A High Performance Implementation of the 2D N-Body Gravitational Problem

Benchmark of the Barnes-Hut algorithm compared to the Brute-Force algorithm

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June 23, 2016

Parallel and High-Performance Computing - Spring Semester 2016
EPFL-CSE

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Project Description

Introduction

Purpose of this project:

- Write a fast program to solve a problem
- Use the knowledge of optimization learned during the course
- Use MPI to implement a parallel version
- Compare the theory with the numerical results

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Use-case: 2D N-Body Gravitational problem

N-Body Gravitational problem - Theory

Gravitational force of body i on body j:

$$\vec{F}_{i\to j} = G \cdot \frac{m_i m_j(\vec{x}_j - \vec{x}_i)}{\|\vec{x}_j - \vec{x}_i\|^3}$$

where G is the gravitational constant, m_i, m_j are the masses and $\vec{x}_i$, $\vec{x}_j$ are the positions.

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At each iteration, we will have for body j:

$$\vec{F}_j = \sum_{i=1}^{n} \vec{F}_{i \to j}$$

We can then update it:

$$\vec{v}_j = \vec{v}_j + \frac{dt}{m_j} \cdot \vec{F}_j \qquad \vec{x}_j = \vec{x}_j + dt \cdot \vec{v}_j$$

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How can we compute all the interactions between all the bodies?

Algorithms

- **Brute-Force**
    - Compute all the interactions between all the bodies
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  - Compute all the interactions between all the bodies
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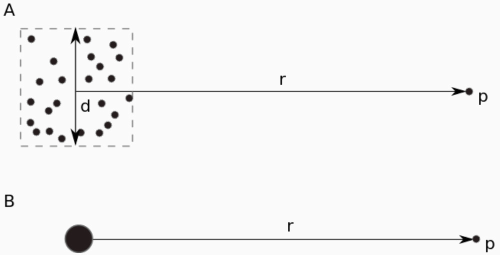
- **Barnes-Hut**
  - Approximation of the far bodies to compute all the forces on a body
  - Not that difficult to implement. (Require more lines of code)
  - Complexity: $\mathcal{O}(n \log n)$

Barnes-Hut algorithm in details

General idea

Idea of this algorithm:

- Use a precision parameter θ to approximate the forces of the far bodies using the center of mass



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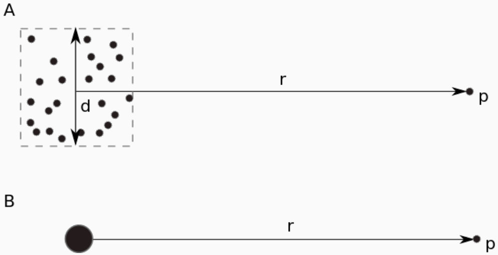
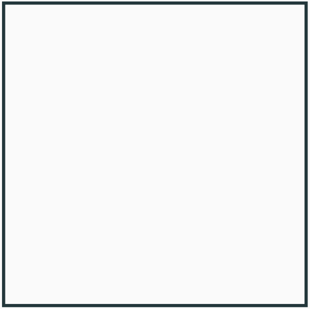


How can we do this? $\Rightarrow$ Use a quadtree and the CM of the nodes.

Quadtree

- A quadtree is a tree with four children
  (for the four directions NE, NW, SE and SW)
- In each leaf, there's a maximum of 1 body.
- If a body is added in a leaf with a body, we split the leaf in 4 parts.
  And we add the two bodies to its children.

Quadtree



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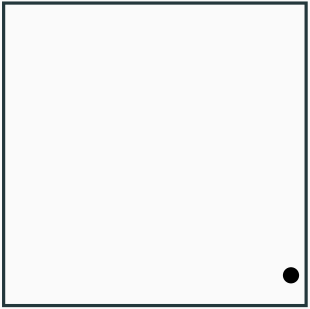

1 body ●

Quadtree

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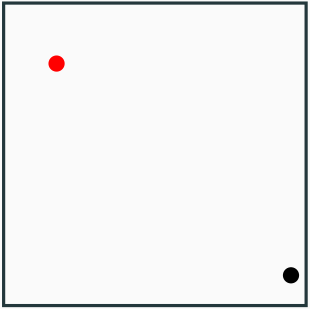

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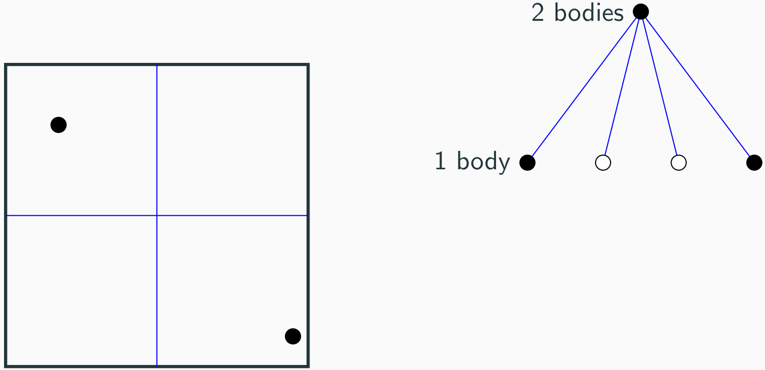

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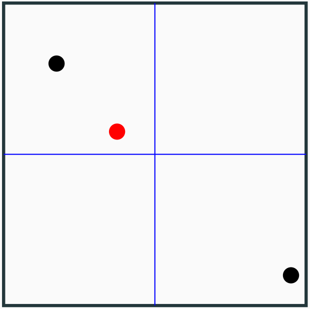

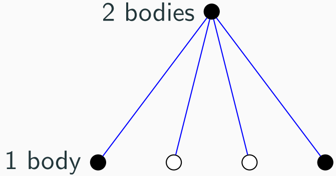

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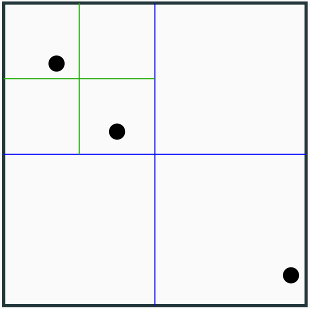

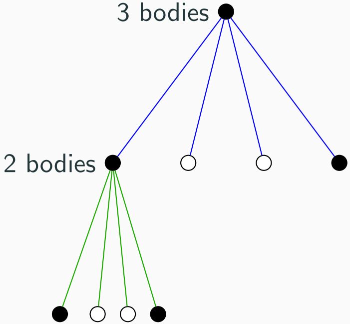

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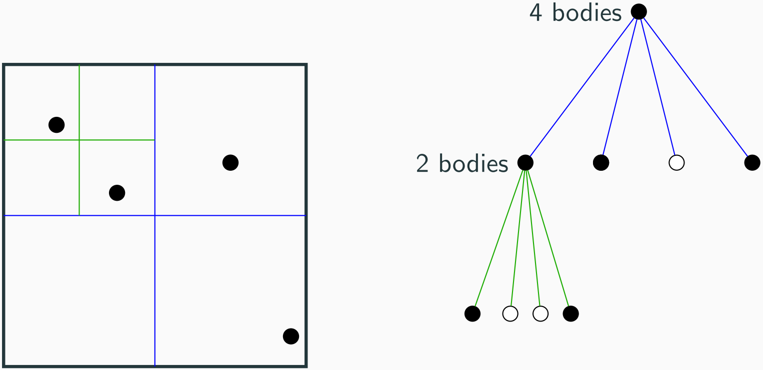

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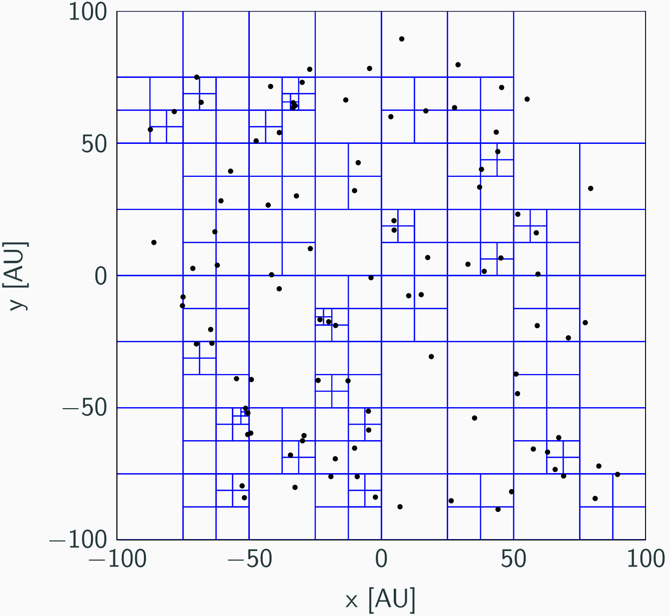

Pseudo-code (with MPI)

Algorithm Barnes-Hut

```
Read config file
Broadcast information to all processes
Build Quadtree
while t < t_end do
    Assign nodes to process
    Compute forces for the bodies in the corresponding nodes
    Update the bodies
    Gather all the bodies
    Rebuild Quadtree
    Write some information in files
```

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Read *config* file
Broadcast information to all processes
Build Quadtree
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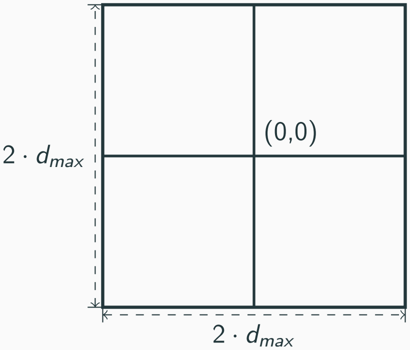
1. Lost bodies and collisions?
2. Load-Balancing?
3. Computing the forces?

Lost bodies and collisions

Define maximum distance maximum distance d_{max} such that:



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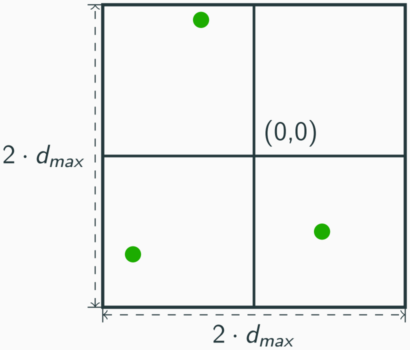

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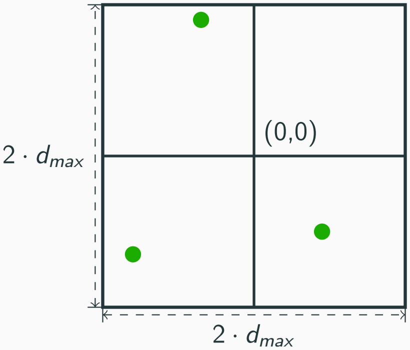

Too far!

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Therefore, we define a distance d_{min}. The conditions to do a collision are:

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2. `0.5*(node.width+node.height)` $< d_{min}$

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The new body is defined by:

$$\vec{x}_{new} = \frac{m_i \vec{x}_i + m_j \vec{x}_j}{m_i + m_j}$$

$$\vec{v}_{new} = \frac{m_i \vec{v}_i + m_j \vec{v}_j}{m_i + m_j}$$

$$m_{new} = m_i + m_j$$

Load-Balancing

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Therefore, we need to put approximately the same number of bodies in each process.

To achieve that, we can walk in the tree and assign nodes to the processes. Each process can contain n_{max} bodies. If we assign a node to a process, then all the bodies in the children nodes will be assigned to the process.

For maximizing the performance, the nodes assigned to a process should be as close as possible.

Computing the forces

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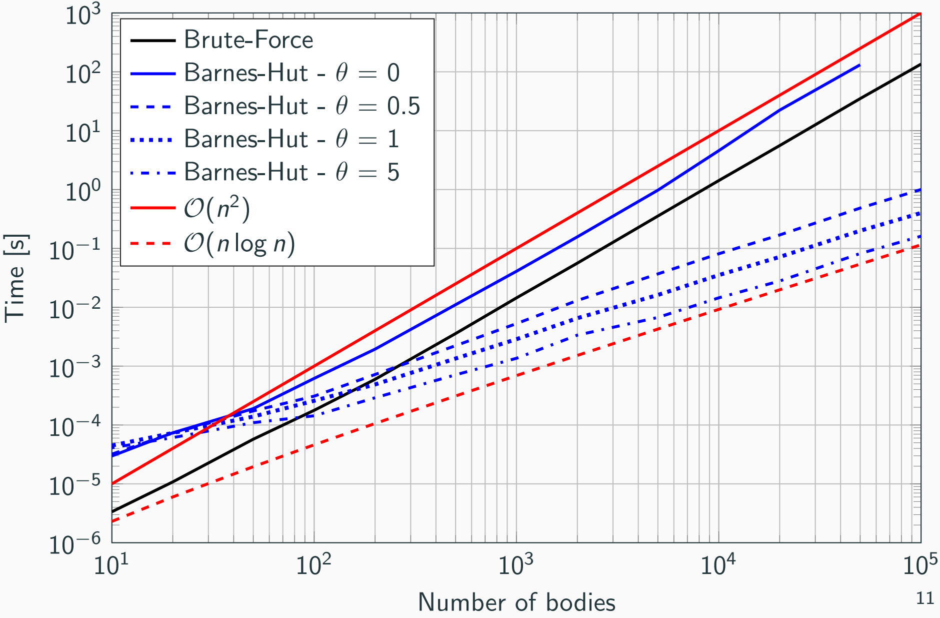
Algorithm Approximation of the force

```
dist = node.distance(body);
if !node.isLeaf then
    if 0.5*(node.width+node.height)/dist <= theta then
        node.applyForcesOnBody(body);
    else
        Continue recursion with the children
else
    if node.containsBody then
        node.localBody.applyForcesOnBody(body);
```

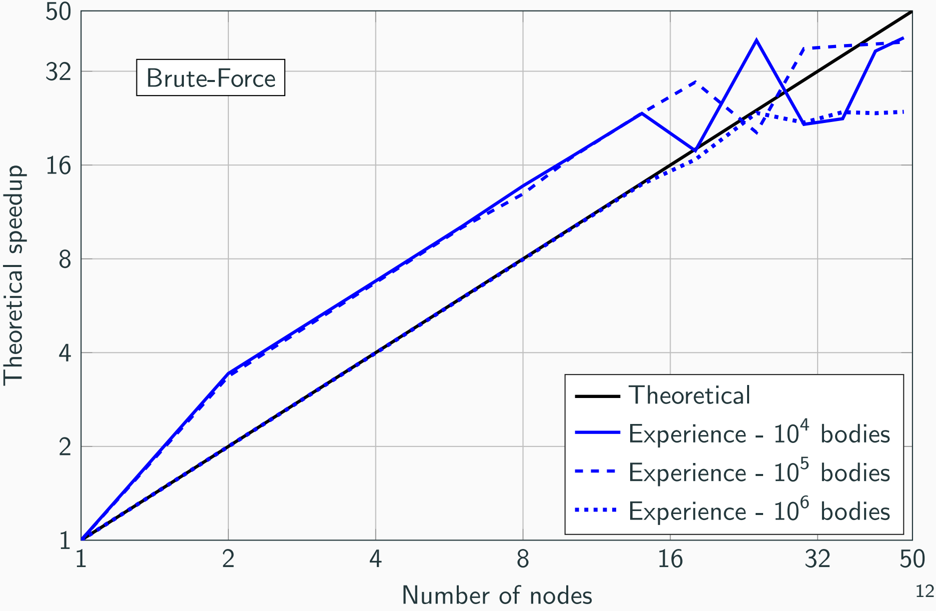
Results

Complexity



Brute-Force
Barnes-Hut - $\theta = 0$
Barnes-Hut - $\theta = 0.5$
Barnes-Hut - $\theta = 1$
Barnes-Hut - $\theta = 5$
$\mathcal{O}(n^2)$
$\mathcal{O}(n \log n)$
Time [s]
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
Number of bodies

Strong Scaling



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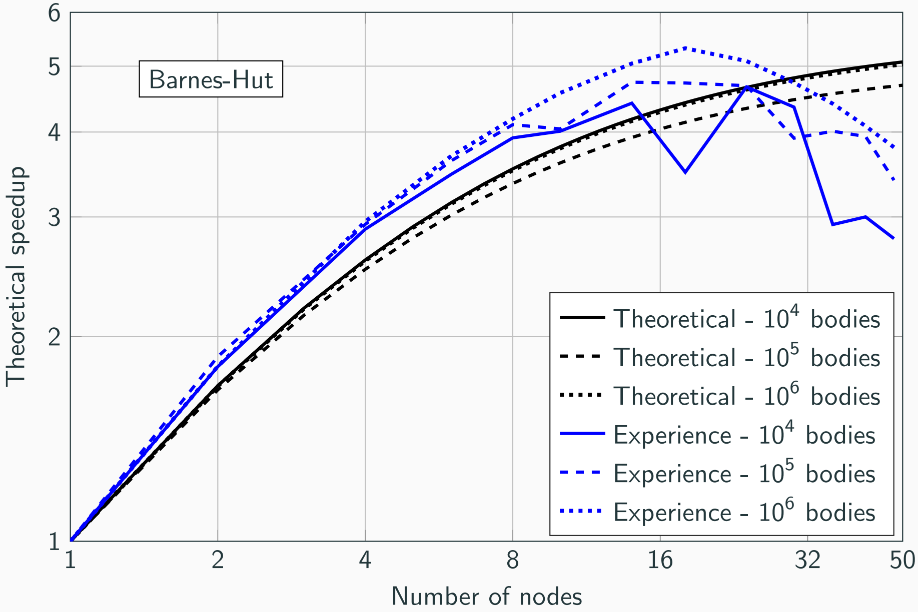
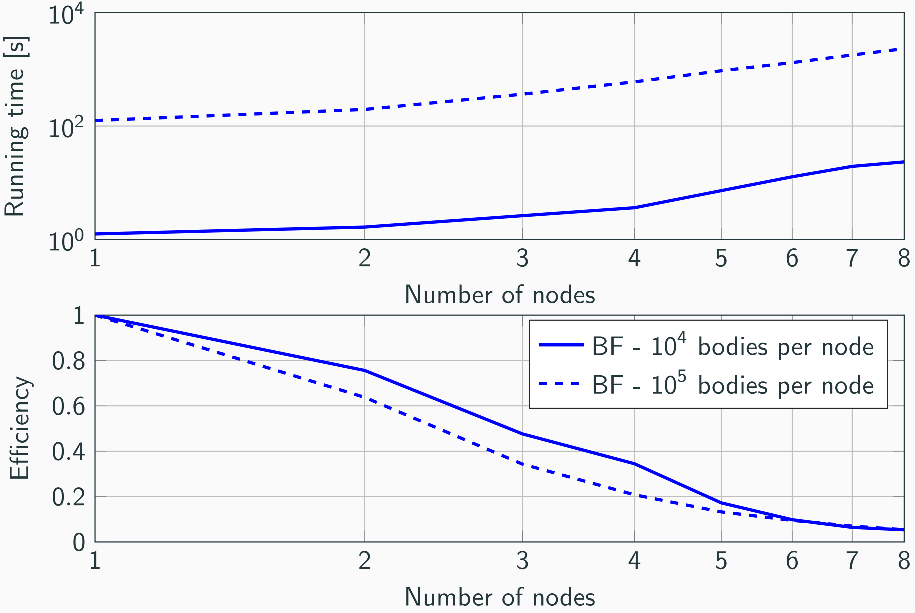


Weak Scaling



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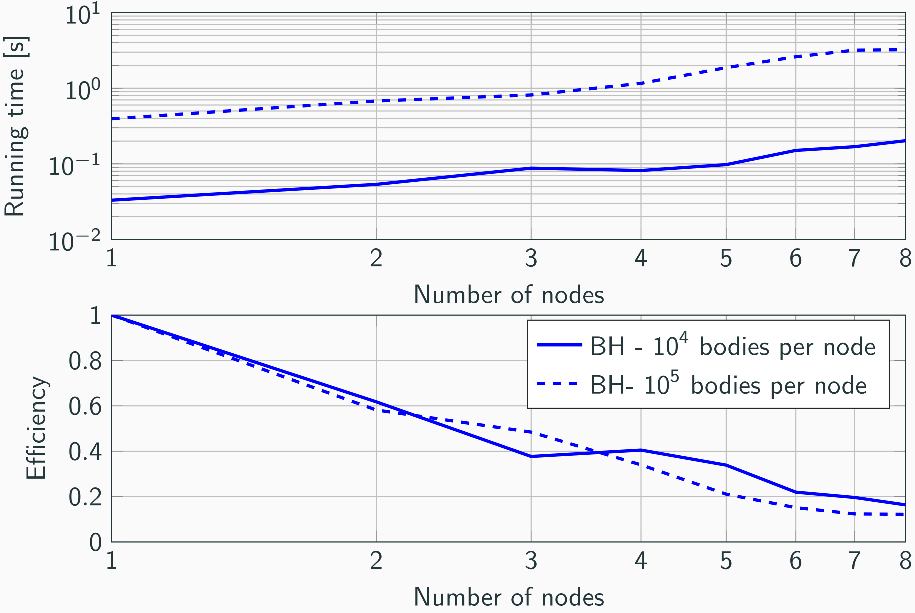

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How can we make it better?

- Use MPI I/O to write the positions of the bodies
- Implement a heuristic for the construction of the tree
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- Use a sorting algorithm for the bodies to build the tree in parallel
- Use RK4 (or another schema) to update the bodies

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What did we learn?

- A clever algorithm in serial can be better (and more ecological) than an easy parallel algorithm.
- Complex serial algorithm can be "easily" updated to a parallel version
- We can always make an algorithm faster. But is it worth it?

Thank you

n-Body simulation of the Solar System

Algorithm: Barnes-Hut

Number of bodies: 1 million

(Sun, 8 planets and 999'991 asteroids)

Length: 10'000 days

(2'000 time steps are shown)