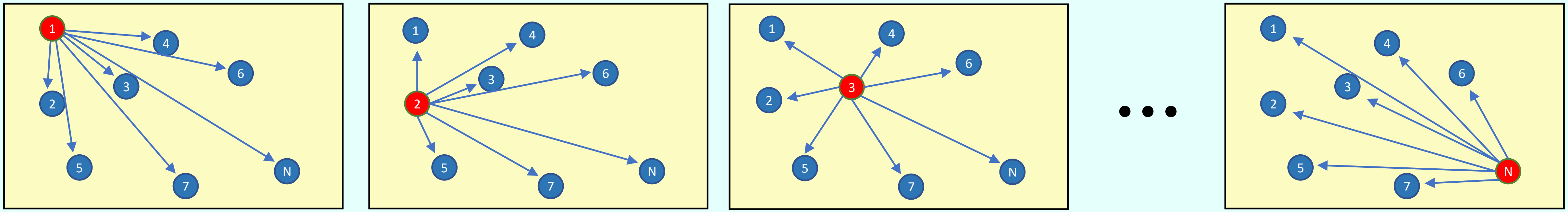
A Fast Algorithm for Particle Simulation

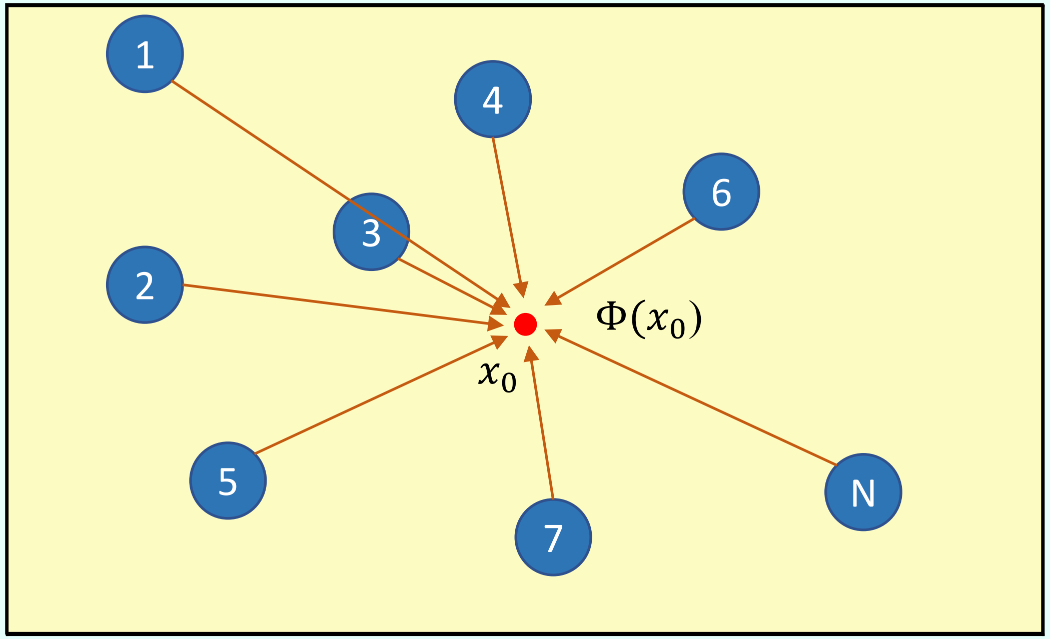
Traditional Method



N work　N work　N work　N work

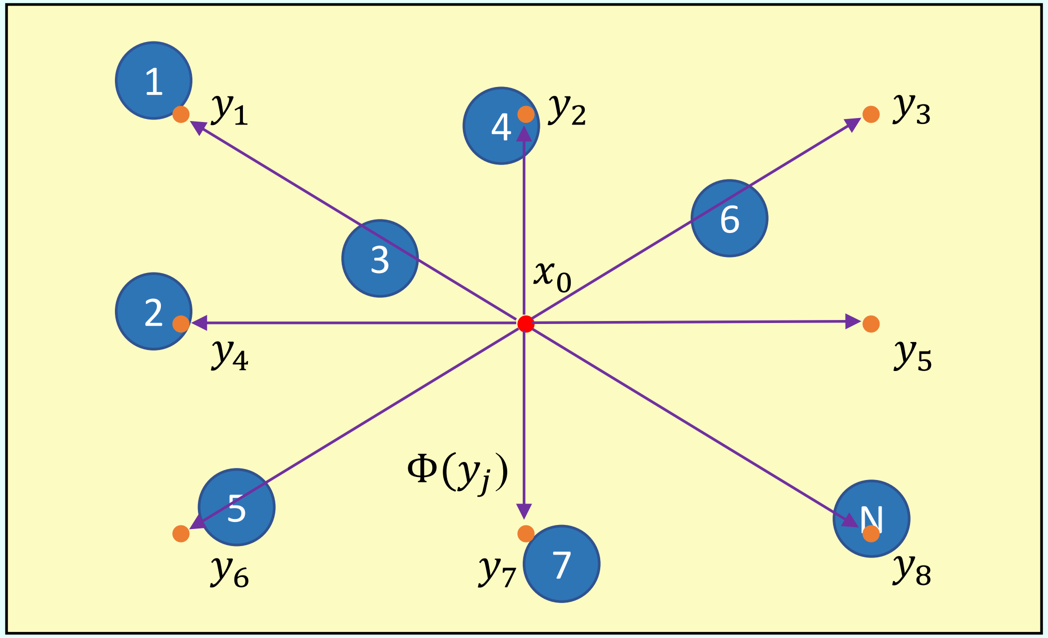
N×N work

Fast Algorithm



1. Computation of the <u>coefficients</u> of $\Phi(x_0)$ due to the charges about x_0.

mp work



2. Evaluation the coefficients of $\Phi(x_0)$ at all points y_j.

np work

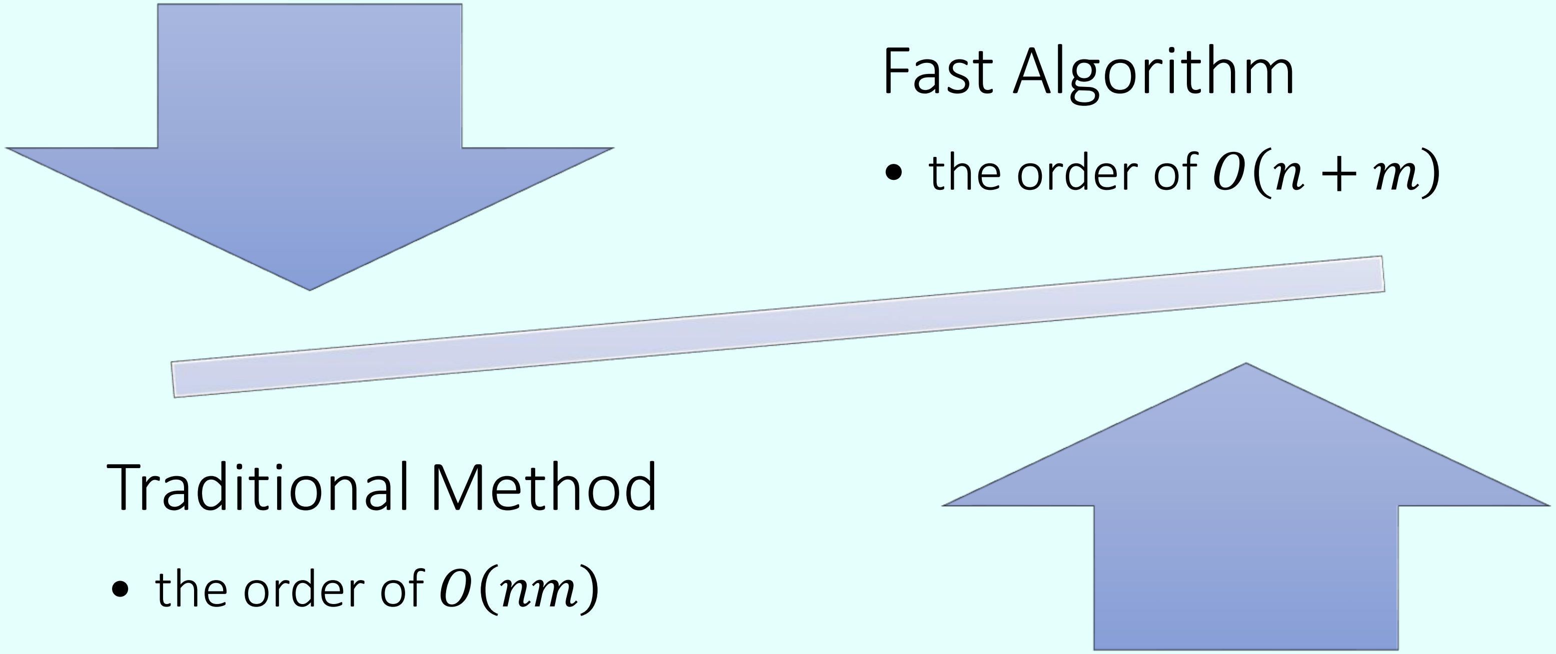
mp + np work

- **Theorem 2.1**. (**Multipole expansion**). Suppose that **m** charges of strengths $\{q_i\ ,\ i = 1\ , \ldots\ , m\}$ are located at points $\{z_i\ ,\ i = 1\ , \ldots\ , m\}$ with $|z_i| < r$. Then for any $z \in C$ with $|z| > r$, the potential $\Phi(z)$ is given by

$$\Phi(z) = Q\log(z) + \sum_{k=1}^{p} \frac{a_k}{z^k} \qquad \left(Q = \sum_{i=1}^{m} q_i \qquad a_k = \sum_{i=1}^{m} \frac{-q_i\, {z_i}^k}{k} \right)$$

$$p \approx -\log_2 \varepsilon$$ ε is relative precision

Traditional Method and Fast Algorithm



Fast Algorithm

- the order of $O(n + m)$

Traditional Method

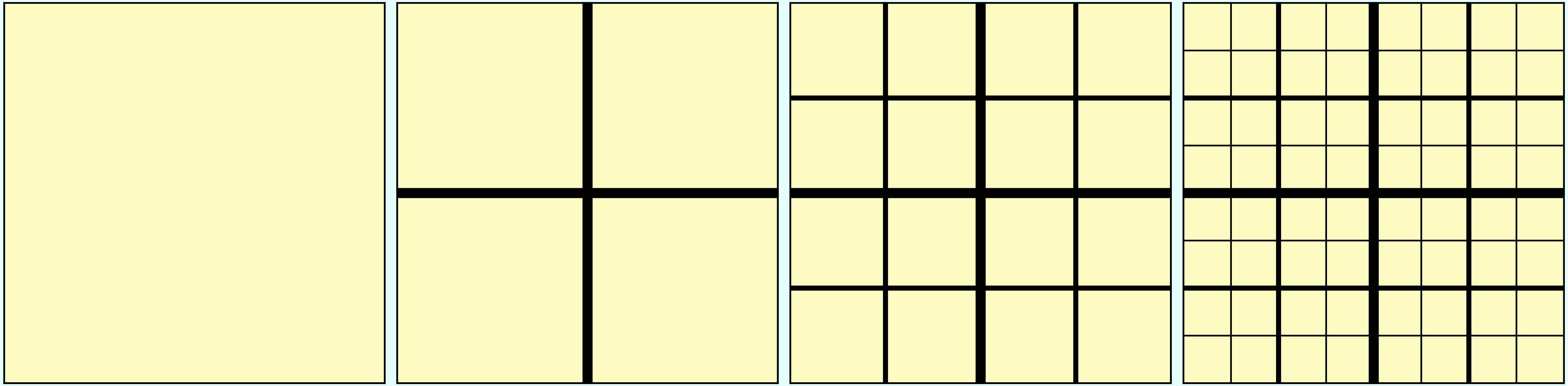
- the order of $O(nm)$

For a system of n particles, **the amount of work** that is needed to evaluate potential at m point

The strategy of fast algorithm

- Clustering particles
  - Interactions with particles which are nearby
  - Interactions with clusters which are sufficiently far away

Computational Box



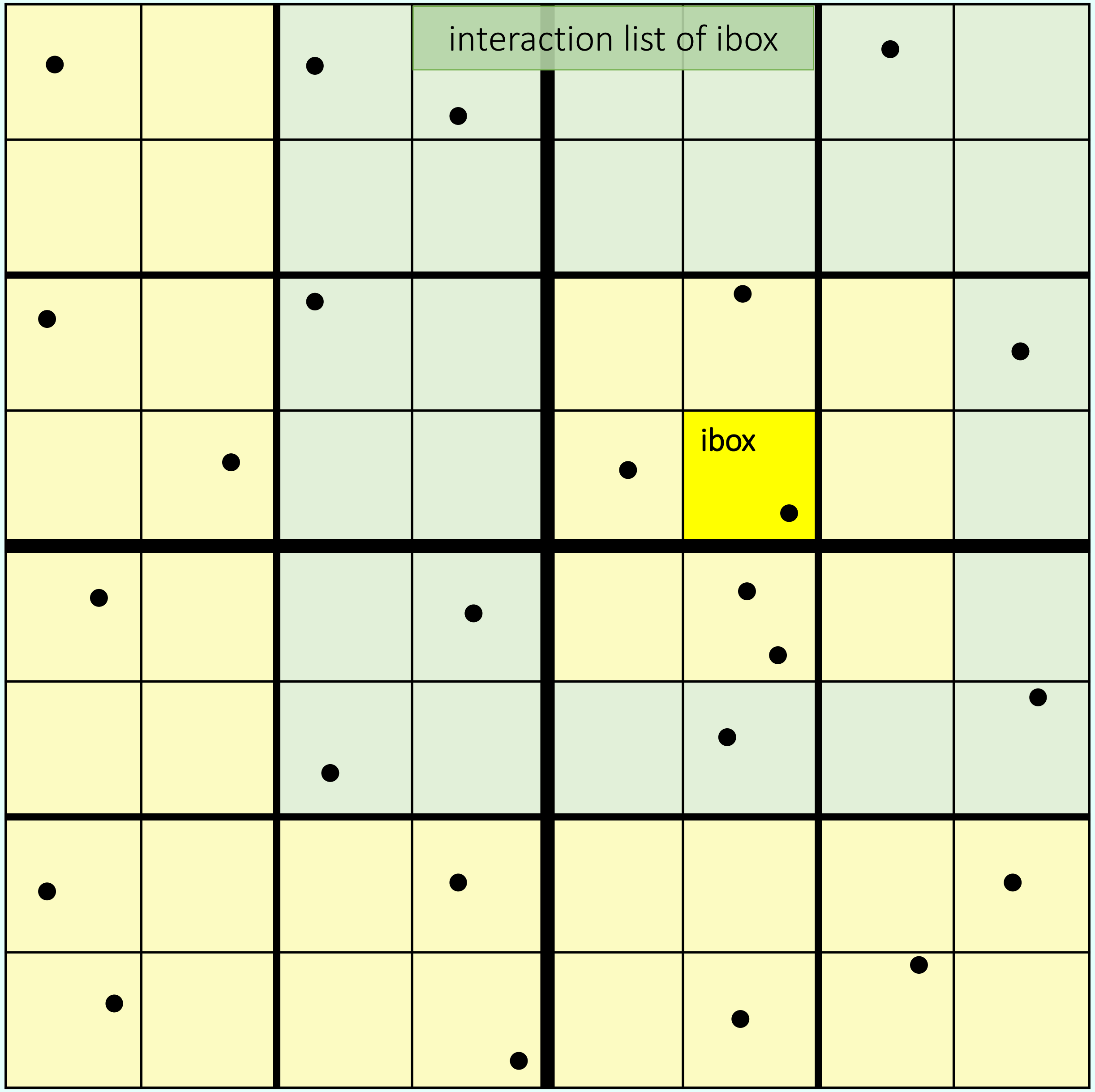
Level 0 Level 1 Level 2 Level 3

- Level of refinement: $n \approx \log_4 N$
- The number of boxes at mesh level l is equal to 4^l

Computational Box

Interaction list:

Children of the nearest neighbors of ibox's parent which are well separated from ibox

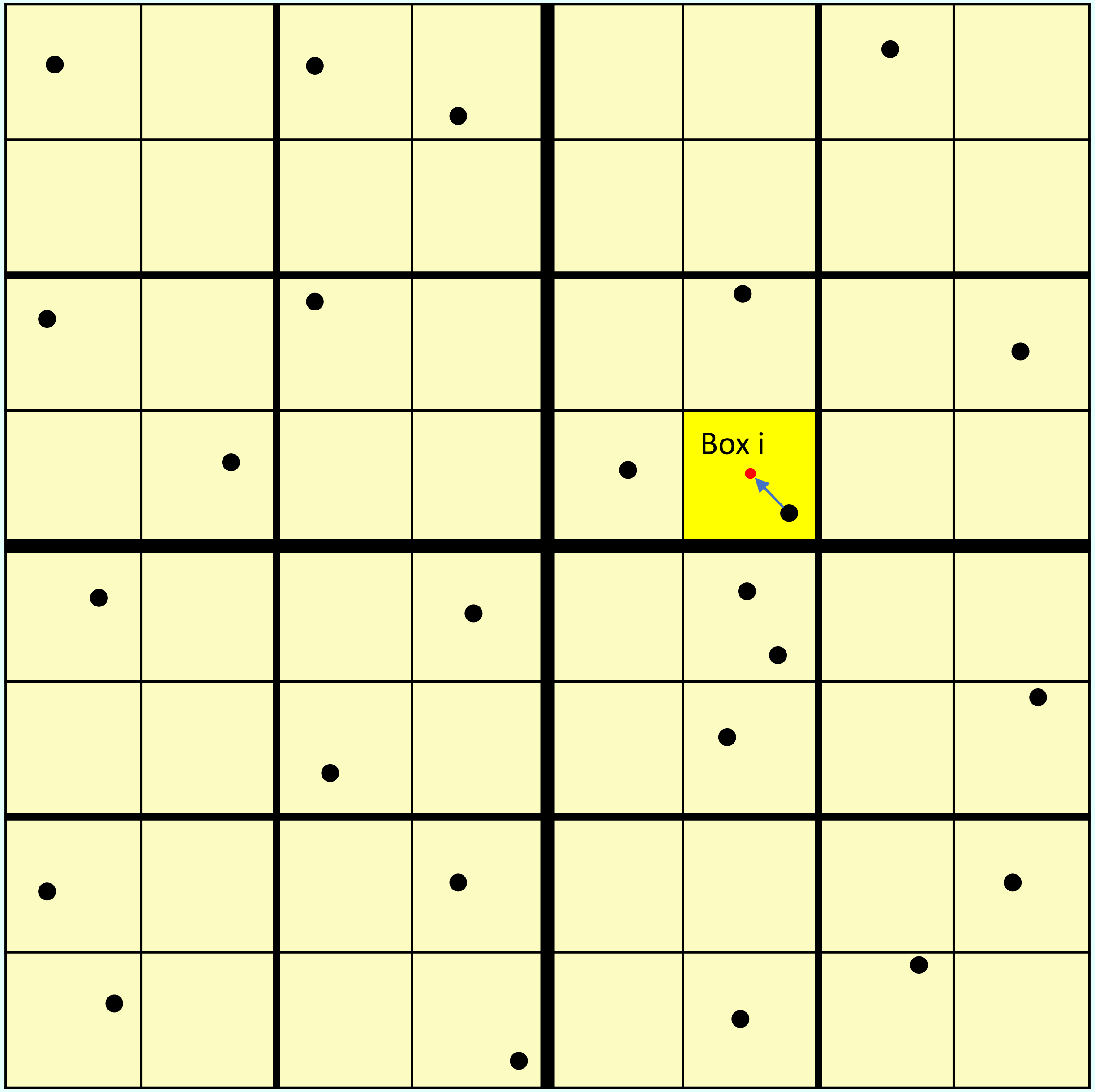


Notation used

p-term multipole expansion

$$\Phi_{l,i}$$

the *p*-term multipole expansion (about the box center) of the potential field created by the particles contained inside box *i* at level *l*.

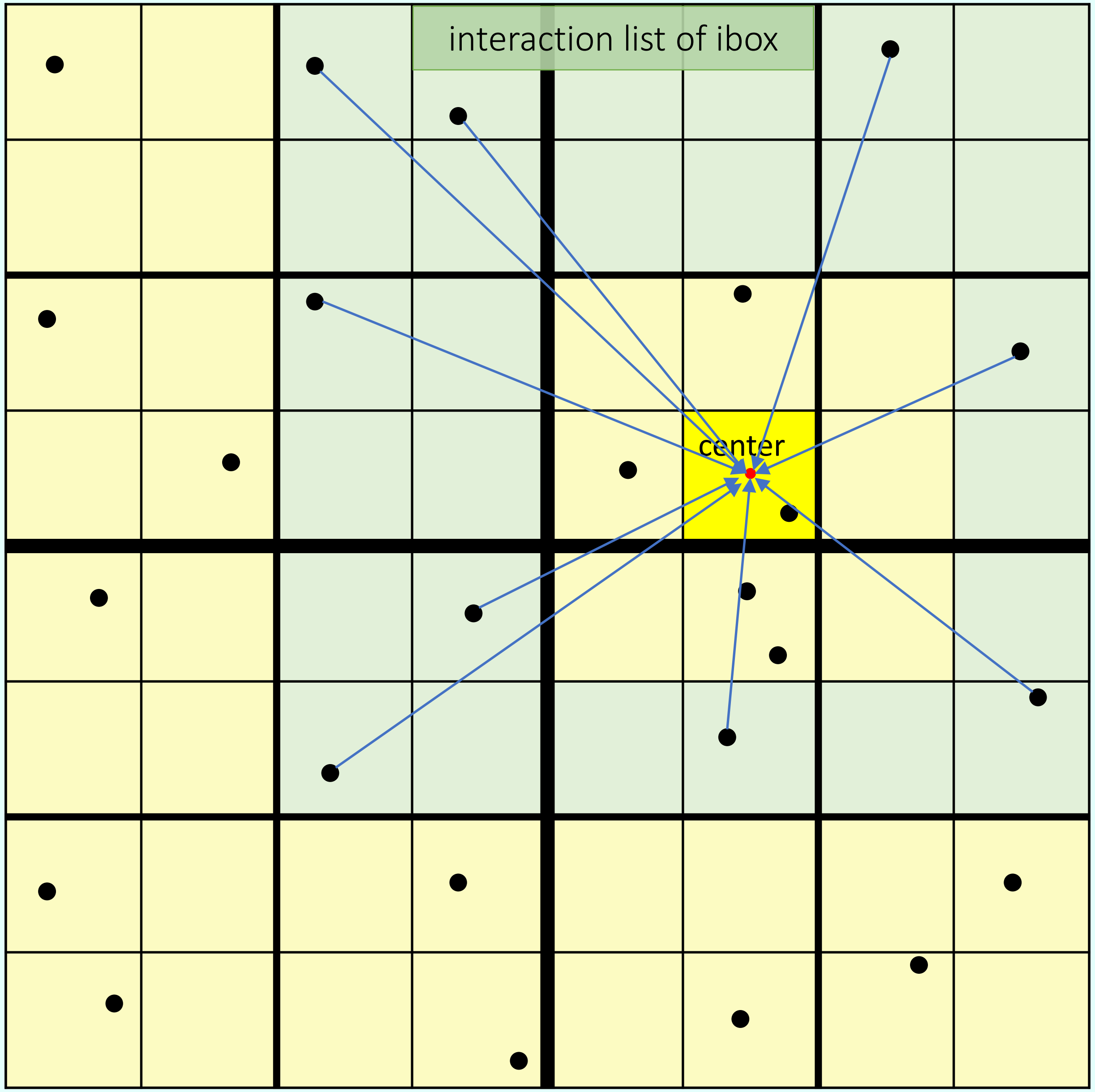


Notation used

p-term expansion

$$\Psi_{l,i}$$

the p-term expansion about the center of ibox at level l, describing the potential field due to <u>all particles inside the interaction list of ibox</u>.

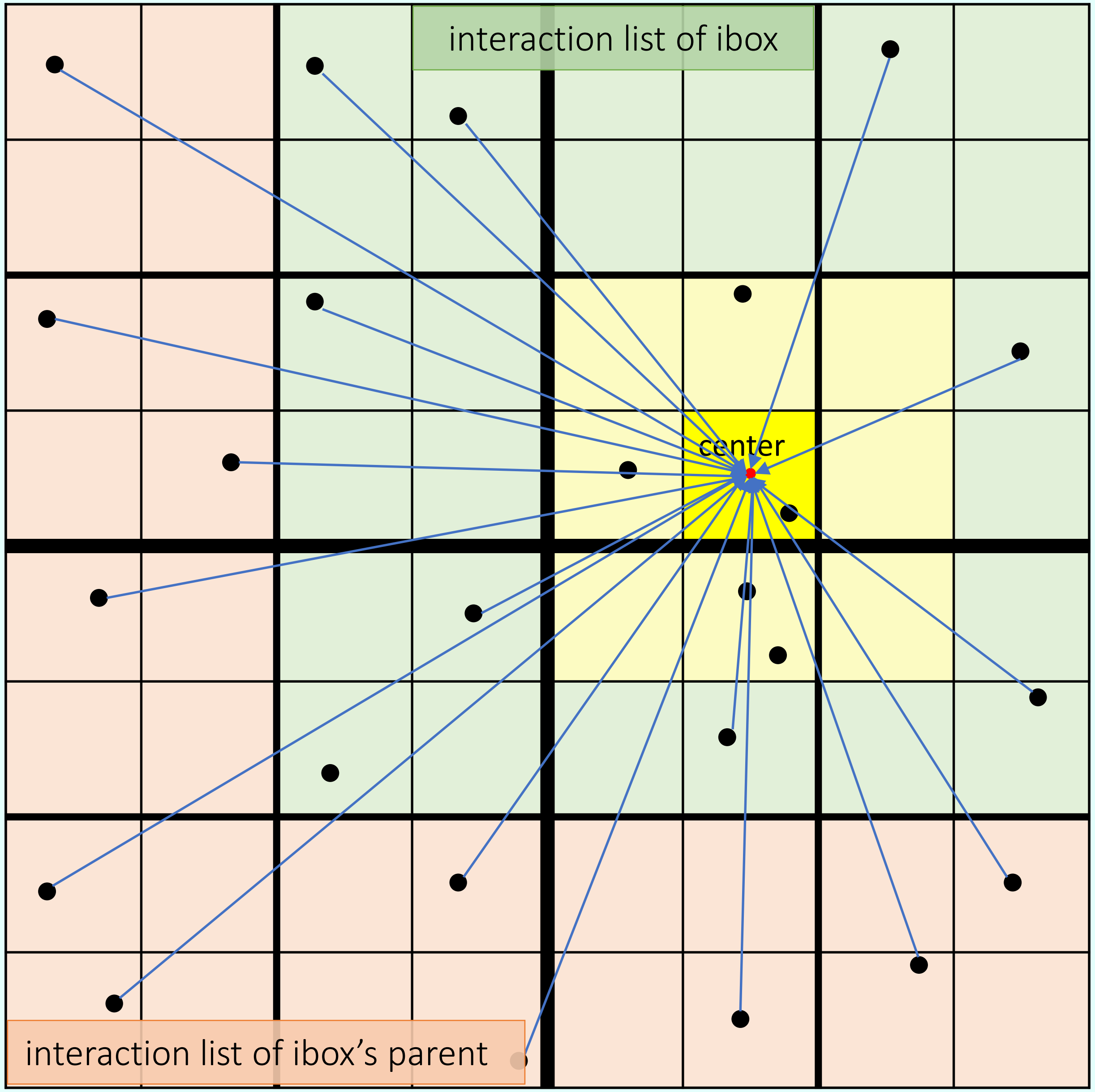


Notation used

p-term local expansion

$$\widetilde{\Psi}_{l,i}$$

the p-term local expansion about the center of ibox at level l, describing the potential field due to all particles inside the interaction list of ibox and ibox's parent.



Algorithm

Step 1. Form $\Phi_{finest\ mesh,ibox}(box\ center)$ due to particles in each child box

- Form a p-term multipole expansion $\Phi_{finest\ mesh,ibox}$, by using Theorem 2.1.

Step 2. Form $\Phi_{coarser\ mesh,ibox}(box\ center)$ due to particles in each child box

- Form a p-term multipole expansion $\Phi_{coarser\ mesh,ibox}$, by using Lemma 2.3 to shift the center of each child box's expansion to the current box center and adding them together.

Step 3. Form a **local expansion** about the center of each box at **coarser** mesh $l \leq n-1$

- Form $\Psi_{l,ibox}$ by using Lemma 2.4 to convert multipole expansion $\Phi_{l,interaction\ list}$ to local expansion, adding these expansions together.
- Adding result to $\widetilde{\Psi}_{l,ibox}$
- Form $\widetilde{\Psi}_{l+1,ibox's\ children}$ by using lemma 2.5 to expand $\Psi_{l,ibox}$ about the children's box centers.

Step 4. Form a **local expansion** at **finest** mesh level $l = n$

- Form $\Psi_{l,ibox}$ by using Lemma 2.4 to convert multipole expansion $\Phi_{l,interaction\ list}$ to local expansion, adding these expansions together.
- Adding result to $\widetilde{\Psi}_{l,ibox}$

Step 5. **Evaluate local expansion** $\widetilde{\Psi}_{n,ibox}(z_j)$ at **particle positions**

Step 6. Compute **potential** due to **nearest neighbors directly**

Step 7. For every particle in box ibox, **add direct** and **far** field terms together

Algorithm

- Step 1

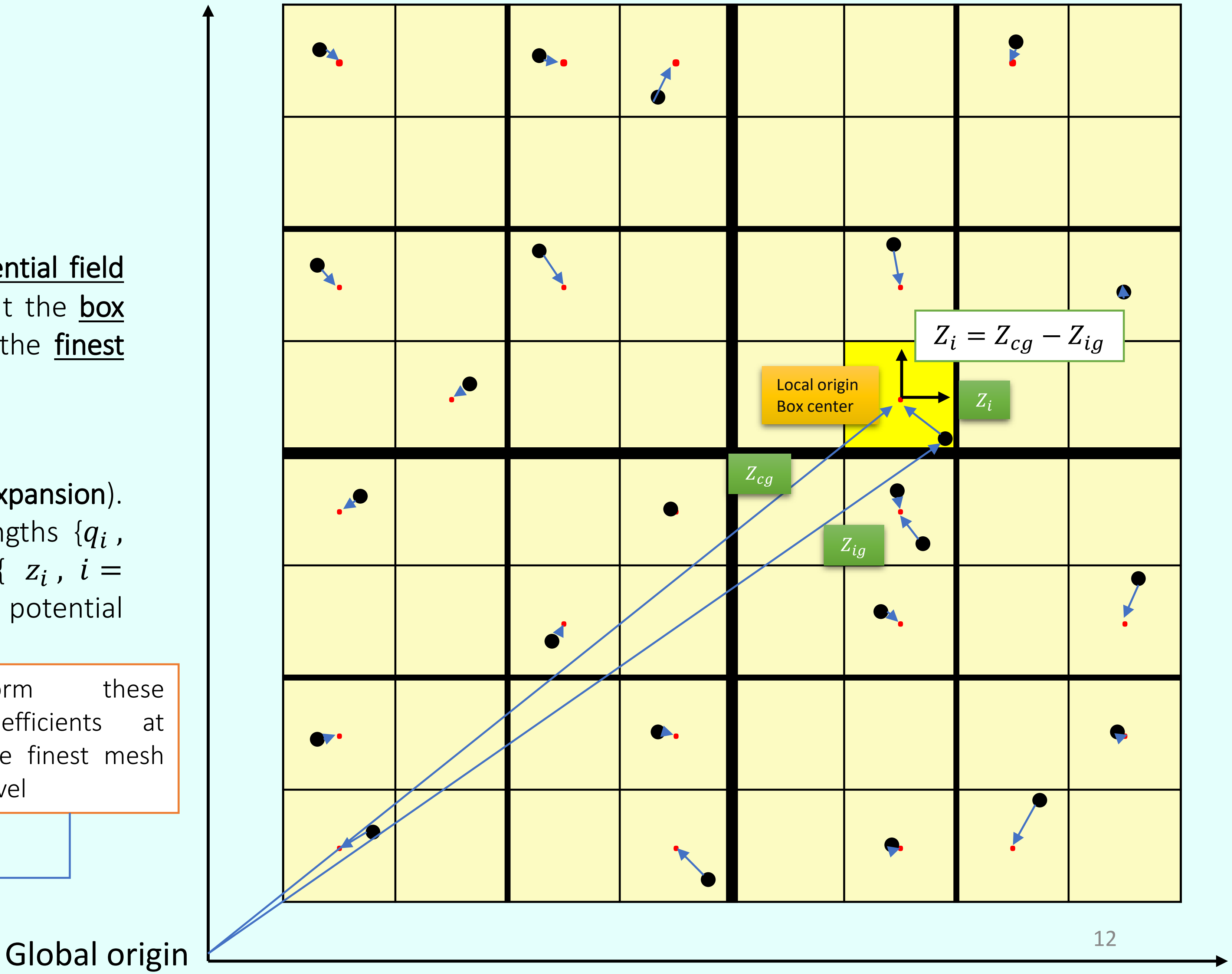
➢ Form coefficients of $\Phi_{n,ibox}$ (potential field due to particles in each box about the box center) by using theorem 2.1 at the finest mesh level.

➢ **Theorem 2.1. (Multipole expansion).** Suppose that m charges of strengths $\{q_i\,,\ i = 1\,,\dots,m\ \}$ are located $\{\ z_i\,,\ i = 1\,,\dots,m\}$. Then for any $z \in C$, the potential $\Phi(z)$ is given by

$$\Phi(z) = Q\log(z) + \sum_{k=1}^{p} \frac{a_k}{z^k}$$

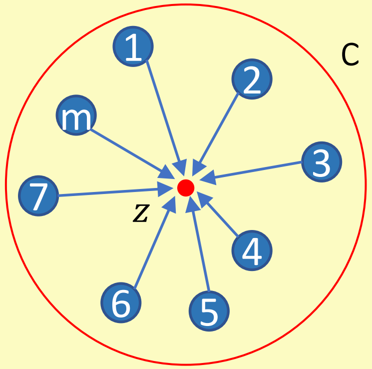
$$\left(Q = \sum_{i=1}^{m} q_i \quad a_k = \sum_{i=1}^{m} \frac{-q_i\, {z_i}^k}{k} \right)$$

Form these coefficients at the finest mesh level

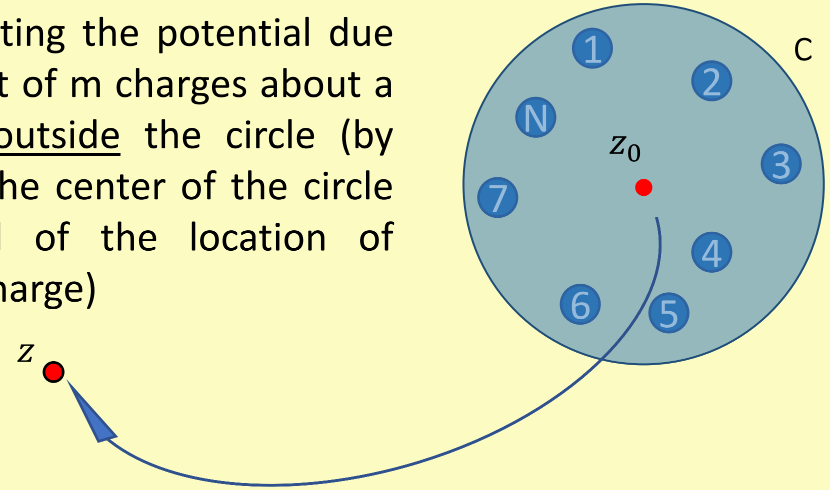


Lemma 2.3.

Calculating the potential due to a set of m charges about a point <u>inside</u> the circle (by using the location of each charge)



Calculating the potential due to a set of m charges about a point <u>outside</u> the circle (by using the center of the circle instead of the location of each charge)



- **Theorem 2.1**. (**Multipole expansion**). Suppose that **m** charges of strengths $\{q_i\ ,\ i = 1\ ,\dots\ ,m\}$ are located <u>inside</u> the circle C. Then for any $z \in C$ <u>inside</u> the circle C, the potential $\Phi(z)$ is given by

- **Lemma 2.3**. Suppose that **m** charges of strengths $\{q_i\ ,\ i = 1\ ,\dots\ ,m\}$ are located <u>inside</u> the circle C with center at z_0. Then for any $z \in C$ <u>outside</u> the circle C, the potential $\Phi(z)$ is given by

$$\Phi(z) = Q\log(z) + \sum_{k=1}^{p} \frac{a_k}{z^k} \quad \left(Q = \sum_{i=1}^{m} q_i \quad a_k = \sum_{i=1}^{m} \frac{-q_i\, {z_i}^k}{k} \right)$$

$$\Phi(z) = Q\log(z) + \sum_{l=1}^{p} \frac{b_l}{z^l} \quad \left(b_l = \left(\sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{Q z_0^l}{l} \right)$$

Algorithm

- Step 2

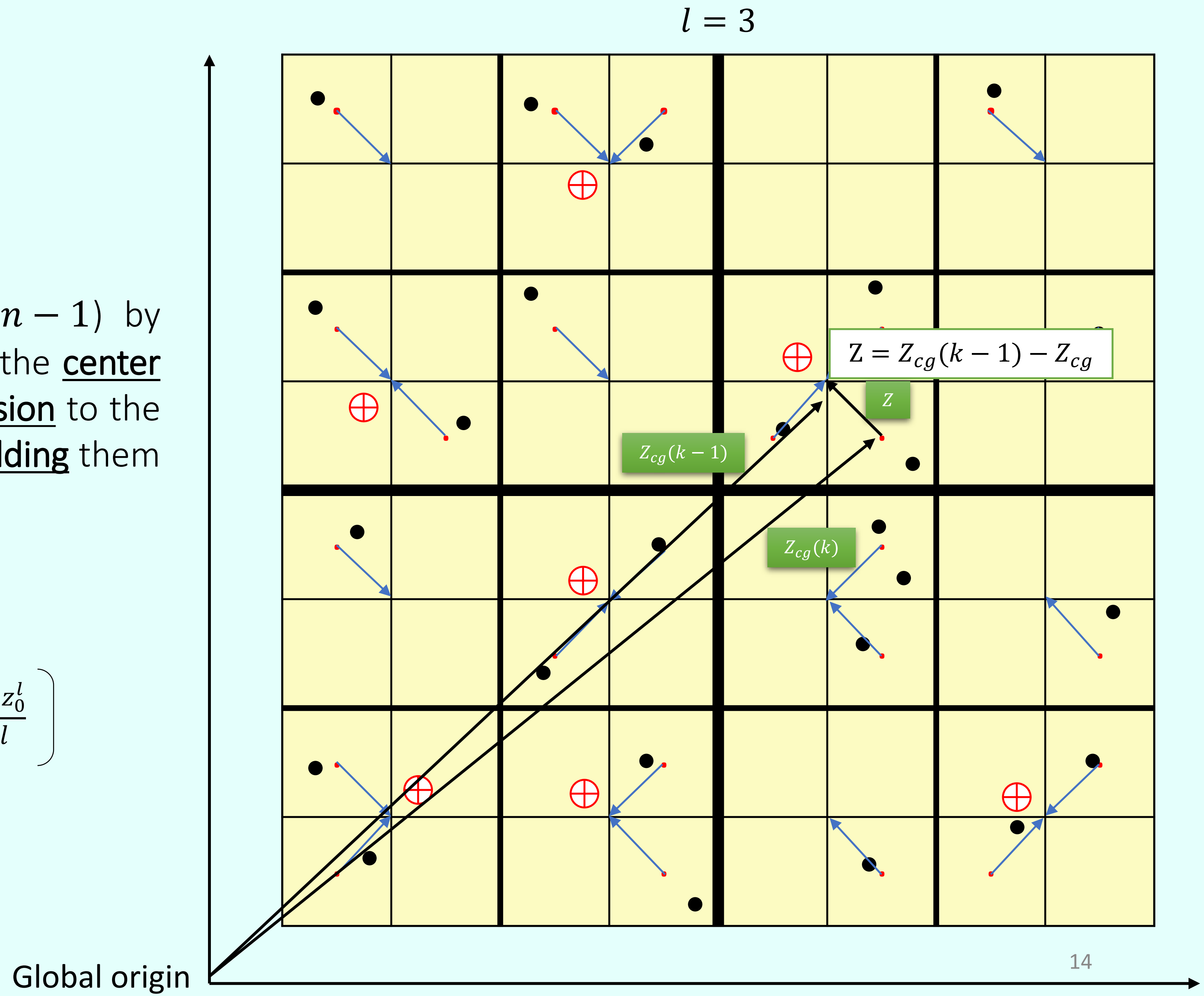
Form $\Phi_{l,ibox}$ $(l = 0, \ldots, n-1)$ by using lemma 2.3 to shift the center of each child box's expansion to the current box center and adding them together.

$$\Phi(z) = Q\log(z) + \sum_{l=1}^{p} \frac{b_l}{z^l}$$

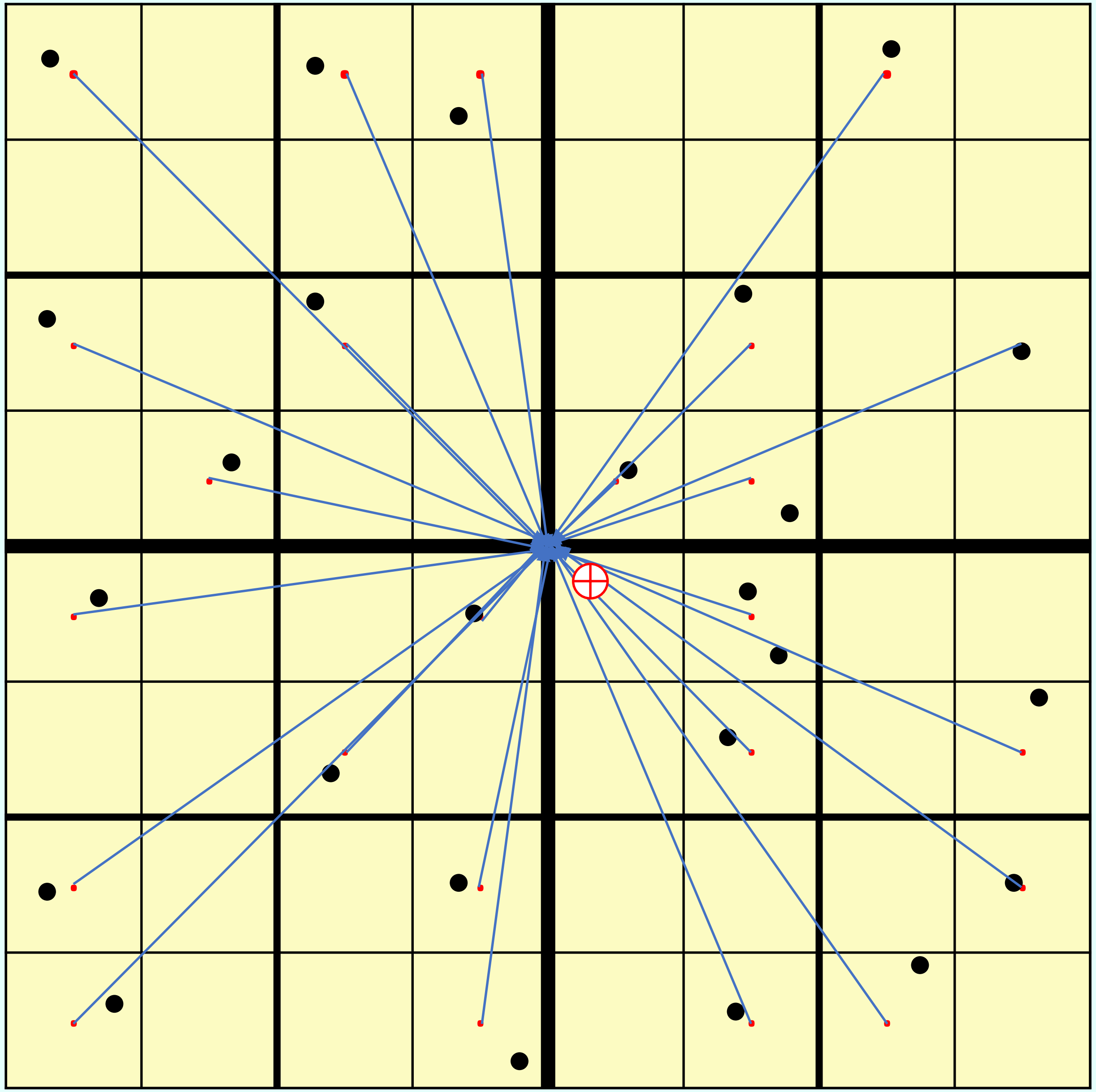
$$\left\{ b_l = \left(\sum_{k=1}^{l} a_k z_0^{l-k} \binom{l-1}{k-1} \right) - \frac{Q z_0^l}{l} \right\}$$

coarser mesh level

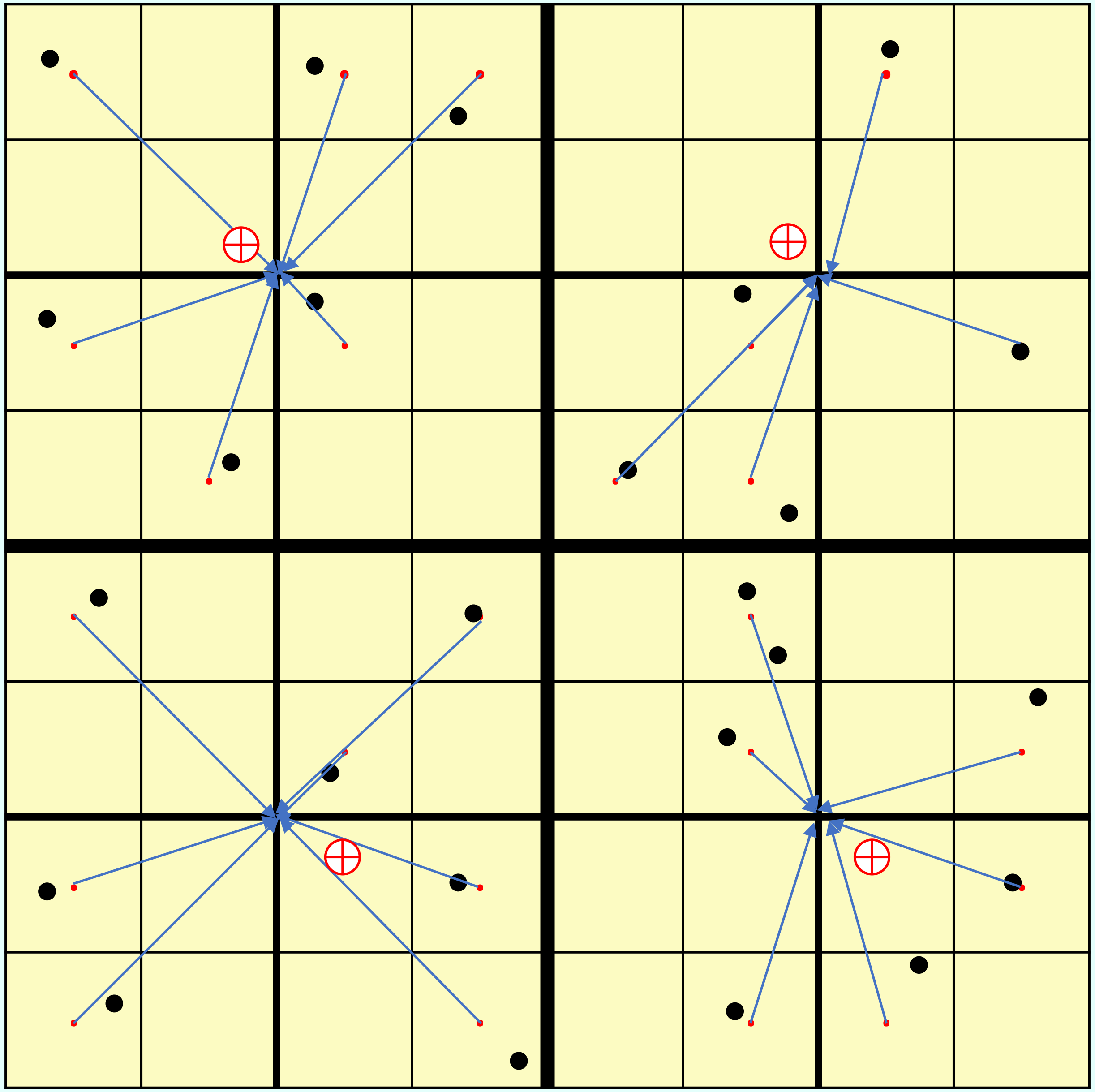
Finest mesh level



$l = 1$

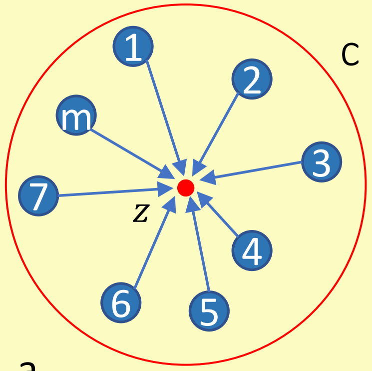


$l = 2$



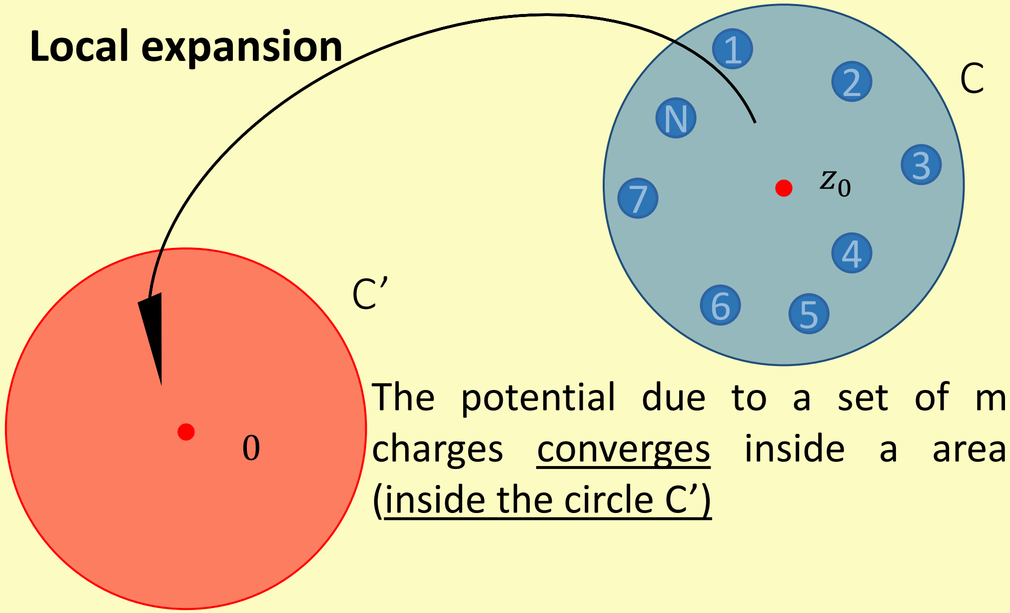
Lemma 2.4.

Multipole expansion



Calculating the potential due to a set of m charges about a point <u>inside</u> the circle (by using the location of each charge)

Local expansion



The potential due to a set of m charges <u>converges</u> inside a area <u>(inside the circle C')</u>

- **Theorem 2.1**. (**Multipole expansion**). Suppose that **m** charges of strengths $\{q_i\ ,\ i = 1\ ,\ldots\ , m\}$ are located <u>inside</u> the circle C. Then for any $z \in C$ <u>inside</u> the circle C, the potential $\Phi(z)$ is given by

$$\Phi(z) = Q\log(z) + \sum_{k=1}^{p} \frac{a_k}{z^k} \qquad \left(Q = \sum_{i=1}^{m} q_i \quad a_k = \sum_{i=1}^{m} \frac{-q_i\, {z_i}^k}{k} \right)$$

- **Lemma 2.4**. Suppose that **m** charges of strengths $\{q_i\ ,\ i = 1\ ,\ldots\ , m\}$ are located <u>inside</u> the circle C with center at z_0 . Then the <u>corresponding multipole expansion converges inside the circle C'.</u>

$$\Phi(z) = \sum_{l=0}^{p} b_l \cdot z^l \quad \left(\begin{aligned} b_0 &= \sum_{k=1}^{p} \frac{a_k}{z_0^k}(-1)^k + Q\log(-z) \\ b_l &= \left(\frac{1}{z_0^l} \sum_{k=1}^{p} \frac{a_k}{z_0^k} \binom{l+k-1}{k-1} (-1)^k \right) - \frac{Q}{l \cdot z_0^l} \end{aligned} \right)$$

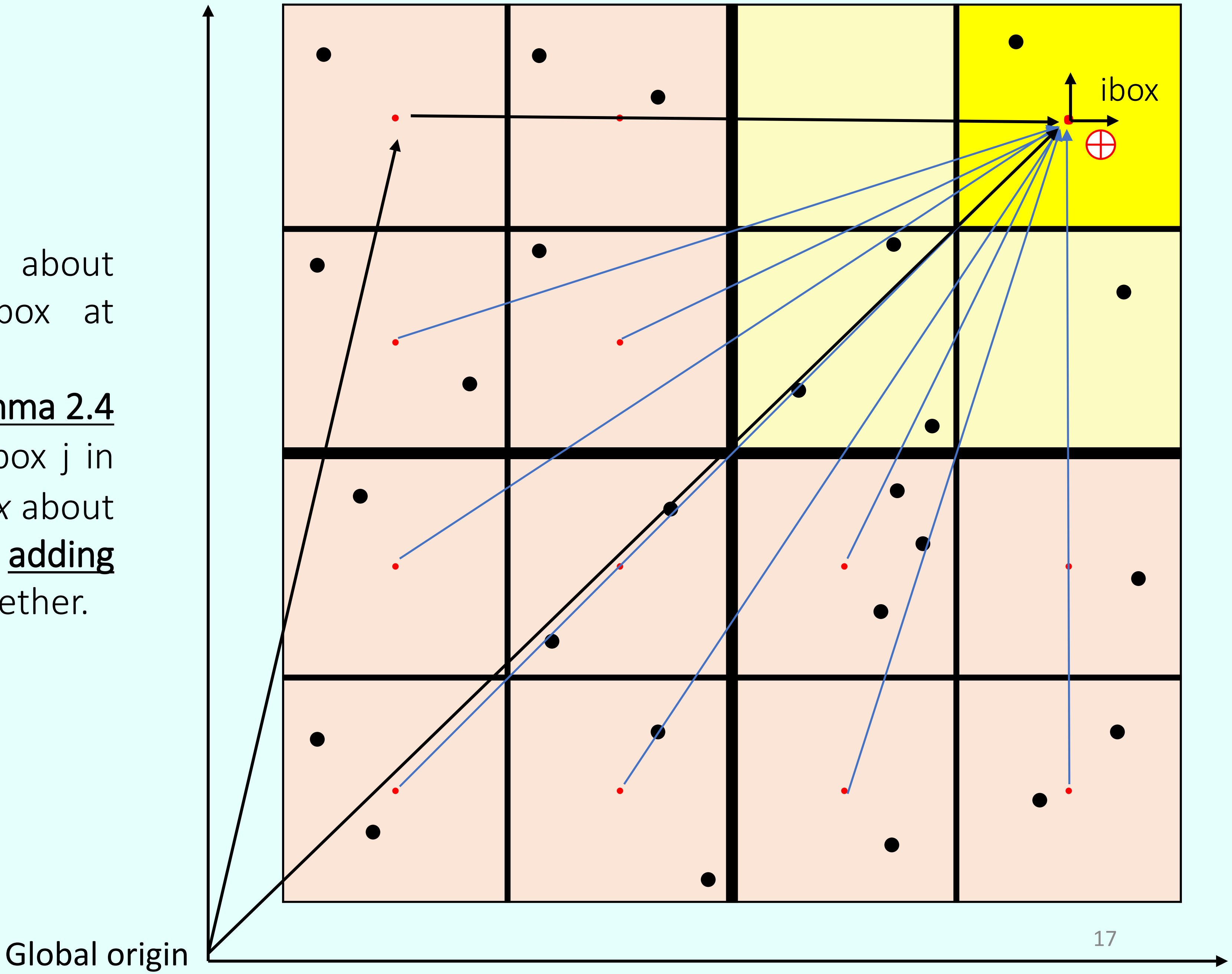
Algorithm

- Step 3

❖ Form a local expansion about the center of each box at coarser mesh $l \le n-1$

❖ Form $\Psi_{l,ibox}$ by using lemma 2.4 to convert $\Phi_{l,j}$ of each box j in interaction list of box *ibox* about the center of box *ibox*, adding these local expansion together.

❖ Adding result to $\widetilde{\Psi}_{l,ibox}$



Algorithm

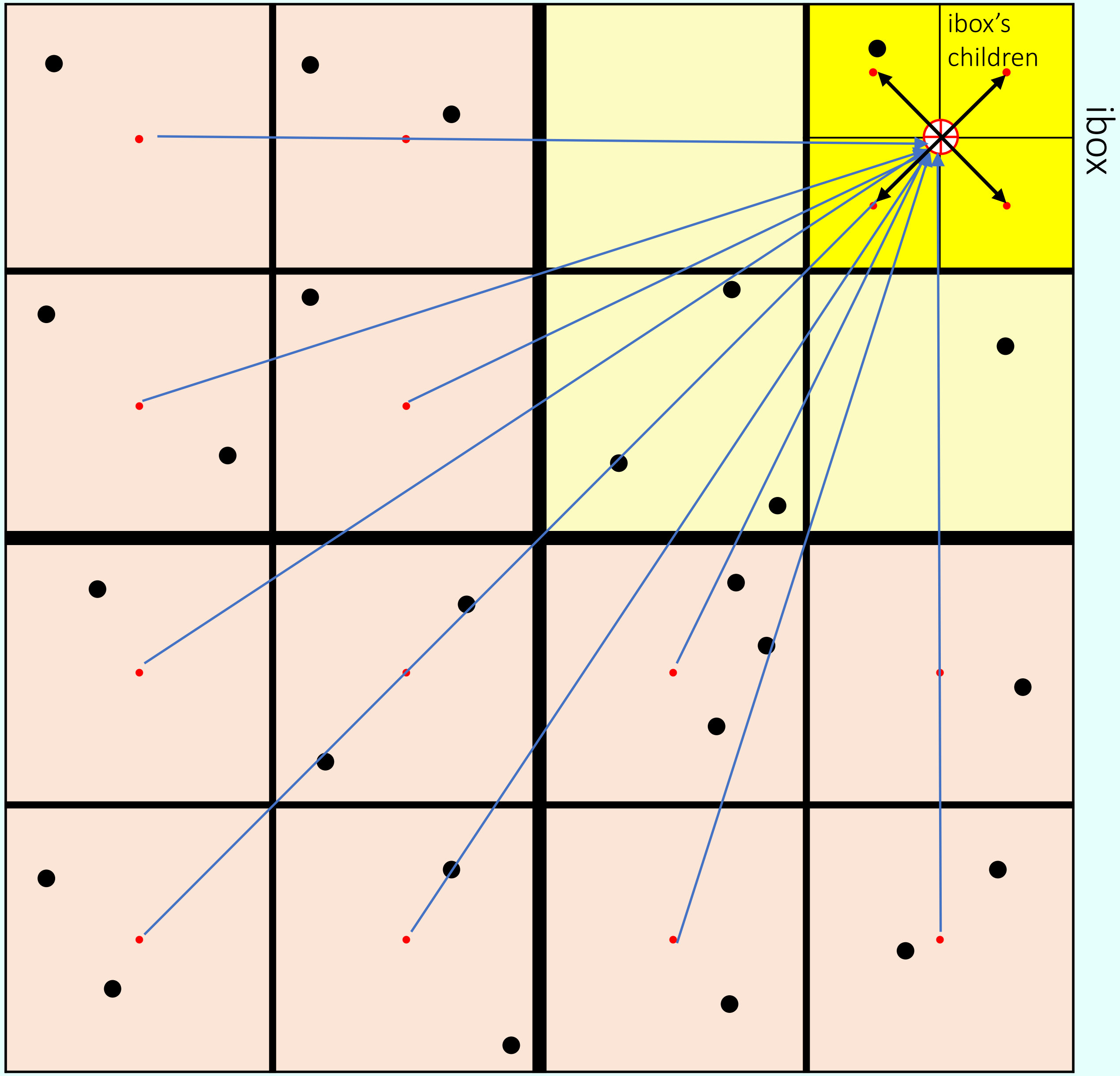
- **Step 3**

  Form $\widetilde{\Psi}_{l+1,ibox's\ children}$ by using <u>lemma 2.5</u> to <u>expand</u> $\Psi_{l,ibox}$ <u>about the children's box centers</u>.

- **Lemma 2.5**

  For any complex z_0, z and $\{a_k\}, k = 0, 1, 2, \dots, n$,

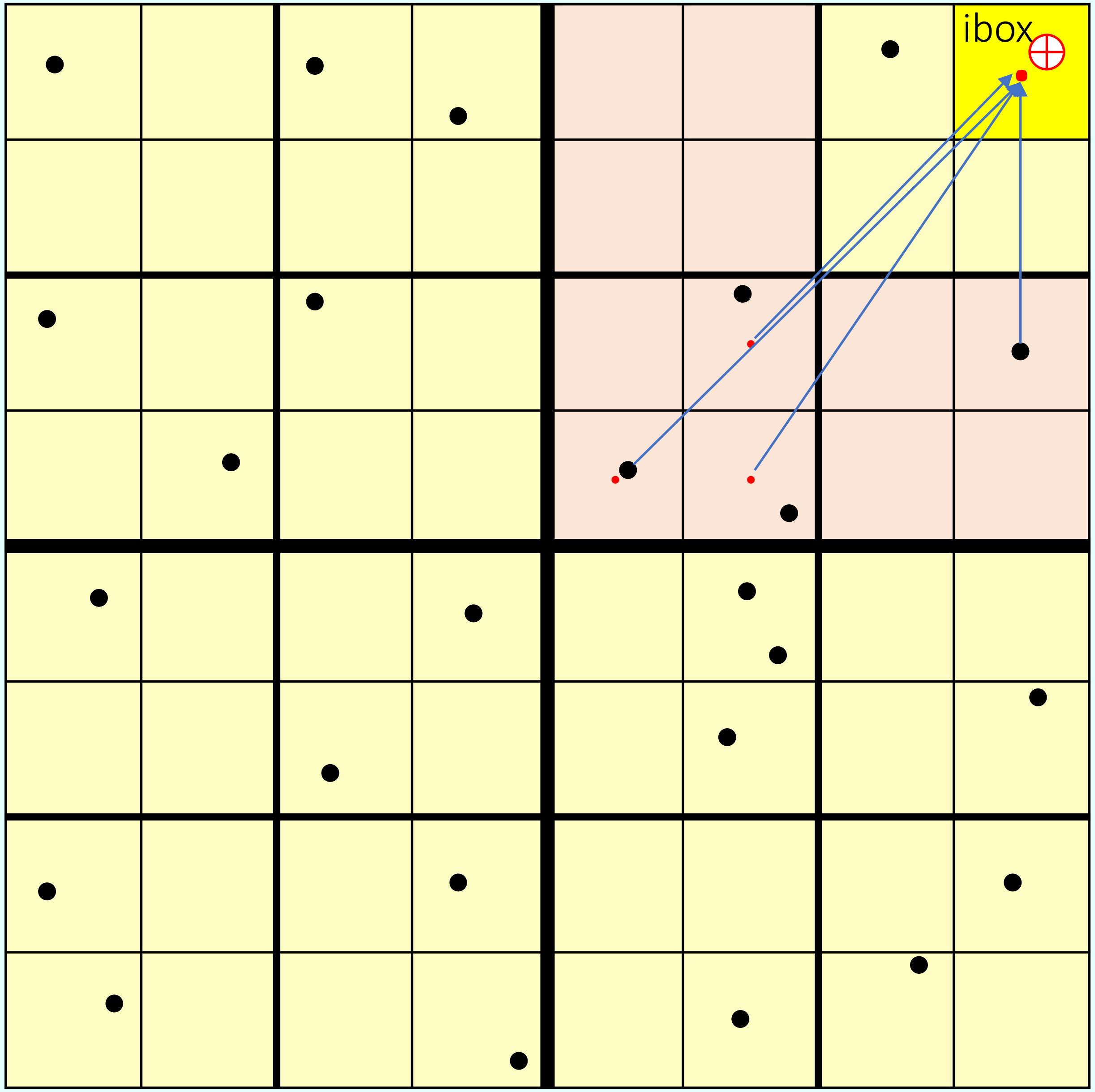
$$\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{k=0}^{n} \left(\sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right) z^l$$



Algorithm

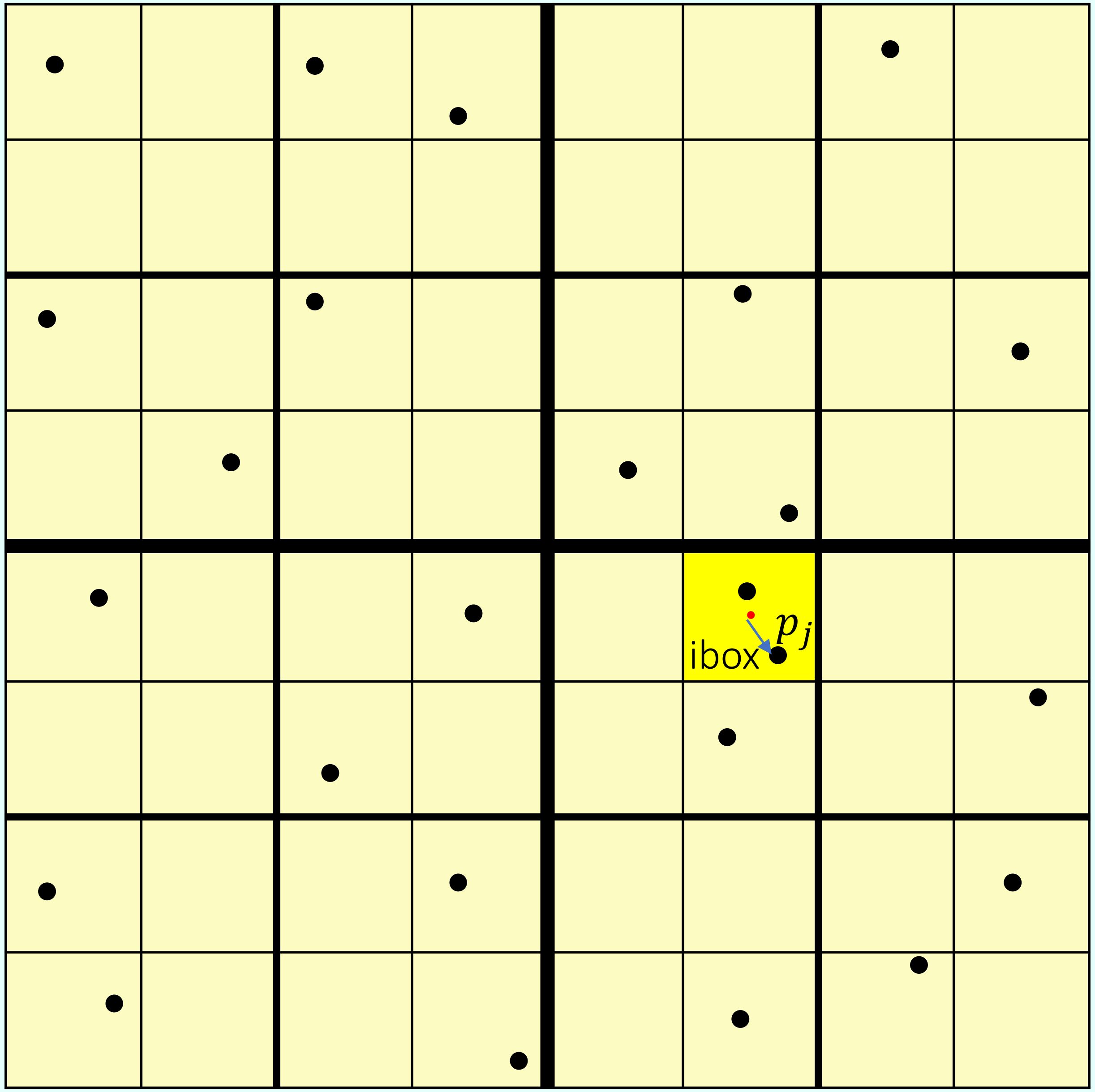
- Step 4

  - Form a <u>local expansion</u> at <u>finest</u> mesh level $l = n$
  - Form $\Psi_{l,ibox}$ by using <u>lemma 2.4</u> to <u>convert</u> $\Phi_{l,j}$ of each box j in <u>interaction</u> list of box *ibox* about the <u>center of box *ibox*</u>, <u>adding</u> these local expansion together.
  - Adding the result to $\widetilde{\Psi}_{l,ibox}$



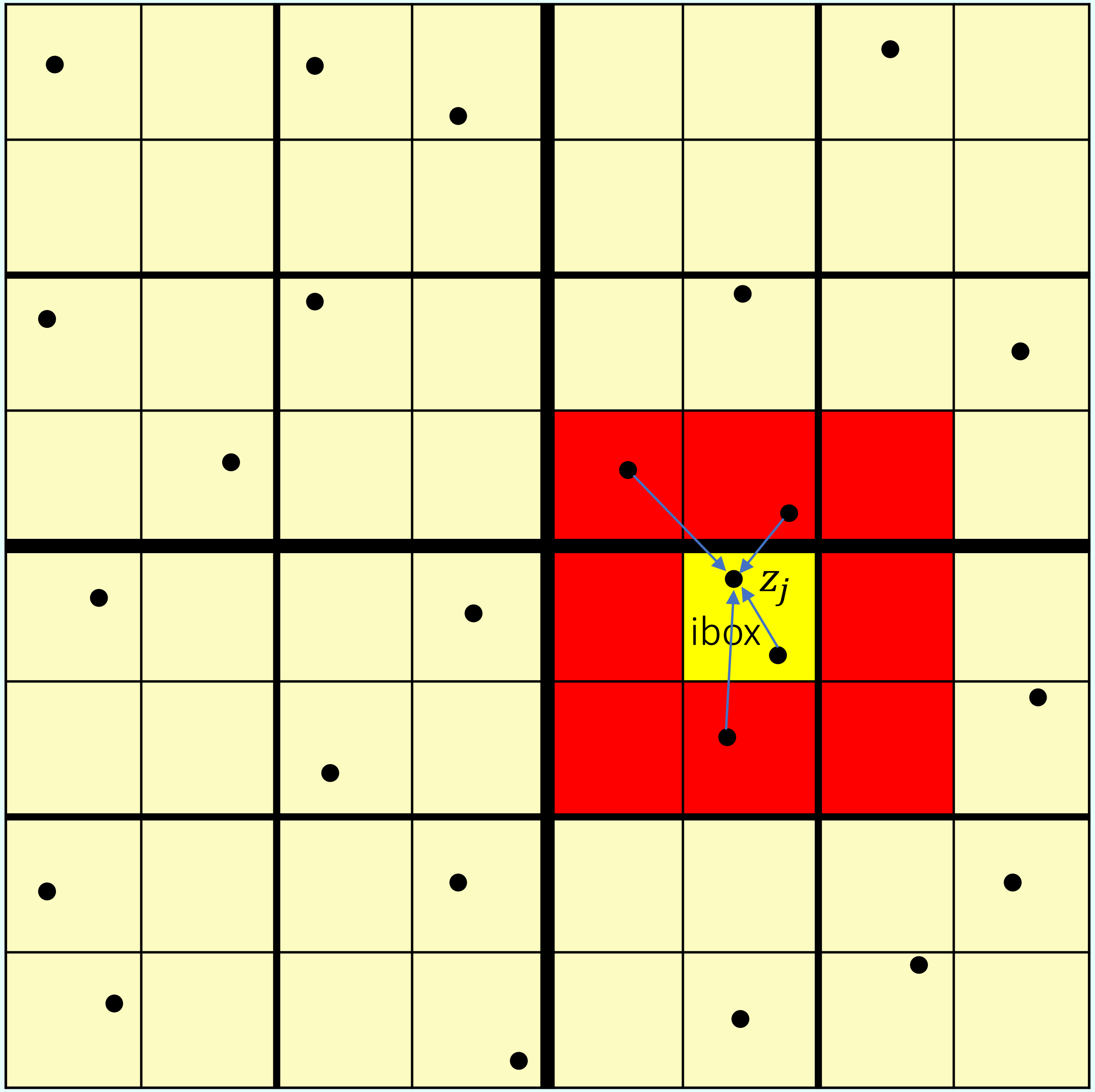
Algorithm

- Step 5
  - ❖ <u>Evaluate local expansion</u> at <u>particle positions</u>
  - ❖ For every particle p_j located at the point z_j in ibox, evaluate $\widetilde{\Psi}_{n,ibox}(z_j)$



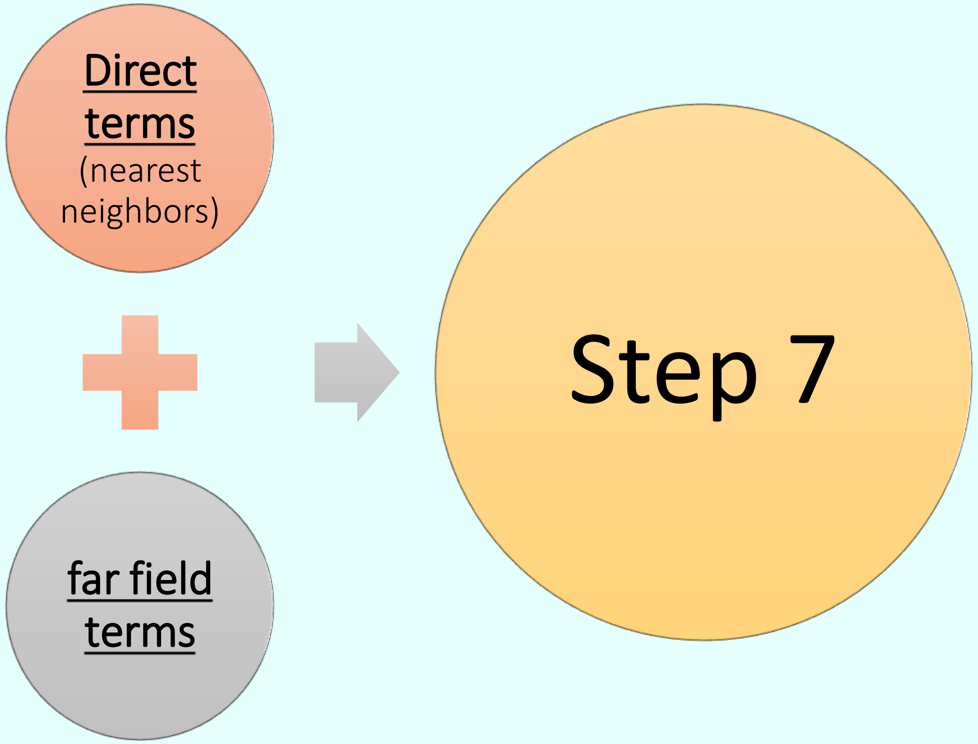
Algorithm

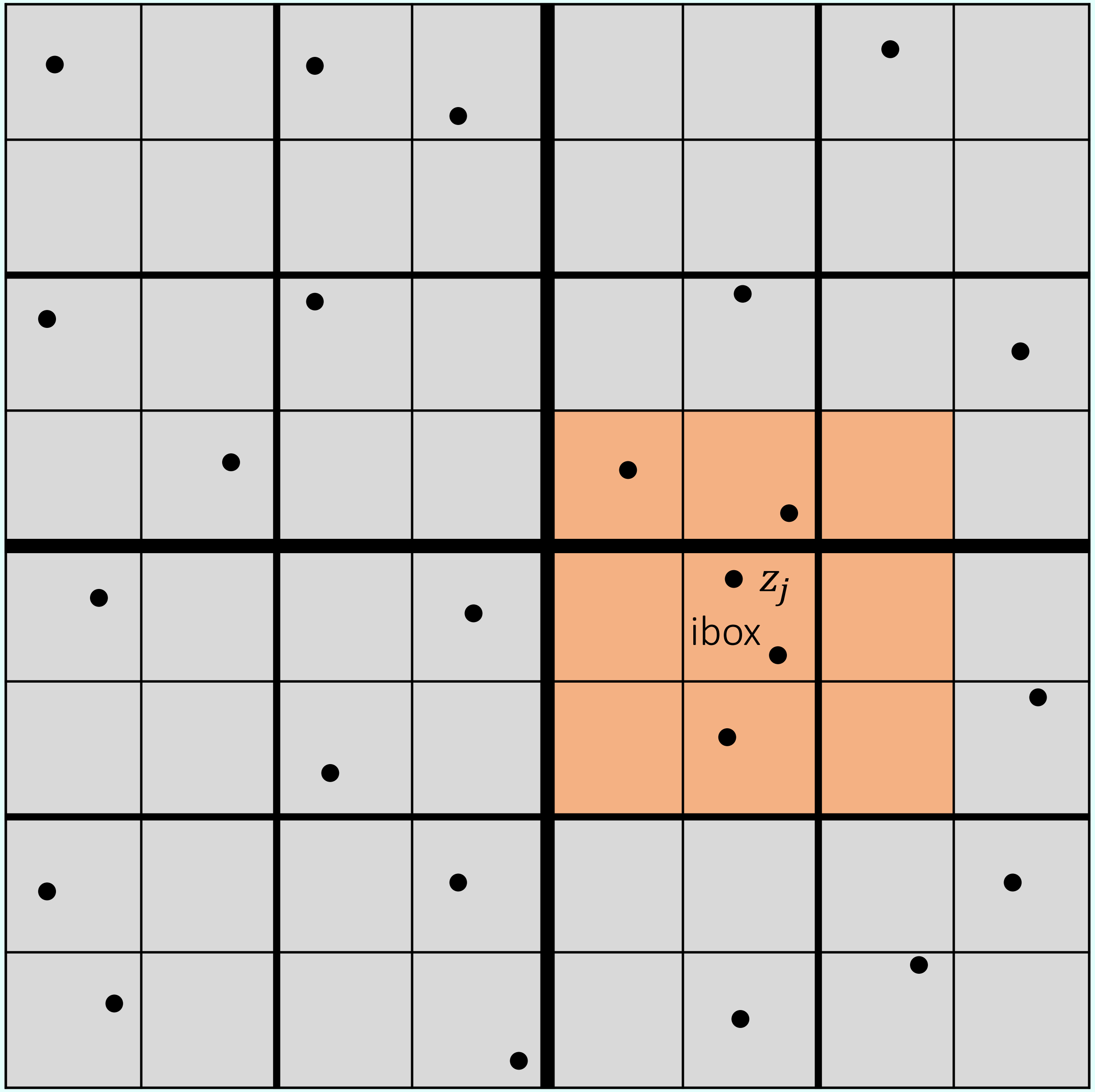
- Step 6
  - ❖ Compute <u>**potential**</u> due to <u>**nearest neighbors directly**</u>
  - ❖ For every particle p_j located at the point z_j compute interactions with all other particles within the box and its nearest neighbors.



Algorithm

- Step 7





Thank you
For your attention