Dagstuhl Seminar on
High-level parallel programming models
April 1999

The Barnes-Hut Algorithm as a case study
for parallel programming models

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Motivation

Why a case study?

- An opportunity to evaluate programming models on
  - Expressiveness
  - Performance
  - Practicality

Why consider the Barnes-Hut algorithm?

- presents non-trivial expression and performance challenges
- has been used as a case study by others
- relatively small and manageable
The *n*-body simulation problem

*Simulate the evolution of a system of *n* bodies over time.*

- Equations of motion
  - pairwise interaction potential \( f(i,j) \) between body *i* and *j*
  - total force \( f(i) \) on body *i*

- Numerical integration of equations of motion

**Applications**

- astrophysics (gravity)
- molecular dynamics (electrostatics)
- computer graphics (radiosity)

Ex: Gravitation

\[
 f(i, j) = G \cdot \frac{m_i \cdot m_j}{r_{ij}^2}
\]

\[
 f(i) = \sum_{j \neq i} f(i, j)
\]

- the basic simulation algorithm:

  ```
  while (t < t_{final}) do
      forall 1 \leq i \leq n do
          ⟨ compute force f(i) on body i ⟩
          ⟨ numerical integration step Δt ⟩
          ⟨ update velocity and position of body i ⟩
      t = t + Δt
  ```

- \( O(n^2) \) interactions per time-step
Reducing the number of interactions

exploit combined effect of “distant” bodies:

Formally

**Multipole expansion** of the interaction of a body with the entire *Andromeda* galaxy

\[ f(i) = G \frac{M m_i}{r_i^2 c} + \cdots \]

Multipole expansion saves work if it can be reused with multiple bodies

Accuracy of truncated multipole expansion improves with

- increasing \( r \)
- decreasing \( d \)
- retained terms in expansion
- uniformity of particle distribution

apply this idea *recursively*:

- determines control-structure
- determines hierarchical decomposition of space
Hierarchical decomposition of space: quad- and octtrees
The Barnes-Hut algorithm

\[
\text{stepSystem():}
\]

\[
T := \text{makeTree}(P(1:n))
\]

\[
\text{forall } 1 \leq i \leq n \text{ do}
\]

\[
f(i) := \text{gravCalc}(P(i), T)
\]

\[
\langle \text{update velocities and positions} \rangle
\]

\[
\text{function gravCalc}(p, q)
\]

\[
\text{if } \text{"q is a leaf"} \text{ then}
\]

\[
\langle \text{return body-body interaction} \rangle
\]

\[
\text{else}
\]

\[
\text{if } \text{"p is distant enough from q"} \text{ then}
\]

\[
\langle \text{return body-cell interaction} \rangle
\]

\[
\text{else}
\]

\[
\text{forall } q' \in \text{nonemptyChildren}(q) \text{ do}
\]

\[
\text{accumulate } \text{gravCalc}(p, q')
\]

\[
\langle \text{return accumulated interaction} \rangle
\]

\[
\text{end if}
\]

\[
\text{end if}
\]

interaction in the case of gravitation:

\[
F = G \frac{m_p \cdot m_q}{r_{pq}^2} \cdot \left[ \frac{x_p - x_q}{r_{pq}}, \frac{y_p - y_q}{r_{pq}}, \frac{z_p - z_q}{r_{pq}} \right]
\]

\[
r = \sqrt{(x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2}
\]

**body-body interaction**: use masses of particles and distance between them.

**body-cell interaction**: use mass of particle and cell and distance between particle and center of mass of cell.

force is additive; individual contributions can be accumulated.
The Barnes-Hut algorithm - Performance issues

```plaintext
stepSystem(P(1:n))

T := makeTree(P(1:n))
forall i := 1 to n do
  f(i) := gravCalc(P(i), T)
  \langle update velocities and positions \rangle
```

Parallelism
- nested parallelism
  - over bodies
  - over recursively divided cells
- load balance
  - different number of interactions for different bodies

Locality
- nearby bodies interact with similar set of nodes in T

```plaintext
function gravCalc(p, q)
  if ("q is a leaf") then
    \langle return body-body interaction \rangle
  else
    if ("p is distant enough from q") then
      \langle return body-cell interaction \rangle
    else
     forall q' \in nonemptyChildren(q) do
        accumulate gravCalc(p, q')
      \langle return accumulated interaction \rangle
    end if
  end if
end function
```
The acceptance criterion

when is a cell “distant enough”? original criterion used by Barnes-Hut:

\[
\frac{d}{r} < \theta \equiv r > \frac{d}{\theta}
\]

where usually \(0.7 < \theta < 1.0\)

problem: detonating galaxy anomaly (one) solution: _add distance between center of mass (cm) and geometric center of cell (c)._

\[
r > \frac{d}{\theta} + |cm - c|
\]
Effects of acceptance criterion … on runtime

Effects of acceptance criterion … on accuracy

Fig. 6.—Magnitude of the typical error (in percent) in the tree force computation, relative to a direct sum, as a function of $\theta$, for selected values of the particle number $N$. The calculations have assumed spherical, isotropic Plummer models with softening parameter $\epsilon = 0$, and only monopole terms have been included in the force computations.


1% accuracy sufficient for most astrophysical simulations. Different techniques with better error control necessary for other systems (*fast multipole methods*).
Effect of body distribution … on tree depth

Plummer model

Uniform distribution
Parameters of the Barnes-Hut algorithm

- Initial configuration of bodies
  - number of bodies \( n \)
  - dimensionality of the simulation
  - distribution of bodies
    - uniform density (random placement)
    - plummer model

- Acceptance criterion
  - when can a body-cell interaction be used?

- Tree properties
  - number of bodies per leaf
  - update strategy

- Retained terms in multipole expansion
  - monopole, quadrupole, ...

- Integration method and time step

- Form of potential
  - gravity, electrostatics, ...

Suggested parameter settings

- Initial configuration
  - parameter \( n \)
  - 3D
  - Plummer 1 (Barnes)

- Acceptance criterion
  - (Barnes)

- Tree properties
  - single body per leaf
  - strict update

- Retained terms
  - monopole, quadrupole

- Integration method
  - (Barnes)

- Form of potential
  - Gravity (Barnes)
Summary of issues for BH

How can it be expressed?
- sophisticated algorithm with
  - complex data and control structure
  - sources of parallelism and locality

What performance can be obtained and how?
- cost model
  - accuracy and tractability
- accessibility of performance factors
  - memory hierarchy
  - communication
  - load-balance
- performance portability
  - architectural requirements and commitments

How practical is the approach?

Workshop presenters who will include some discussion of BH
- Manuel Chakravarty
- Ralf Ebner
- Kevin Hammond
- Gabi Keller
- Paul Kelly
- Christoph Kessler
- Jan Prins

Website for details
http://www.score.is.tsukuba.ac.jp/~chak/dagstuhl/bh