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

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

Gael Lederrey

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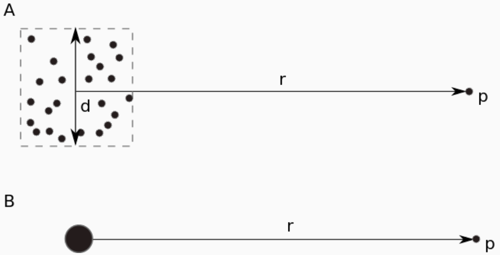
- **Barnes-Hut**
  - Approximation of the far bodies to compute all the forces on a body
  - Not that difficult to implement. (Require more lines of code)
  - Complexity: $\mathcal{O}(n \log n)$

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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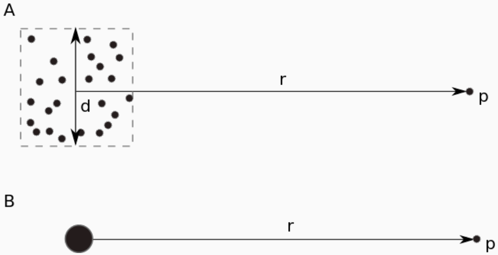
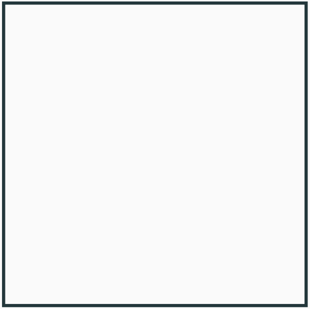


How can we do this? $\Rightarrow$ Use a quadtree and the CM of the nodes.

Quadtree

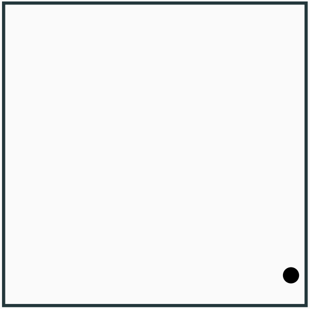
- A quadtree is a tree with four children
  (for the four directions NE, NW, SE and SW)
- In each leaf, there's a maximum of 1 body.
- If a body is added in a leaf with a body, we split the leaf in 4 parts.
  And we add the two bodies to its children.

Quadtree



Quadtree

1 body ●



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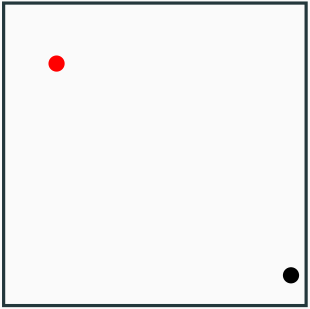

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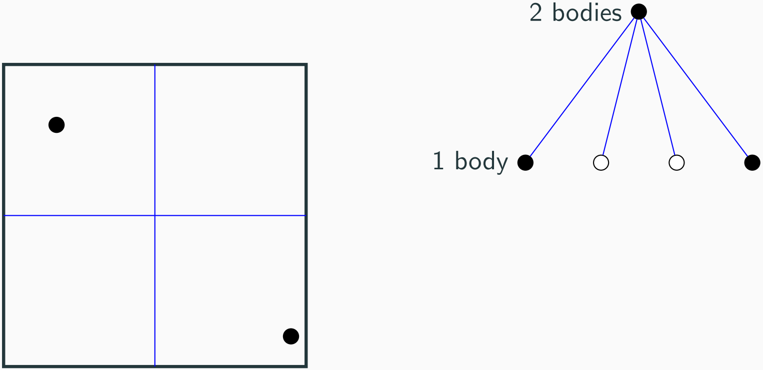

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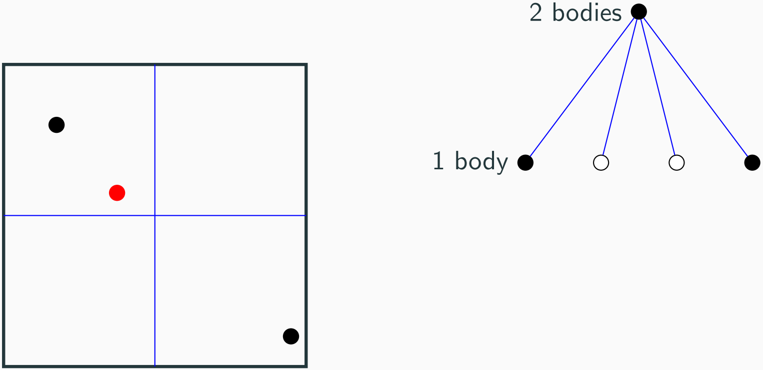

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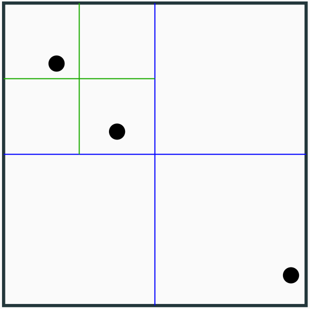

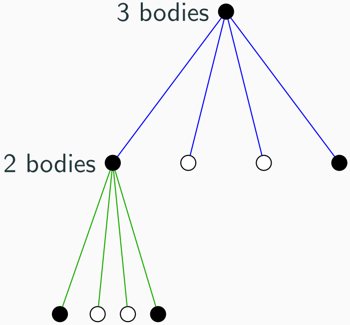

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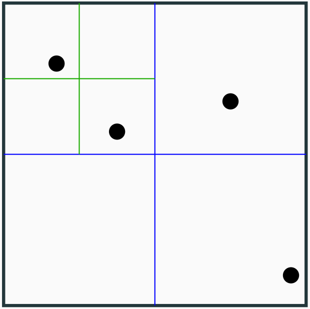

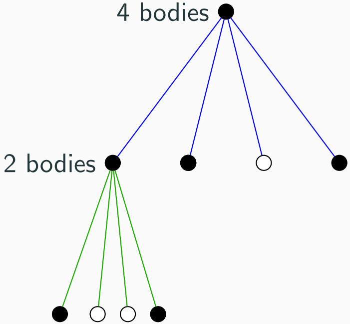

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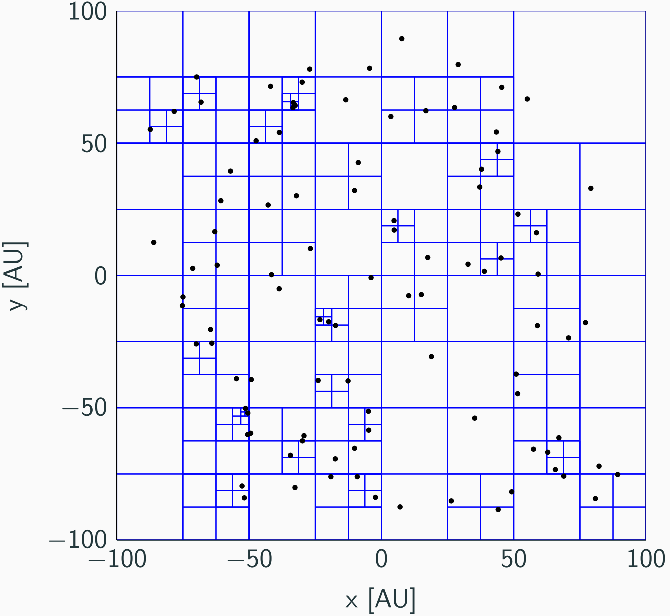

Pseudo-code (with MPI)

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
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Write some information in files

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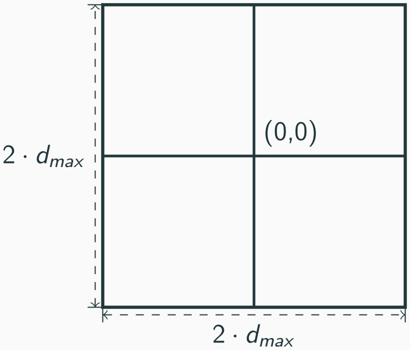
```

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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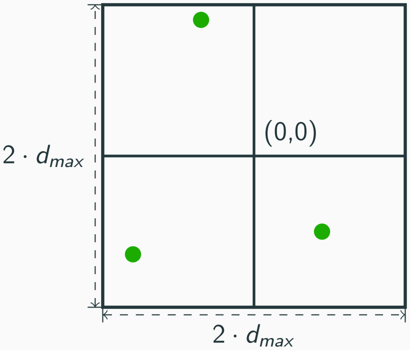

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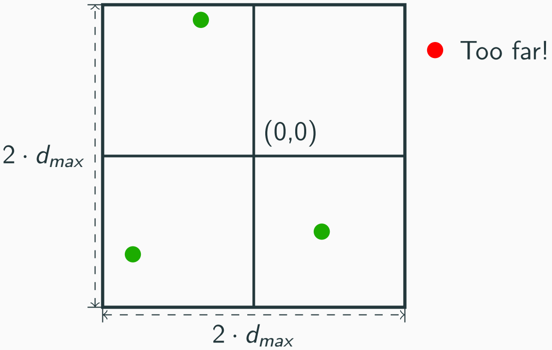

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The new body is defined by:

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

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

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

Load-Balancing

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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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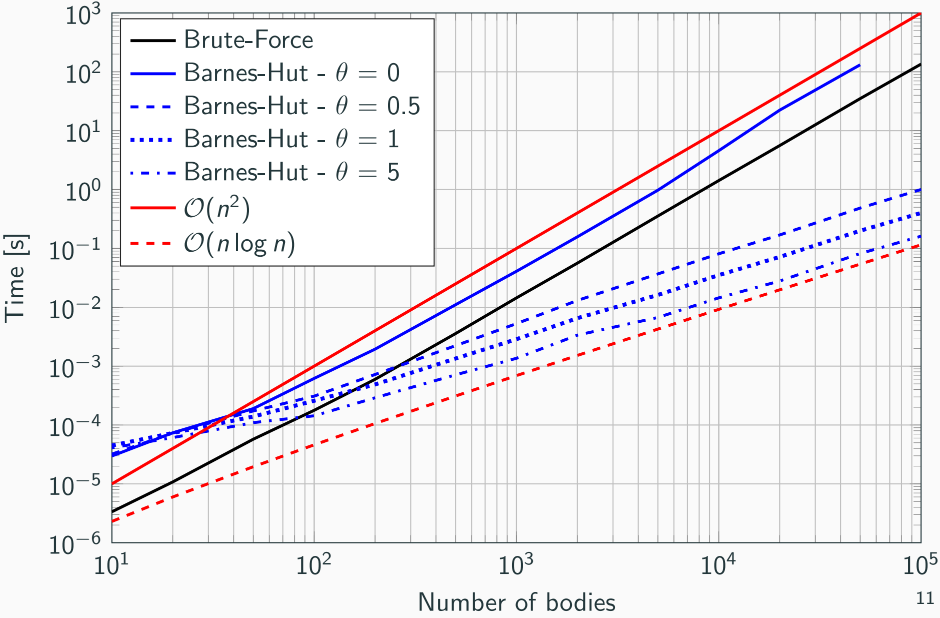
Algorithm Approximation of the force

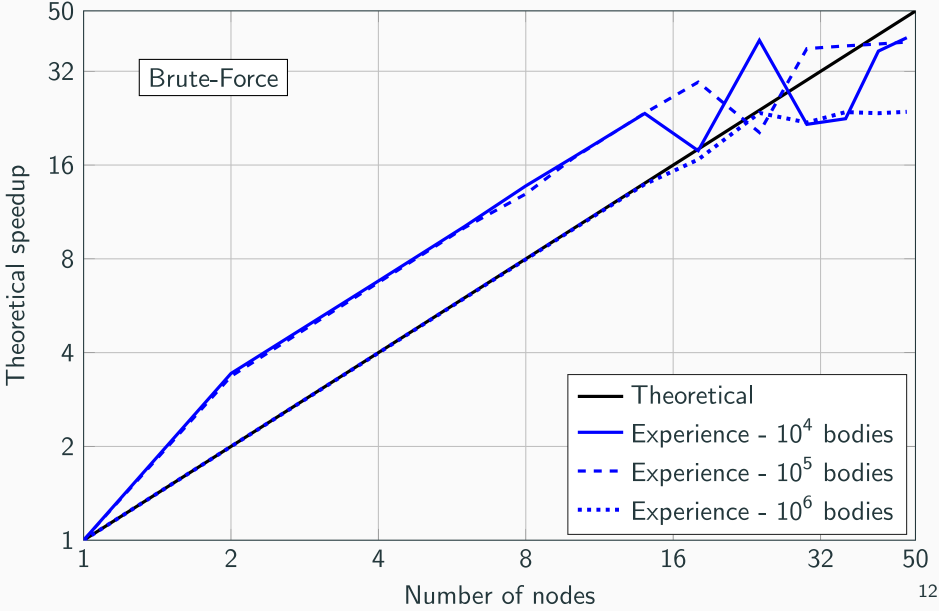
```
dist = node.distance(body);
if !node.isLeaf then
    if 0.5*(node.width+node.height)/dist <= theta then
        node.applyForcesOnBody(body);
    else
        Continue recursion with the children
else
    if node.containsBody then
        node.localBody.applyForcesOnBody(body);
```

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]
Number of bodies
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

Strong Scaling



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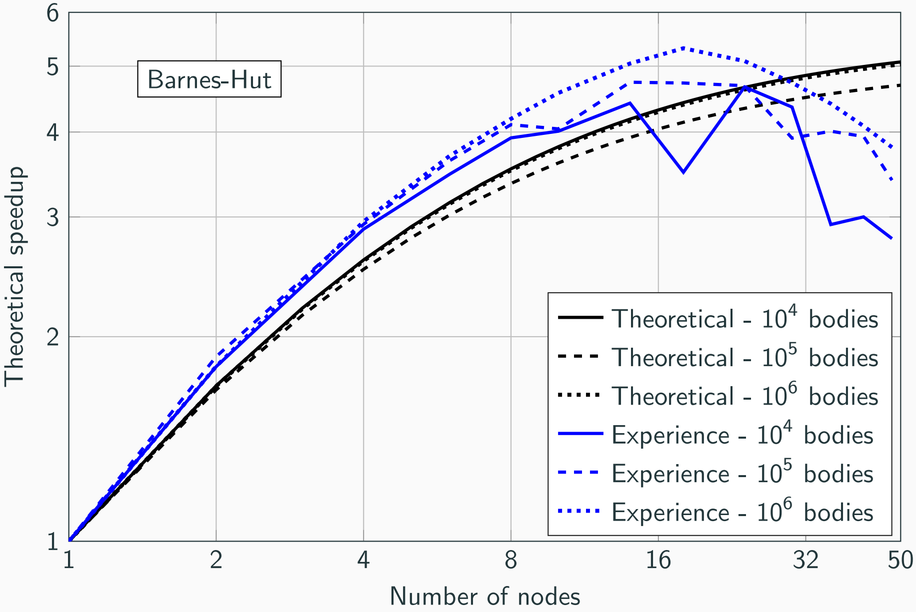
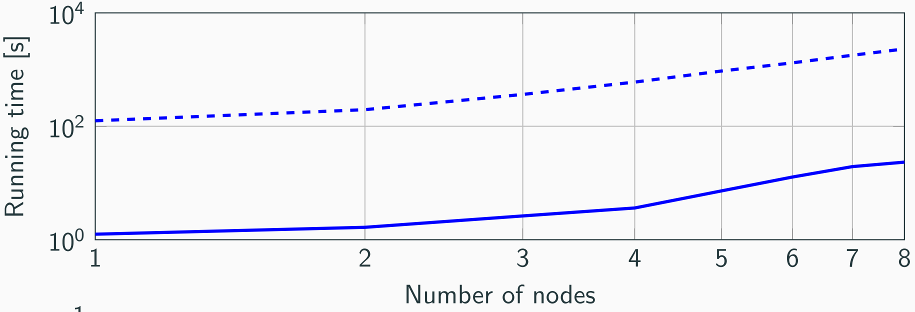
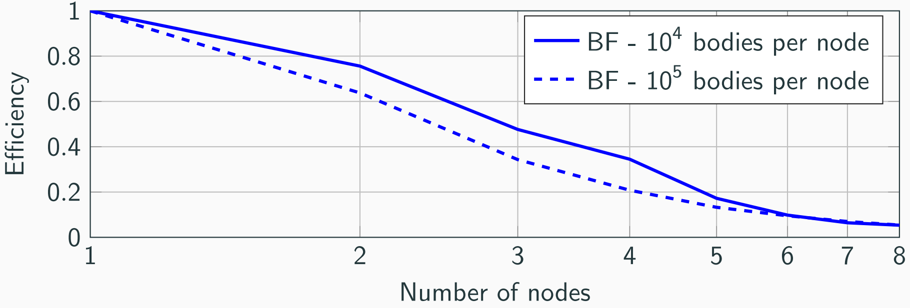


Weak Scaling





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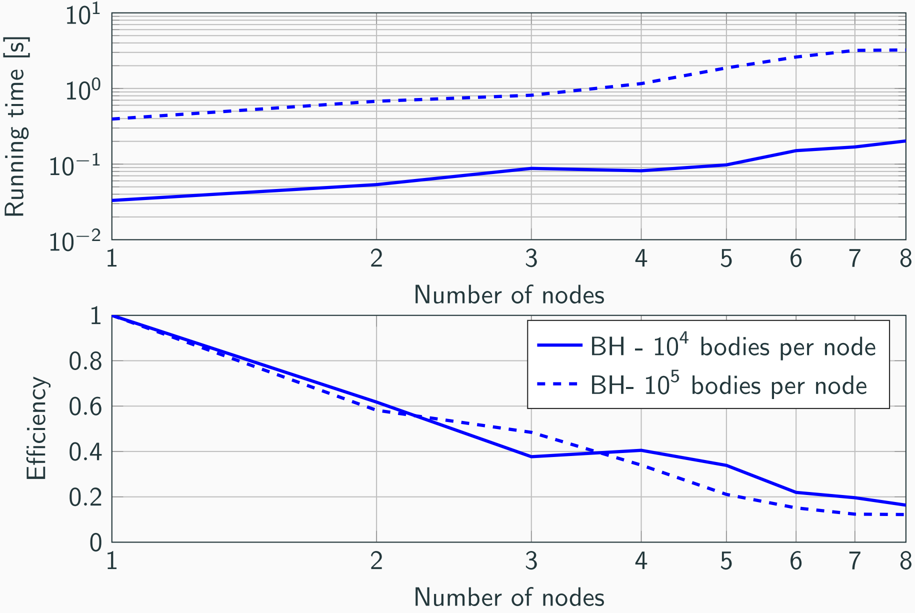

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How can we make it better?

- Use MPI I/O to write the positions of the bodies
- Implement a heuristic for the construction of the tree
  (don't rebuild it at each iteration)
- 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)