Parallel N-Body simulation with Barnes-Hut algorithm

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1. Introduction

This report is a part of 4th assignment of course HY342 - Parallel Programming of Computer Science Department, University of Crete. It presents an implementation of Barnes-Hut algorithm for N-Body simulation and proposes methods to parallel this algorithm using C++ and Java. The following report is organized as follows: Section 2 Describes the input, Section 3 is about the implementation and Section 4 presents measurements and comparisons among the different programming languages and configurations.

2. Input

By default, input is represented as a physical system in an external file containing description about the entities. This description informs us about the name of each entity, the starting coordinates and initial speed on regarding the 2D environment and their corresponding mass. It also configures the size of the universe. These bodies are saved into a dynamic list structure upon the start of the simulation. After the simulation is ended, their final coordinates and speed are printed in an output dataset file following the same format as the input.

3. Implementation

In this section the implementation of the algorithm and the parallelism method are described. The Barnes-Hut approximation algorithm runs for a fixed number of iterations, with each iteration representing the time difference of 1 time unit: dt = 1. For every iteration, the algorithm has three phases: Phase 1 is about the BHTree construction, phase 2 calculates the Sum of all powers acting on every entity using the Newton's Gravitational Law, while phase 3 calculates the new positions of the bodies for the current iteration. Thus we proceed by describing each one of these phases:

3.1 BHTrees

BHTrees are the core of the efficiency of Barnes-Hut, as they reduce the calculations needed to be done by splitting the universe recursively in quads and subquads, till every leaf has at most one entity. Thus, inner nodes represent the mass center of all bodies below them, allowing us to approximate the total force acting on a specific entity by considering that entities belonging to another quad of the universe to be a general body generated by the mass center of all the bodies above it.

3.1.1 BHTree Structure

The structure of BHTree contains some other supporting structures:

```
class Point {
    double x;
    double y;
}
class Region {
    Point center;
    double dimension;
}
class Entity {
```

```
double Vy;
    double Vx;
    double mass;
    double SFx = 0;
    double SFy = 0;
    String name;
    Point point;
    Region currentRegion;
}
class BHTree {
    Region region;
    //When the current node is not leaf represents the mass center of the region
    Entity *entity = NULL;
    BHTree *quad1 = NULL;
    BHTree *quad2 = NULL;
    BHTree *quad3 = NULL;
    BHTree *quad4 = NULL;
}
```

3.1.2 BHTree Insert

The most powerful yet confusing BHTree functionality is the insert:

```
procedure insertEntity(Entity *_entity){
    if (!region.containsPoint(_entity -> getPoint()))
        return false;
    if (isLeaf()){
        //empty leaf case, inserting safely!
        if (entity == NULL) {
            _entity ->setCurrentRegion(region);
            entity = _entity;
            return true;
        }
        patchIfCollision();
        //else divide the tree
        createSubQuads();
        if (quad1->insertEntity(entity) ||
                quad2->insertEntity(entity) ||
                quad3->insertEntity(entity) ||
                quad4->insertEntity(entity)) {
            //success
        }
    }
    if (quad1->insertEntity(_entity) ||
        quad2->insertEntity(_entity) ||
        quad3->insertEntity(_entity) ||
        quad4->insertEntity(_entity)) {
```

```
entity = massCenter(entity, _entity);
    return true;
}

procedure createSubQuads() {
    quad1 = new BHTree(Region(Point(xCenter + dim / 2, yCenter + dim / 2), dim / 2));
    quad2 = new BHTree(Region(Point(xCenter - dim / 2, yCenter + dim / 2), dim / 2));
    quad3 = new BHTree(Region(Point(xCenter - dim / 2, yCenter - dim / 2), dim / 2));
    quad4 = new BHTree(Region(Point(xCenter + dim / 2, yCenter - dim / 2), dim / 2));
}
```

3.2. Calculating Netforce

```
The netforce on each body is calculated for every single entity by traversing the BHTree, as following:
```

```
procedure netForce(Entity *e, BHTree *bh) {
    if (bh = NULL)
        return:
    if (bh—>isLeaf()) {
        Entity *body = bh->getEntity();
        if (body != e && body != NULL) {
            double r = distance(*e, *body);
            double f = F(*e, *body, r);
            double fx = Fx(*e, *body, f, r);
            double fy = Fy(*e, *body, f, r);
            e->addToSFx(fx);
            e->addToSFy(fy);
        return;
    }
    BHTree *quads [4] = \{bh->getQuad1(), bh->getQuad2(), bh->getQuad3(), bh->getQuad4()\}; \\
    BHTree *quadToGo = NULL;
    for (int i = 0; i < 4; i++) {
        if (quads[i]!= NULL) {
            Entity *cent = quads[i]->getEntity();
            Region reg = quads[i]->getRegion();
            if (cent == NULL)
                continue;
            if (reg.containsPoint(e->getPoint(), i + 1))
                quadToGo = quads[i]; //saving the destination quad
            else {
                /*In this case, entity cent represents the mass center of the current adjacer
                double s = 2 * e->getCurrentRegion().getDimension();
                double r = distance(*e, *cent);
                if (r > s \mid | quads[i] -> isLeaf()) {
                    double f = F(*e, *cent, r);
                    double fx = Fx(*e, *cent, f, r);
```

As stated above, to calculate the netforce on a body, the Newton's Gravitational Law is Used:

$$F = G \frac{m_1 m_2}{r^2}$$

where

$$G = \frac{6.67}{10^{11}} \frac{Nm^2}{kq^2}$$

and from trigonometry and Pythagorean theorem we have

$$F_x = F \frac{x_2 - x_1}{r}$$

and

$$F_y = F \frac{y_2 - y_1}{r}$$

3.3. Calculating the New Positions

The most powerful yet confusing BHTree functionality is the insert:

```
\begin{array}{lll} & \textbf{procedure calcNewPos}(Entity~*e\,,~\textbf{double}~dt\,,~\textbf{double}~dims)~\{\\ & \textbf{double}~SFy = e{-}{>} getSFy\,()\,;\\ & \textbf{double}~SFx = e{-}{>} getSFx\,()\,;\\ & \textbf{double}~m = e{-}{>} getMass\,()\,;\\ & \textbf{double}~oldVx = e{-}{>} getVx\,()\,;\\ & \textbf{double}~oldVy = e{-}{>} getVy\,()\,;\\ & \textbf{double}~oldX = e{-}{>} getPoint\,()\,.\,getX\,()\,;\\ & \textbf{double}~oldY = e{-}{>} getPoint\,()\,.\,getY\,()\,;\\ & \textbf{double}~oldY = e{-}{>} getPoint\,()\,.\,getY\,()\,;\\ & \textbf{double}~Ax = SFx~/~m;\\ & \textbf{double}~Ay = SFy~/~m;\\ & \textbf{double}~newVx = oldVx~+~Ax~*~dt\,;\\ \end{array}
```

```
double newVy = oldVy + Ay * dt;
double newX = oldX + newVx * dt;
double newY = oldY + newVy * dt;

patchIfOutOfUniverse();

e->setPoint(Point(newX, newY));

e->setSFx(0);
e->setSFy(0);
e->setVx(newVx);
e->setVy(newVy);
```

It's clear that we are able to calculate the new positions we need to use:

$$a_x = \frac{F_x}{m}, a_y = \frac{F_y}{m}$$

thus

}

$$V_x = V_x + \Delta t \times a_x, V_y = V_y + \Delta t \times a_y$$

meaning that the new positions are:

$$x = x + \Delta t \times V_x, y = y + \Delta t \times V_y$$

3.4. Parallelization

3.4.1 Parallelization Method

The way we described the implementation leads us to think that phase two and three can be paralleled. The most simple and efficient way to do this, it to parallel the loop of phase 2, without the deal of data race as every single thread will modify the total force only for the chunk of bodies that it edits, and wont modify any coordinates or speed. Then, using a barrier between phase two and three, we can also parallel the new position calculation loop for every body, without the fear for data race, for the same reason as above.

Thus, for C++ using TBB we could implement the following:

```
for (int i = 0; i < iterations; i++) {
    bh = createBHTree(entities, dims);

    parallel_for(blocked_range < size_t > (0, size),
        [&](const blocked_range < size_t > &r) -> void {
        for (size_t i = r.begin(); i != r.end(); i++) {
            netForce(entities[i], bh);
        }
    }); //barrier

parallel_for(blocked_range < size_t > (0, size),
        [&](const blocked_range < size_t > &r) -> void {
        for (size_t i = r.begin(); i != r.end(); i++) {
            newPosition(entities[i], dt, dims);
        }
    }); //barrier
```

```
freeBHTree(bh);
}
and for Java Threads we have:

for (int k = 0; k < iters; k++) {
    try {
        BHTree bh = BHUtils.createBHTree(entities, dims);
        barrier.await();

    for (int i = from; i < to; i++) {
            BHUtils.netForce(entities.get(i), bh);
    }

    barrier.await();

    for (int i = from; i < to; i++) {
            BHUtils.newPosition(entities.get(i), dt, dims);
        }
        barrier.await();
}

catch (Exception e)
        e.printStackTrace();
}
for each thread.</pre>
```

3.4.1 Load Balancing

Considering C++: As this algorithm is implemented with the help of TBB, we could just use two parallel for generics to create the above idea. Also, doing measurements it's obvious that automated grain size of TBB could provide better results by manually setting the chunk size or grain size for each thread.

Considering Java: Using Java threads, we could create the chunks manually and synchronize the threads with a custom barrier. We could also use parallel streams of Java 8. Considering Java threads, a chunk size can be considered as the fraction of number of total bodies and the threads number.

3.4.2 BHTree as a parallel container

As insertion on BHTree probably needs to extensively divide the universe more and more, paralleling this procedure would need a great amount of synchronization among the different thread, resulting in a high overhead. For this reason this structure is implement sequentially.

3.5 Collision and Error Handling

Its possible for collisions to occur, and there are also cases that a body can leave the region of the universe, mainly when the dimensions are small. Such cases are patched differently: When 2 bodies collide (aka they have the same coordinates) the coordinates of one body are patched by a small dx,dy, so that the two bodies will never be considered to have the same coordinates. A possible variation of the algorithm could consider calculating the collision outcome, other than patching the coordinates. On the other hand, when a body gets out of bounds, it's kept at the border so as to show that it got out of bounds during the simulation. Note that such cases are extremely rare for actual big datasets (e.g. for datasets simulation solar systems), but they are common for small testing datasets.

4. Measurements

In this sections, the execution time results are presented for all configurations. These execution times where gathered and calculates using an automated Python script.

4.1 Speedup and Standard Deviation

For speedup, two versions of the calculations are used, SpeedUp(C) and SpeedUp(N). SpeedUp(C) is the speedup in comparison with the sequential code (compiled with 0 threads arg), while SpeedUp(N) is the speedup between thread N and N-1 (etc. the speedup between thread 2 and thread 4):

$$SpeedUp(C) = \frac{t_{seq}}{t_{par}} = \frac{Sequential_{average}}{threadN_{average}} = C$$

$$SpeedUp(N) = \frac{t_{seq}}{t_{par}} = \frac{threadN - 1_{average}}{threadN_{average}} = N$$

Standard Deviation is calculated for each configuration and input size using the equation:

$$Stdev = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2} = Vseconds$$

4.2 C++ Implementation using TBB

4.2.1 Input1

• 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	0.138	0.141	0.14	0.139	0.14	0.1396	0	0	0.00114
1	0.174	0.169	0.168	0.166	0.173	0.17	0.82118	0.82118	0.00339
2	0.148	0.146	0.146	0.146	0.217	0.1606	0.86924	1.05853	0.03154
4	0.205	0.188	0.135	0.138	0.137	0.1606	0.86924	1.00000	0.03334

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	1.351	1.265	1.215	1.25	1.241	1.2644	0	0	0.05171
1	1.583	1.514	1.482	1.481	1.534	1.5188	0.83250	0.83250	0.04230
2	1.407	2.05	1.325	1.405	1.32	1.5014	0.84215	1.01159	0.30951
4	1.711	1.537	1.358	2.02	1.379	1.601	0.78976	0.93779	0.27390

4.2.2 Input2

• 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	6.482	6.265	6.402	6.319	6.296	6.3528	0	0	0.08830
1	6.899	6.682	6.757	6.845	6.687	6.774	0.93782	0.93782	0.09616
2	5.471	4.803	4.679	4.687	4.698	4.8676	1.30512	1.39165	0.34103
4	3.456	3.395	3.39	3.91	3.416	3.5134	1.80816	1.38544	0.22323

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	64.985	62.992	63.186	62.641	61.268	63.0144	0	0	1.33253
1	67.879	67.588	67.37	67.353	68.062	67.6504	0.93147	0.93147	0.31330
2	47.153	46.422	46.041	48.97	52.443	48.2058	1.30720	1.40337	2.62272
4	40.794	38.583	39.613	37.83	35.834	38.5308	1.63543	1.25110	1.87482

4.2.3 Input3

\bullet 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	5.539	5.391	5.501	5.396	5.391	5.4436	0	0	0.07105
1	5.993	5.872	5.924	5.789	5.771	5.8698	0.92739	0.92739	0.09275
2	3.725	3.947	4.001	4.172	3.963	3.9616	1.37409	1.48167	0.15970
4	2.906	2.856	2.878	2.856	3.254	2.95	1.84529	1.34292	0.17118

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	53.686	52.782	52.928	53.62	53.118	53.2268	0	0	0.40756
1	57.698	57.543	57.428	59.305	57.097	57.8142	0.92065	0.92065	0.86213
2	41.105	40.006	40.167	39.822	39.82	40.184	1.32458	1.43874	0.53473
4	33.895	29.655	34.099	31.822	33.173	32.5288	1.63630	1.23534	1.83748

4.2.4 Input4

• 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	85.419	82.537	82.31	82.595	82.941	83.1604	0	0	1.28266
1	83.144	82.349	82.834	82.045	84.205	82.9154	1.00295	1.00295	0.83671
2	56.978	56.447	56.295	55.894	57.764	56.6756	1.46731	1.46298	0.72182
4	42.007	41.399	42.194	42.825	42.002	42.0854	1.97599	1.34668	0.51065

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	850.73	913.379	886.605	868.92	848.703	873.6674	0	0	27.00128
1	848.109	850.635	922.492	913.214	920.318	890.9536	0.98060	0.98060	38.12386
2	600.91	607.797	593.318	598.404	602.097	600.5052	1.45489	1.48367	5.29006
4	451.665	454.782	449.434	456.092	448.046	452.0038	1.93288	1.32854	3.42106

4.2.5 Input5

\bullet 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	111.618	112.925	115.301	112.727	111.119	112.738	0	0	1.61861
1	110.397	111.592	111.304	110.809	111.155	111.0514	1.01519	1.01519	0.46200
2	68.641	67.859	69.499	71.967	68.373	69.2678	1.62757	1.60322	1.62153
4	48.205	47.683	48.299	47.925	48.419	48.1062	2.34352	1.43989	0.29863

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	1111.05	1113.23	1110.34	1079.19	1084.44	1099.65	0	0	16.42109
1	1121.85	1094.34	1096.85	1111.38	1095.19	1103.922	0.99613	0.99613	12.19745
2	668.853	686.979	683.197	685.753	654.066	675.7696	1.62726	1.63358	14.13657
4	453.219	468.754	464.745	465.6	466.599	463.7834	2.37104	1.45708	6.09233

4.3 Java Implementation using Java Threads

4.3.1 Input1

\bullet 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	0.098	0.089	0.113	0.108	0.088	0.0992	0	0	0.01117
1	0.119	0.11	0.117	0.117	0.117	0.116	0.85517	0.85517	0.00346
2	0.335	0.327	0.373	0.35	0.355	0.348	0.28506	0.33333	0.01794
4	0.691	0.729	0.685	0.636	0.67	0.6822	0.14541	0.51011	0.03376

\bullet 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	0.484	0.482	0.478	0.469	0.478	0.4782	0	0	0.00576
1	0.516	0.492	0.494	0.479	0.504	0.497	0.96217	0.96217	0.01386
2	1.895	1.862	1.893	1.747	1.796	1.8386	0.26009	0.27031	0.06499
4	4.713	4.663	4.809	4.681	4.702	4.7136	0.10145	0.39006	0.05670

4.3.2 Input2

\bullet 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	1.121	1.122	1.065	1.114	1.089	1.1022	0	0	0.02471
1	1.093	1.088	1.096	1.107	1.114	1.0996	1.00236	1.00236	0.01064
2	1.195	1.128	1.132	1.106	1.144	1.141	0.96599	0.96372	0.03317
4	1.962	1.832	1.732	1.748	1.795	1.8138	0.60767	0.62907	0.09175

• 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	8.075	7.934	7.863	7.851	7.857	7.916	0	0	0.09503
1	7.996	7.958	8.089	8.025	8.11	8.0356	0.98512	0.98512	0.06342
2	7.606	7.613	7.621	7.557	7.447	7.5688	1.04587	1.06167	0.07252
4	9.584	9.619	9.443	9.648	9.619	9.5826	0.82608	0.78985	0.08127

4.3.3 Input3

\bullet 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	0.921	0.894	0.889	0.894	0.894	0.8984	0	0	0.01282
1	0.928	0.909	0.913	0.908	0.883	0.9082	0.98921	0.98921	0.01621
2	0.946	0.978	0.936	0.975	0.956	0.9582	0.93759	0.94782	0.01817
4	1.581	1.359	1.389	1.419	1.319	1.4134	0.63563	0.67794	0.10073

\bullet 100000 iterations

	Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
Π	0	6.277	6.206	6.21	6.259	6.214	6.2332	0	0	0.03252
T	1	6.498	6.4	6.338	6.351	6.392	6.3958	0.97458	0.97458	0.06290
\prod	2	6.2	6.327	6.249	6.146	6.136	6.2116	1.00348	1.02965	0.07885
	4	8.856	9.32	8.702	8.83	9.174	8.9764	0.69440	0.69199	0.25900

4.3.4 Input4

• 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	11.389	10.778	11.039	10.629	10.781	10.9232	0	0	0.29926
1	11.041	11.064	10.741	11.081	11.175	11.0204	0.99118	0.99118	0.16429
2	8.909	8.703	8.578	8.515	8.648	8.6706	1.25980	1.27101	0.15098
4	8.698	9.792	9.504	9.185	9.136	9.263	1.17923	0.93605	0.41212

• 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	104.807	103.116	103.264	103.09	103.15	103.4854	0	0	0.74178
1	104.381	103.112	102.364	102.655	103.293	103.161	1.00314	1.00314	0.77451
2	79.973	77.141	79.678	81.017	77.268	79.0154	1.30969	1.30558	1.72694
4	72.352	73.713	72.725	70.233	71.706	72.1458	1.43439	1.09522	1.29290

4.3.5 Input5

• 10000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	11.986	12.163	12.148	12.035	12.115	12.0894	0	0	0.07609
1	12.098	11.867	11.959	11.926	11.94	11.958	1.01099	1.01099	0.08548
2	9.084	9.044	9.463	9.088	9.087	9.1532	1.32078	1.30643	0.17416
4	8.966	9.285	8.208	8.201	8.158	8.5636	1.41172	1.06885	0.52554

• 100000 iterations

Threads	Run 1	Run 2	Run 3	Run 4	Run 5	Average	Speedup(C)	Speedup(N)	Stdev
0	115.758	110.113	113.002	116.448	115.902	114.2446	0	0	2.66957
1	114.71	114.07	115.393	115.129	115.504	114.9612	0.99377	0.99377	0.58450
2	85.386	85.223	85.724	85.998	85.261	85.5184	1.33591	1.34429	0.33292
4	72.98	73.558	74.892	76.848	73.396	74.3348	1.53689	1.15045	1.57693

4.4 Comparing the Implementations

From the results above we conclude that JVM Warm-ups and optimizations could result in execution speeds even higher than C++ although the thread speedup is less. In both implementations, we notice that we don't always have speedups. This is normal, as the speedup relies on the number of different bodies a simulation needs to process. When a dataset has many bodies (eg. Dataset input5) we notice that using threads to split the calculations can be really efficient. In any case, someone could conclude that C++ multi-threading using TBB is better than Java multi-threading based on the results presented above. Although TBB is a great tool for concurrent programming, that result is not fully true, as the Java implementation used manual chunk creation and classic Java threads, which means that this implementation is not the best possible.

SOLUTION: Java 8 provides parallel streams, which are really useful and efficient to parallel simple for loops, like this:

```
public static void BarnesHutStream(ArrayList<Entity> entities, int iters, double dims, int th
   ForkJoinPool customThreadPool = new ForkJoinPool(threadsNum);
   for (int i = 0; i < iters; i++) {
    BHTree bh = BHUtils.createBHTree(entities, dims);</pre>
```

customThreadPool.submit(() -> entities.parallelStream().forEach(

```
e -> { BHUtils.netForce(e, bh); }));

customThreadPool.submit(() -> entities.parallelStream().forEach(
    e -> { BHUtils.newPosition(e, dt, dims); }));
}

customThreadPool.shutdownNow();
}
```

However CSD computers do not support these streams, so the measurements could not be done. Also, there is another problem, which could occur if one TBB was used in the place of classic TBB: Although these streams offer methods to customize the thread pool, it's the schedulers choice to run on as many threads as the optimal solution could be. That means that measurements to compare difference among thread running times could be impossible.