Fast Multipole Method

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Problem Statement

Goal: solve the N-body problem
Requires evaluating the sum

\[ \phi_{x_i} = \sum_{j=1}^{N} G(x_i, x_j) q_j, \quad i = 1, \ldots, N \]

where the kernel G in 2-D is given by

\[
G(x, y) = \begin{cases} 
  -\log(x - y), & x \neq y \\
  0, & x \neq y
\end{cases}
\]
Multipole Expansion

Consider the case where \( N \) sources and \( M \) targets are separated.

Direct evaluation cost is \( O(MN) \).

Separation of variables yields

\[
\log(x - y) = \log(x - c) + \sum_{p=1}^{\infty} \frac{-1}{p} \frac{1}{(x - c)^p} (y - c)^p
\]

\[
\phi(x) = \log(x - c) \hat{q}_0 + \sum_{p=1}^{P} \frac{1}{(x - c)^p} \hat{q}_p
\]

\[
\hat{q}_0 = \sum_{j=1}^{N} q_j \quad \hat{q}_p = \frac{-1}{p} \sum_{j=1}^{N} (y_j - c)^p q_j
\]

Multipole expansion cost is \( O(P(M+N)) \)
Matrix Interpretation

Define $A$ such that

$$A(i, j) = \log(x_i - y_j)$$

We can rewrite $A$ as

$$A \approx BC$$

where

$$B(i, p) = \begin{cases} 
\log(x_i - c), & p = 0 \\
1/(x_i - c)^p, & p \neq 0 
\end{cases}$$

$$C(p, j) = \begin{cases} 
1, & p = 0 \\
-1/p(y_j - c)^p, & p \neq 0 
\end{cases}$$
Algorithm

Subdivide domain into grid with each box containing roughly equal number of particles
Algorithm

Form multipole expansions about box centers at finest grid level
Algorithm

Translate multipole expansions to parent box and repeat
**Algorithm**

Convert multipole expansions of boxes in interaction list to local expansion at all levels
Algorithm

Translate local expansion to children boxes and repeat
Algorithm

At leaf box level, we now have influence due to particles outside nearest neighbor boxes
Translate local expansion to particles within leaf box
Perform direct computation of potential from particles in the same leaf box and nearest neighbors
Data Decomposition: Fieldspaces

Particle
- ID
- Source strength
- Position
- Potential
- Boxes

Box
- Position
- Side length
- Parent
- Children
- Interaction list
- Neighbors
- Particle
- Expansion coefficients
Tasks

initialize_particles
create_tree
create_neighb
create_ilist

P2M
  ●  r_particles, r_boxes at leaf level

M2M
  ●  r_boxes at current and child level

M2L
  ●  r_boxes at current level

L2L
  ●  r_boxes at current and child level
eval_forces
  ●  r_particles, r_boxes at leaf level
Tasks

initialize_particles
create_tree
create_neighb
create_ilist
P2M
  •  r_particles, r_boxes at leaf level
M2M
  •  r_boxes at current and child level
M2L
  •  r_boxes at current level
L2L
  •  r_boxes at current and child level
eval_forces
  •  r_particles, r_boxes at leaf level

Partitions

•  p_particles: equal, disjoint, based on CPUs
•  p_boxes: disjoint, based on grid level
•  p_boxes_child: disjoint, children of p_boxes
•  p_boxes_ilist: aliased, interaction list of p_boxes
Scaling
Scaling

![Graph showing Strong Scaling (50000 Particles)]
Scaling (Without Initialization)
Future Work

Speed up interaction list initialization
Use unstructured regions for grid
Implement tasks for particle motion
Make scheme adaptive for non-uniform distributions