Fast Multipole Method Algorithm in 2D

- Input

N : number of particles $\rightarrow$ int npar

$\rightarrow$ double z[Max_particle][2]

$\{z_j = x_j + i y_j \mid x_j, y_j \in [0,1]; i = \sqrt{-1}; j = 0, \dots, N\}$: particle positions

$\rightarrow$ double q[Max_particle]

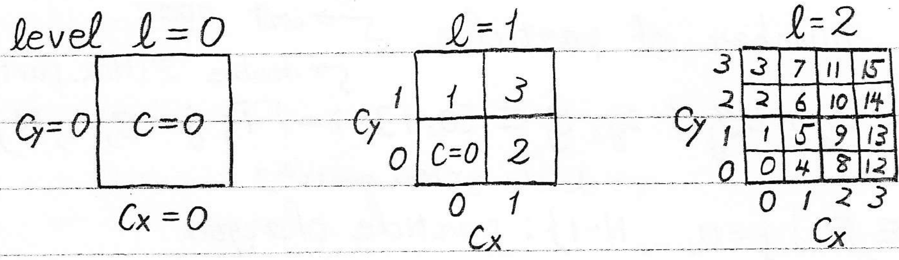
$\{q_j \in \mathbb{R} \mid j = 0, \dots, N-1\}$: particle charges.

- Output

$\rightarrow$ double pot[Max_Npar][2]

$\{\phi(z_j) = \sum_{\substack{k=1 \\ (k \neq j)}}^{N} q_k \log(z_j - z_k) \mid j = 1, \dots, N\}$: electrostatic potentials

Data structures: cell quadtree



int L

L: maximum level of refinement

Level $l=0$ is the root level, and the only one cell $c=0$ at $l=0$ is the entire simulation system $[0,1]^2$. At level $l \geq 1$, each mother cell at level $l-1$ is subdivided into 2×2 square daughters of equal area, so that there are 4^l cells at level l. The recursive subdivision is repeated until the leaf level, $l=L$.

(Cell index)

At level l, the 4^l cells, $c=0,\ldots,4^l-1$, are indexed using a vector index, $\vec{c}=(C_x,C_y)$ $(C_x,C_y=0,\ldots,2^l-1)$, where C_x and C_y are the column and row indices in the x and y directions, respectively. The serial cell index is numbered in the column-major order:

$$\begin{cases} C_x = c/2^l & \text{(quotient)} \quad (1) \\ C_y = c \bmod 2^l & \text{(remainder)} \quad (2) \end{cases}$$

or

$$c = C_x \cdot 2^l + C_y \qquad (3)$$

– Data structures : multipoles and local expansions

$\to$ int P

P : Truncation degree of multipole and local expansions

$\{\Phi_c^{(l)}(\alpha) \mid l=0,\dots,L;\ c=0,\dots,4^l-1;\ \alpha=0,\dots,P\}$: α-th order multipole around the center of cell c at level l

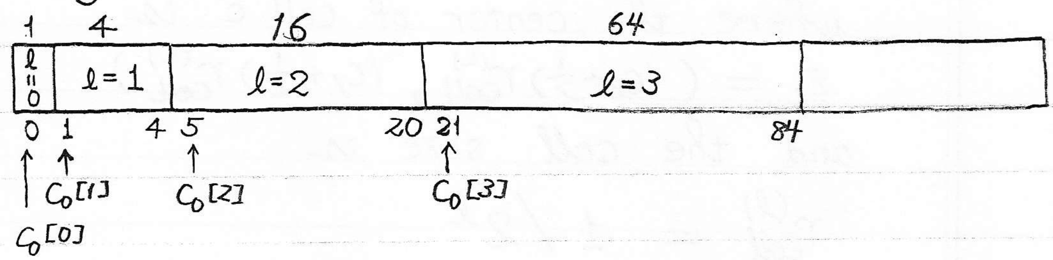
$\hookrightarrow$ phi[Max_cell][Max_term][2]

$\overbrace{\text{real(0) / imaginary(1)}}$

$\{\Psi_c^{(l)}(\alpha) \mid l=0,\dots,L;\ c=0,\dots,4^l-1;\ \alpha=0,\dots,P\}$: local expansion terms

$\hookrightarrow$ psi[Max_cell][Max_term][2]

In the arrays phi & psi, cells are sequentially stored starting from 0th level.



$C_0(l)$ $(l=0,\dots,L)$: the starting position, in arrays phi & psi, of the cell at level l.

$\hookrightarrow$ int C0[Max_level]

phi[$C_0(l)$+c][α][] stores $\Phi_c^{(l)}(\alpha)$
psi Ψ

$$C_0(l) = \begin{cases} 0 & (l=0) \\ 1+4^k+\cdots+4^{l-1} = \dfrac{4^l-1}{3} & (l \geq 1) \end{cases} \tag{4}$$

— Algorithm

1. Form the multipoles of all leaf cells at level L

$$
\begin{aligned}
&\text{for } c = 0 \text{ to } 4^L - 1 \\
&\qquad \Phi_c^{(L)}(0:P) \leftarrow 0 \\
&\text{for } j = 0 \text{ to } N-1 \qquad \text{// scan } \forall \text{ particles} \\
&\qquad c_x \leftarrow \lfloor x_j / r_{cell}^{(L)} \rfloor ; \; c_y \leftarrow \lfloor y_j / r_{cell}^{(L)} \rfloor \qquad \text{// particle} \rightarrow \text{cell mapping} \\
&\qquad c \leftarrow c_x \cdot 2^L + c_y
\end{aligned}
$$

$$
\Phi_c^{(L)}(\alpha) \mathrel{+}= \begin{cases} q_j & (\alpha = 0) \\ -\dfrac{q_j (z_j - z_c)^\alpha}{\alpha} & (\alpha \geq 1) \end{cases} \tag{5}
$$

where the center of cell c is

$$
z_c = \left(\left(c_x + \tfrac{1}{2}\right) r_{cell}^{(L)}, \left(c_y + \tfrac{1}{2}\right) r_{cell}^{(L)} \right) \tag{6}
$$

and the cell size is

$$
r_{cell}^{(l)} = 1/2^l \tag{7}
$$

2. Upward pass to compute the multipoles

for $l = L-1$ down to 0

  for $c = 0$ to $4^l - 1$

$$\Phi_c^{(l)} \leftarrow \sum_{c' \in \mathrm{daughters}(c)} T^{M \leftarrow M}_{\mathbb{Z}_{c'} - \mathbb{Z}_c} \Phi_{c'}^{(l+1)} \quad (\alpha = 0, \dots, P) \qquad (8)$$

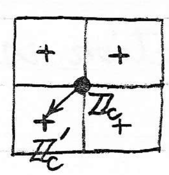
Here, daughters(c) is the set of 4 daughter cells of cell c,

$$\mathrm{daughters}(c) = \left\{ c' \mid c'_\mu = 2c_\mu \text{ or } 2c_\mu + 1 \ (\mu = x, y) \right\} \qquad (9)$$

$$\mathbb{Z}_{c'} - \mathbb{Z}_c = \left(c'_x + \tfrac{1}{2}, c'_y + \tfrac{1}{2}\right) r_{\mathrm{cell}}^{(l+1)} - \left(c_x + \tfrac{1}{2}, c_y + \tfrac{1}{2}\right) r_{\mathrm{cell}}^{(l)} \qquad (10)$$

and the multipole-to-multipole transformation is

$$T^{M \leftarrow M}_{\mathbb{Z}} \Phi_{c'}^{(l+1)}(\alpha) = \begin{cases} \Phi_{c'}^{(l+1)}(0) & (\alpha = 0) \\ \left[\sum_{\beta=1}^{\alpha} \Phi_{c'}^{(l+1)}(\beta) \, \mathbb{Z}^{\alpha-\beta} \, {}_{\alpha-1}C_{\beta-1} \right] - \dfrac{\Phi_{c'}^{(l+1)}(0) \, \mathbb{Z}^{\alpha}}{\alpha} & (\alpha \geq 1) \end{cases} \qquad (11)$$



3. Downward pass to compute the local expansion

for $c = 0$ to 4^1

$\Psi_c^{(2)}(0:P) \leftarrow 0$

for $l = 2$ to L

for $c = 0$ to 4^l

$$\Psi_c^{(l)} \leftarrow T^{L\leftarrow L}_{Z_{mother(c)} - Z_c} \Psi^{(l-1)}_{mother(c)} + \sum_{c' \in interactive(c)} T^{L\leftarrow M}_{Z_{c'} - Z_c} \Phi^{(l)}_{c'} \tag{12}$$

Here, the mother cell of cell c is

$$mother(c) = (c_x/2,\ c_y/2) \tag{13}$$

and the set of interactive cells is

$$interactive(c) = \{ c' \mid c'_\mu = 2(\underbrace{c_\mu/2}_{mother} - 1), \ldots, 2(c_\mu/2+1)+1 \quad (\mu = x,y)$$

$$\text{but any } c'_\mu \neq c_\mu \text{ or } c_\mu \pm 1 \quad (\mu = x,y) \} \tag{14}$$

The multipole-to-local transformation is

$$T^{L\leftarrow M}_{Z} \Phi^{(l)}_{c'}(\alpha) = \begin{cases} \displaystyle\sum_{\beta=1}^{P} \frac{\Phi^{(l)}_{c'}(\beta)}{Z^\beta} (-1)^\beta + \Phi^{(l)}_{c'}(0) \log(-Z) & (\alpha = 0) \\ \displaystyle\left[\frac{1}{Z^\alpha} \sum_{\beta=1}^{P} \frac{\Phi^{(l)}_{c'}(\beta)}{Z^\beta} {}_{\alpha+\beta-1}C_{\beta-1} (-1)^\beta \right] - \frac{\Phi^{(l)}_{c'}(0)}{\alpha Z^\alpha} & (\alpha \geq 1) \end{cases} \tag{15}$$

The local-to-local transformation is

$$T^{L\leftarrow L}_{\mathbb{Z}}\,\Psi^{(l-1)}_{c'}(\alpha) = \sum_{\beta=\alpha}^{P} \Psi^{(l-1)}_{c'}(\beta)\,{}_{\beta}C_{\alpha}(-z)^{\beta-\alpha} \qquad (16)$$

(Detailed pseudocode for Eq. (12))

$c'_x \leftarrow c_x/2;\; c'_y \leftarrow c_y/2;\; c' \leftarrow c'_x \cdot 2^{l-1} + c'_y$ // mother

$z \leftarrow (c'_x+\frac{1}{2}, c'_y+\frac{1}{2})\, r^{(l-1)}_{\text{cell}} - (c_x+\frac{1}{2}, c_y+\frac{1}{2})\, r^{(l)}_{\text{cell}}$ // $\mathbb{Z}^{\text{mother}} - \mathbb{Z}^{\text{daughter}}$

$\Psi^{(l)}_{c}(\alpha) \leftarrow \sum_{\beta=\alpha}^{P} \Psi^{(l-1)}_{c'}(\beta)\,{}_{\beta}C_{\alpha}(-z)^{\beta-\alpha}$ $(\alpha=0,\ldots,P)$ // inherit mother's local expansion

for $c'_x = 2(c_x/2-1)$ to $2(c_x/2+1)+1$
for $c'_y = 2(c_y/2-1)$ to $2(c_y/2+1)+1$
  if $|c'_x - c_x| \geq 2$ or $|c'_y - c_y| \geq 2$ then
    $z \leftarrow (c'_x - c_x, c'_y - c_y)\, r^{(l)}_{\text{cell}}$
    for $\alpha = 0$ to P

$$\Psi^{(l)}_{c}(\alpha) \mathrel{+}= \begin{cases} \displaystyle\sum_{\beta=1}^{P} \frac{\Phi^{(l)}_{c'}(\beta)}{z^{\beta}}(-1)^{\beta} + \Phi^{(l)}_{c'}(0)\log(-z) & (\alpha=0) \\ \displaystyle\left[\frac{1}{z^{\alpha}}\sum_{\beta=1}^{P} \frac{\Phi^{(l)}_{c'}(\beta)}{z^{\beta}}\,{}_{\alpha+\beta-1}C_{\beta-1}(-1)^{\beta}\right] - \frac{\Phi^{(l)}_{c'}(0)}{\alpha z^{\alpha}} & (\alpha\geq 1) \end{cases}$$

// interactive-cell contribution

4. Direct calculation of nearest-neighbor leaf-cell contribution

for $j = 0$ to $N-1$

$$\phi(z_j) \leftarrow \sum_{\alpha=0}^{P} \Psi_{c(j)}^{(L)}(\alpha)\,(z_j - z_{c(j)})^{\alpha} + \sum_{\substack{j' \in nn(c(j)) \\ j' \neq j}} q_{j'} \log(z_j - z_{j'}) \qquad (17)$$

Here, $c(j)$ is the leaf cell that particle j belong to

$$c_x = \lfloor x_j / r_{\mathrm{cell}}^{(L)} \rfloor, \quad c_y = \lfloor y_j / r_{\mathrm{cell}}^{(L)} \rfloor$$

and $nn(c(j))$ is the 27 nearest-neighbor leaf cells of cell $c(j)$, including $c(j)$ itself.

The first term in Eq. (17) is the local expansion of the potential from non-nearest-neighbor leaf cells; the second term is the direct sums over particles in the nearest-neighbor leaf cells. Use the linked-list cell method in pmd.c to calculate the second contribution.

Slightly Modified Presentation of Downward Pass

3. Downward pass to compute the local expansion

for $c = 0$ to 4^1

$\quad \Psi_c^{(1)}(0:P) \leftarrow 0$

for $l = 2$ to L

$\quad$ for $c = 0$ to 4^l

$$\Psi_c^{(l)} \leftarrow T^{L\leftarrow L}_{\mathbb{Z}_{mother(c)} - \mathbb{Z}_c} \Psi^{(l-1)}_{mother(c)} \tag{12}$$

$\quad$ for $c = 0$ to 4^l

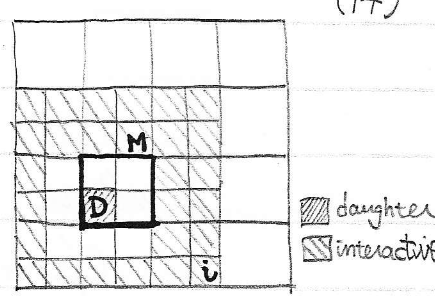
$$\Psi_c^{(l)} \leftarrow \Psi_c^{(l)} + \sum_{c' \in interactive(c)} T^{L\leftarrow M}_{\mathbb{Z}_{c'} - \mathbb{Z}_c} \Phi^{(l)}_{c'} \tag{12'}$$

Here, the mother cell of cell c is

$$mother(c) = (c_x/2,\ c_y/2) \tag{13}$$

and the set of interactive cells is

$$interactive(c) = \{ c' \mid c'_\mu = 2(\underbrace{c_\mu/2}_{mother} - 1), \ldots, 2(c_\mu/2 + 1) + 1 \quad (\mu = x, y)$$
$$\text{but } |c'_x - c_x| > 1 \text{ or } |c'_y - c_y| > 1 \} \tag{14}$$



The multipole-to-local transformation is

$$T^{L\leftarrow M}_{\mathbb{Z}} \Phi^{(l)}_{c'}(\alpha)$$

$$= \begin{cases} \displaystyle\sum_{\beta=1}^{P} \Phi^{(l)}_{c'}(\beta)\left(-\frac{1}{z}\right)^\beta + \Phi^{(l)}_{c'}(0)\log(-z) & (\alpha = 0) \\ \displaystyle\left[\frac{1}{z^\alpha}\sum_{\beta=1}^{P} \Phi^{(l)}_{c'}(\beta)\, {}_{\alpha+\beta-1}C_{\beta-1}\left(-\frac{1}{z}\right)^\beta\right] - \frac{\Phi^{(l)}_{c'}(0)}{\alpha z^\alpha} & (\alpha \geq 1) \end{cases} \tag{15}$$

The local-to-local transformation is

$$T^{L\leftarrow L}_{\mathbb{Z}} \Psi^{(l-1)}_{c'}(\alpha) = \sum_{\gamma=0}^{P-\alpha} \Psi^{(l-1)}_{c'}(\alpha+\gamma)\, {}_{\alpha+\gamma}C_\alpha (-z)^\gamma \tag{16}$$

(Detailed pseudocode for Eq.(12))

$C'_x \leftarrow C_x/2$; $C'_y \leftarrow C_y/2$; $C' \leftarrow C'_x \cdot 2^{l-1} + C'_y$ // mother

$z \leftarrow (C'_x+\frac{1}{2}, C'_y+\frac{1}{2})\, r^{(l-1)}_{cell} - (C_x+\frac{1}{2}, C_y+\frac{1}{2})\, r^{(l)}_{cell}$ // $z^{mother} - z^{daughter}$

$$\Psi^{(l)}_C(\alpha) \leftarrow \sum_{\gamma=0}^{P-\alpha} \Psi^{(l-1)}_{C'}(\alpha+\gamma)\, {}_{\alpha+\gamma}C_\alpha\, (-z)^\gamma \quad (\alpha = 0, \ldots, P)$$

// inherit mother's local expansion

(Detailed pseudocode for Eq.(12′))

for $C'_x = C'_{x}$_begin to C'_{x}_end
for $C'_y = C'_{y}$_begin to C'_{y}_end
if $|C'_x - C_x| > 1$ or $|C'_y - C_y| > 1$ then

// interactive cells

$z \leftarrow (C'_x - C_x, C'_y - C_y)\, r^{(l)}_{cell}$

for $\alpha = 0$ to P

$$\Psi^{(l)}_C(\alpha) \mathrel{+}= \begin{cases} \sum_{\beta=1}^{P} \Phi^{(l)}_{C'}(\beta)\left(-\frac{1}{z}\right)^\beta + \Phi^{(l)}_{C'}(0)\log(-z) & (\alpha=0) \\ \left[\frac{1}{z^\alpha}\sum_{\beta=1}^{P} \Phi^{(l)}_{C'}(\beta)\, {}_{\alpha+\beta-1}C_{\beta-1}\left(-\frac{1}{z}\right)^\beta\right] - \frac{\Phi^{(l)}_{C'}(0)}{\alpha z^\alpha} & (\alpha \geq 1) \end{cases}$$

where

C'_μ_begin $= \max(2(C_\mu/2 - 1), 0)$
C'_μ_end $= \min(2(C_\mu/2+1)+1, 2^l - 1)$ $\quad (\mu = x, y)$