

N-Body Methods

Source:

Load Balancing and Data Locality in Adaptive Hierarchical
N-Body Methods: Barnes-Hut, Fast Multipole, and Radiosity
by Singh, Holt, Totsuka, Gupta, and Hennessy

(except Sections 4.1.2., 4.2, 9, and 10)

N-body problems

- Given are N bodies (molecules, stars, ...)
- The bodies exert *forces* on each other (Coulomb, gravity, ...)
- Problem: simulate behavior of the system over time
- Many applications:
 - Astrophysics (stars in a galaxy)
 - Plasma physics (ion/electrons)
 - Molecular dynamics (atoms/molecules)
 - Computer graphics (radiosity)

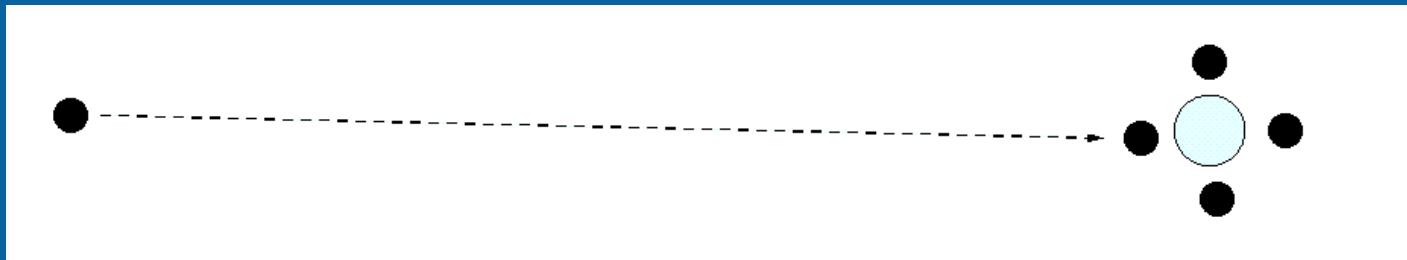
Basic N-body algorithm

```
for each timestep do
    Compute forces between all bodies
    Compute new positions and velocities
od
```

- $O(N^2)$ compute time per timestep
- Too expensive for realistic problems (e.g., galaxies)
- Barnes-Hut is $O(N \log N)$ algorithm for hierarchical N-body problems

Hierarchical N-body problems

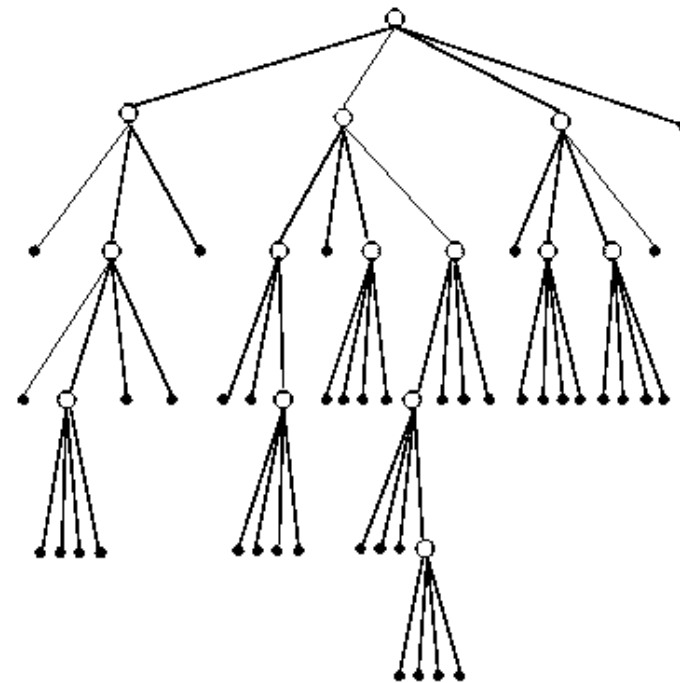
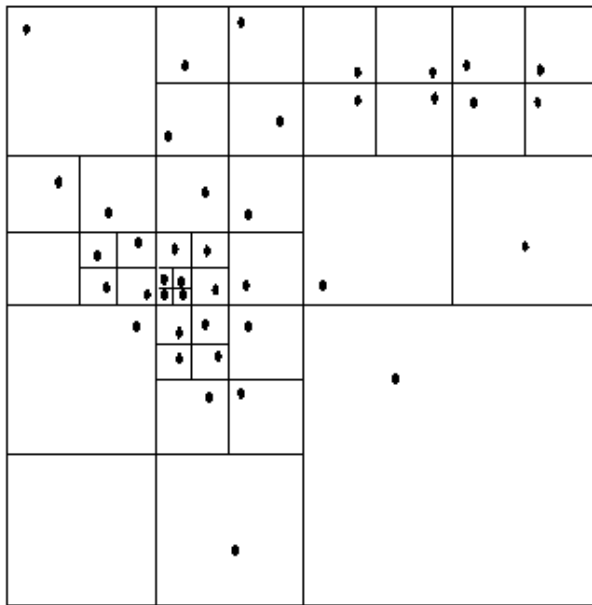
- Exploit physics of many applications:
 - Forces fall very rapidly with distance between bodies
 - Long-range interactions can be approximated
- Key idea: *group* of distant bodies is approximated by a *single* body with same mass and center-of-mass



Data structure

- Octree (3D) or quadtree (2D):
Hierarchical representation of physical space
- Building the tree:
Start with one cell with all bodies (bounding box)
Recursively split cells with multiple bodies into subcells

Example (Fig. 5 from paper)



Barnes-Hut algorithm

```
for each timestep do
  Build tree
  Compute center-of-mass for each cell
  Compute forces between all bodies
  Compute new positions and velocities
od
```

- Building the tree: recursive algorithm (can be parallelized)
- Center-of-mass: upward pass through the tree
- Compute forces: 90% of the time
- Update positions and velocities: simple (given the forces)

Force computation of Barnes-Hut

```
for each body B do
    B.force := ComputeForce(tree.root, B)
od

function ComputeForce(cell, B): float;
    if distance(B, cell.CenterOfMass) > threshold then
        return DirectForce(B.position, B.Mass,
                             cell.CenterOfMass, cell.Mass)
    else
        sum := 0.0
        for each subcell C in cell do
            sum += ComputeForce(C, B)
        return sum
```


Parallelizing Barnes-Hut

- Distribute bodies over all processors
 - In each timestep, processors work on different bodies
- Communication/synchronization needed during
 - Tree building
 - Center-of-mass computation
 - Force computation
- Key problem is efficient parallelization of force-computation
- Issues:
 - Load balancing
 - Data locality

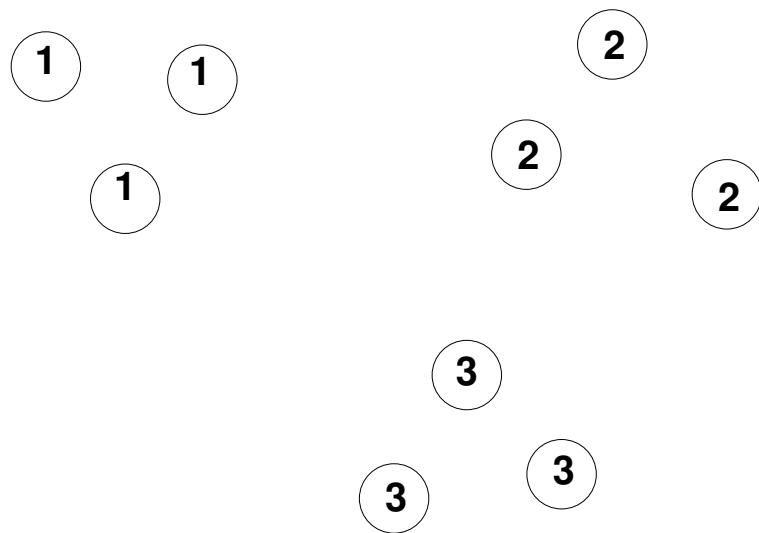
Load balancing

- Goal:
Each processor must get same amount of work
- Problem:
Amount of work per body differs widely

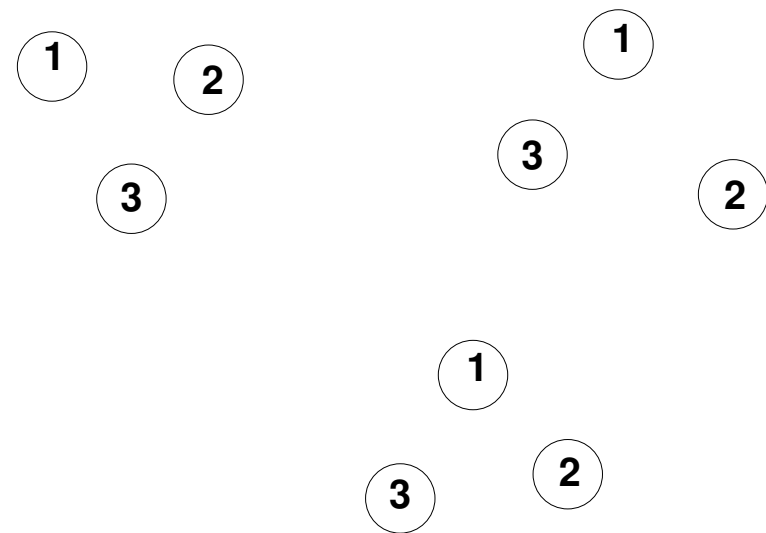
Data locality

- Goal:
 - ★ Each CPU must access small number of bodies many times
 - ★ Reduces communication overhead
- Problems
 - ★ Access patterns to bodies not known in advance
 - ★ Distribution of bodies in space changes (slowly)

Example Data locality



Good locality



Bad locality

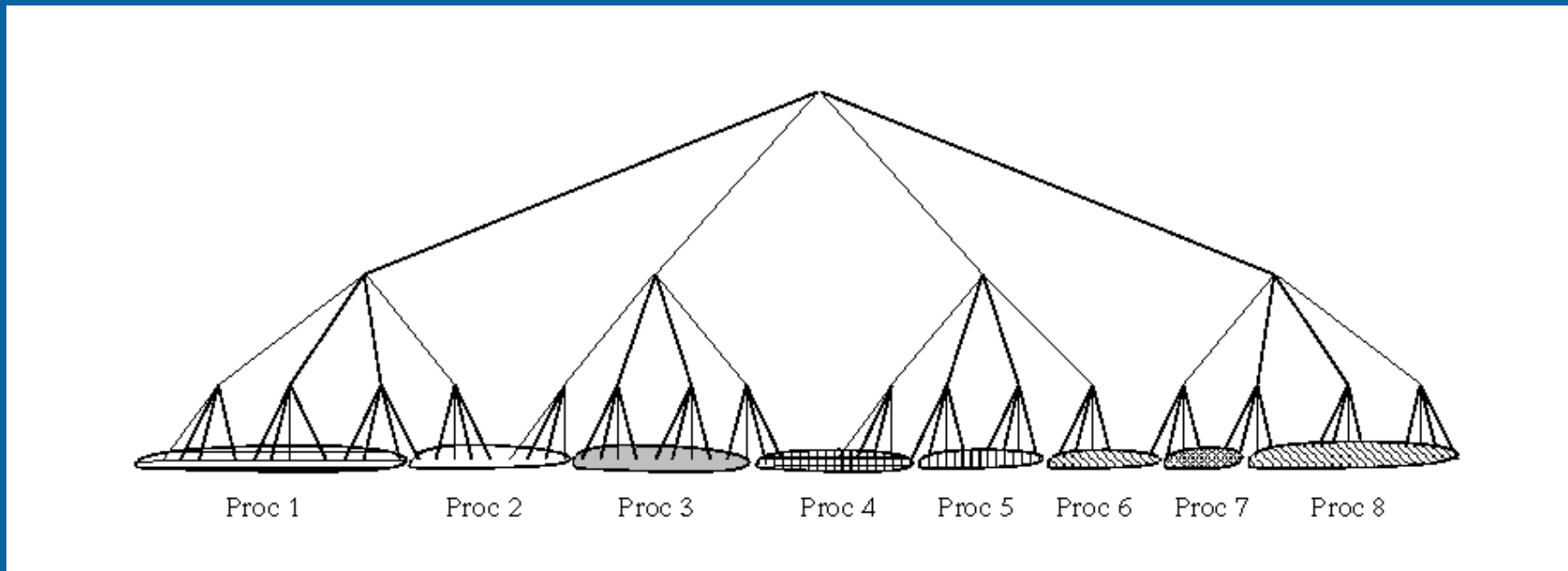
Simple distribution strategies

- Distribute iterations
Iteration = computations on single body in 1 timestep
- Strategy-1: Static distribution
Each processor gets equal number of iterations
- Strategy-2: Dynamic distribution
Distribute iterations dynamically
- Problems
Distributing iterations does not take locality into account
Static distribution leads to load imbalances

More advanced distribution strategies

- Load balancing: cost model
 - Associate a computational *cost* with each body
 - Cost = amount of work (number of interactions) during previous timestep
 - Each processor gets same total cost
 - Works well, because system changes slowly
- Data locality: costzones
 - Observation: octree more or less represents spatial (physical) distribution of bodies
 - Thus: partition the tree, not the iterations
 - Costzone: contiguous zone of costs

Example costzones



Optimization: improve locality using clever child numbering scheme

Experimental system–DASH

- DASH multiprocessor

 - Designed at Stanford university

 - One of the first NUMAs (Non-Uniform Memory Access)

- DASH architecture

 - Memory is physically distributed

 - Programmer sees shared address space

 - Hardware moves data between processors and caches it

 - Implemented using directory-based cache coherence protocol

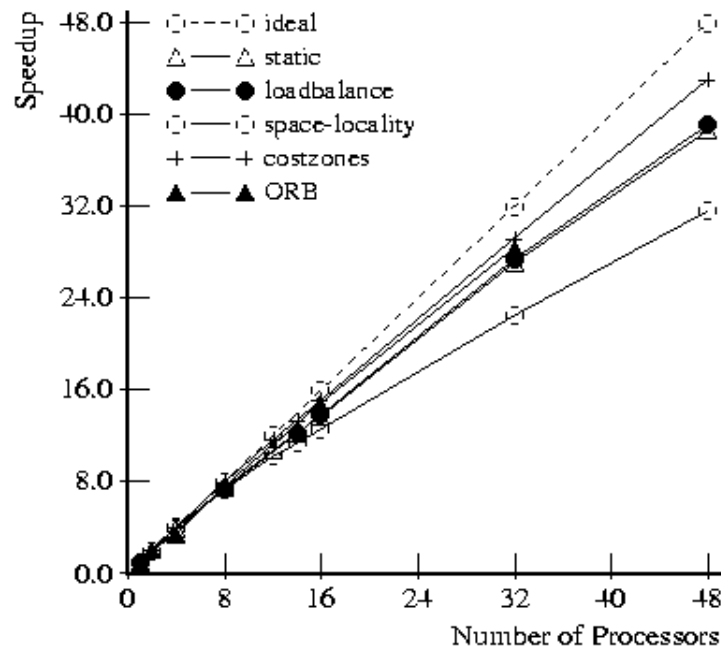
DASH prototype

- 48-node DASH system
 - 12 clusters of 4 processors (MIPS R3000) each
 - Shared bus within each cluster
 - Mesh network between clusters
 - Remote reads 4x more expensive than local reads
- Also built a simulator
 - More flexible than real hardware
 - Much slower

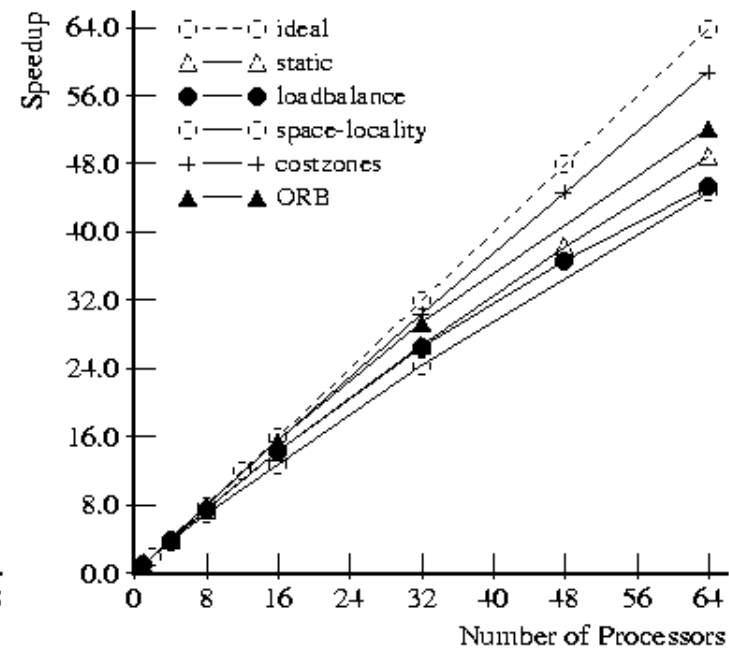
Performance results on DASH

- Costzones reduce load imbalance and communication overhead
- Moderate improvement in speedups on DASH
Low communication/computation ratio

Speedups measured on DASH (figure 17)

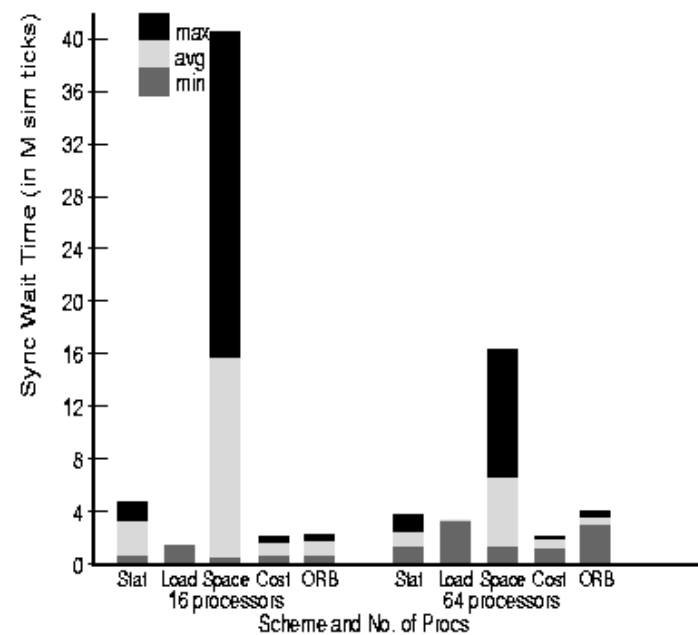


(a) 32K Particles on DASH

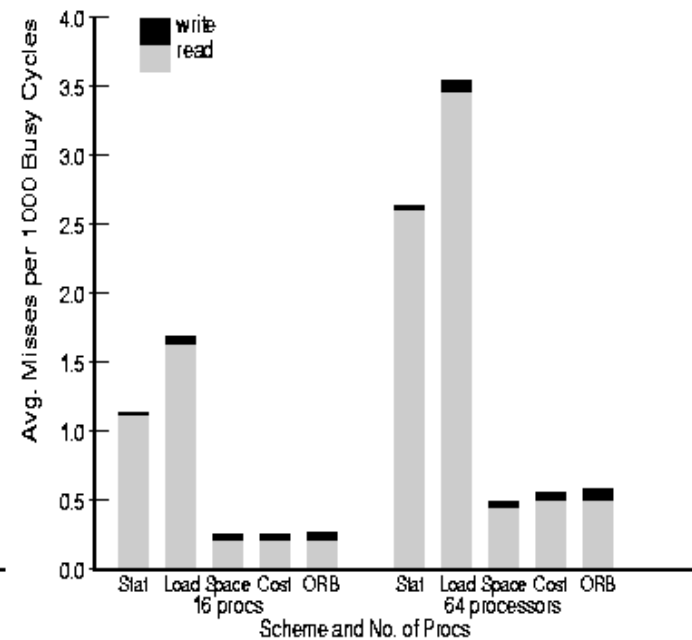


(b) 8K Particles on Simulator

Simulator statistics (figure 18)



(a) Synchronization Wait Times



(b) Communication

Conclusions

- Parallelizing efficient $O(N \log N)$ algorithm is much harder than parallelizing $O(N^2)$ algorithm
- Barnes-Hut has nonuniform, dynamically changing behavior
- Key issues to obtain good speedups for Barnes-Hut
 - Load balancing \rightarrow cost model
 - Data locality \rightarrow costzones
- Optimizations exploit physical properties of the application