_z$ versus $N_e^{\text{emit}}$ for the extended electron sources with sizes $\sigma_r$ (100 $\mu$m, 1mm), thermionic guns, Schottky, cold (CFEG) and heated (HFEG) field-emission guns$^1$

- Degeneracy ($\eta = B_6D\varepsilon_0$, $B_6D = N_e/(\varepsilon_x^2\varepsilon_z)$) can improved with flat photoemission cathode until the virtual cathode threshold.
- Increasing extraction field is helpful, because it defers the onset of virtual cathode effect.
- Large emitting area increases the $N_e^{\text{emit}}$, but not necessary degeneracy (brightness).
- No gain by using sharp emitters (FEGs or atom-sized emitters) due to their poor emittance scaling with $N_e$.

1. The Multiple Level Fast Multipole Algorithm
   - Grid-free, works for any arbitrary charge distribution with an efficiency $O(N)$.
   - Calculate both the potential/field and its derivatives

2. Studied the virtual cathode effect quantitatively in femtosecond electron generation
   - $N_{\text{emit}}^e, \varepsilon_x, \eta$
   - Increase $F_a$ can defer the onset of virtual cathode effect

3. Transition into virtual cathode regime might be described by two fluids

4. $\eta$ is affected by different factors.
THANK YOU!