

i.En variant le nombre de threads (2, 4, 8, 16) pour un nombre de particules = 500. Nombre d'itérations = 400.

```
Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 500

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 2

ND, the spatial dimension, is 3
NP, the number of particles in the simulation, is 500
STEP_NUM, the number of time steps, is 400
DT, the size of each time step, is 0.100000

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.
The sum of these energies should be a constant.
As an accuracy check, we also print the relative error
in the total energy.
```

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 124433.847243 | 0.000000 | 0.000000e+00 |
| 40 | 124244.521135 | 1261.977812 | 8.620257e-03 |
| 80 | 124589.861837 | 1261.409496 | 1.139099e-02 |
| 120 | 124712.954747 | 1215.629632 | 1.201230e-02 |
| 160 | 124737.617850 | 1209.146002 | 1.215840e-02 |
| 200 | 124743.793304 | 1210.432323 | 1.221837e-02 |
| 240 | 124747.806292 | 1208.848522 | 1.223789e-02 |
| 280 | 124749.448048 | 1207.553512 | 1.224068e-02 |
| 320 | 124748.834586 | 1209.154327 | 1.224861e-02 |
| 360 | 124749.794722 | 1209.341428 | 1.225783e-02 |
| 400 | 124749.999367 | 1209.093603 | 1.225748e-02 |

```
Elapsed time for main computation:
7.475321 seconds.
```

```

Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 500

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 4

ND, the spatial dimension, is 3
NP, the number of particles in the simulation, is 500
STEP_NUM, the number of time steps, is 400
DT, the size of each time step, is 0.100000

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.
The sum of these energies should be a constant.
As an accuracy check, we also print the relative error
in the total energy.

Step      Potential      Kinetic      (P+K-E0)/E0
Energy P      Energy K      Relative Energy Error

    0      124433.847243          0.000000      0.000000e+00
   40      124244.521135      1261.977812      8.620257e-03
   80      124589.861837      1261.409496      1.139099e-02
  120      124712.954747      1215.629632      1.201230e-02
  160      124737.617850      1209.146002      1.215840e-02
  200      124743.793304      1210.432323      1.221837e-02
  240      124747.806292      1208.848522      1.223789e-02
  280      124749.448048      1207.553512      1.224068e-02
  320      124748.834586      1209.154327      1.224861e-02
  360      124749.794722      1209.341428      1.225783e-02
  400      124749.999367      1209.093603      1.225748e-02

Elapsed time for main computation:
7.502234 seconds.

```

3 -

```
Enter ND, the spatial dimension : 3
```

```
Enter NP, the number of particles : 500
```

```
Enter step_num, the number of time steps : 400
```

```
Enter DT, the size of the time step (0.1, for instance) : 0.1
```

```
Enter nbrThreads, the number of threads to use : 8
```

```
ND, the spatial dimension, is 3
```

```
NP, the number of particles in the simulation, is 500
```

```
STEP_NUM, the number of time steps, is 400
```

```
DT, the size of each time step, is 0.100000
```

```
Initializing positions, velocities, and accelerations.
```

```
Computing initial forces and energies.
```

```
At each step, we report the potential and kinetic energies.
```

```
The sum of these energies should be a constant.
```

```
As an accuracy check, we also print the relative error  
in the total energy.
```

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 124433.847243 | 0.000000 | 0.000000e+00 |
| 40 | 124244.521135 | 1261.977812 | 8.620257e-03 |
| 80 | 124589.861837 | 1261.409496 | 1.139099e-02 |
| 120 | 124712.954747 | 1215.629632 | 1.201230e-02 |
| 160 | 124737.617850 | 1209.146002 | 1.215840e-02 |
| 200 | 124743.793304 | 1210.432323 | 1.221837e-02 |
| 240 | 124747.806292 | 1208.848522 | 1.223789e-02 |
| 280 | 124749.448048 | 1207.553512 | 1.224068e-02 |
| 320 | 124748.834586 | 1209.154327 | 1.224861e-02 |
| 360 | 124749.794722 | 1209.341428 | 1.225783e-02 |
| 400 | 124749.999367 | 1209.093603 | 1.225748e-02 |

```
Elapsed time for main computation:
```

```
8.267904 seconds.
```

4 -

```
Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 500

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 16

ND, the spatial dimension, is 3
NP, the number of particles in the simulation, is 500
STEP_NUM, the number of time steps, is 400
DT, the size of each time step, is 0.100000

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.
The sum of these energies should be a constant.
As an accuracy check, we also print the relative error
in the total energy.
```

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 124433.847243 | 0.000000 | 0.000000e+00 |
| 40 | 124244.521135 | 1261.977812 | 8.620257e-03 |
| 80 | 124589.861837 | 1261.409496 | 1.139099e-02 |
| 120 | 124712.954747 | 1215.629632 | 1.201230e-02 |
| 160 | 124737.617850 | 1209.146002 | 1.215840e-02 |
| 200 | 124743.793304 | 1210.432323 | 1.221837e-02 |
| 240 | 124747.806292 | 1208.848522 | 1.223789e-02 |
| 280 | 124749.448048 | 1207.553512 | 1.224068e-02 |
| 320 | 124748.834586 | 1209.154327 | 1.224861e-02 |
| 360 | 124749.794722 | 1209.341428 | 1.225783e-02 |
| 400 | 124749.999367 | 1209.093603 | 1.225748e-02 |

```
Elapsed time for main computation:
8.155169 seconds.
```

ii. En variant la taille des particules (200, 500, 1000) pour un nombre de threads= 4. Nombre d'itérations = 400.

Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 200

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 4

ND, the spatial dimension, is 3

NP, the number of particles in the simulation, is 200

STEP_NUM, the number of time steps, is 400

DT, the size of each time step, is 0.100000

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.

The sum of these energies should be a constant.

As an accuracy check, we also print the relative error
in the total energy.

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 19849.695286 | 0.000000 | 0.000000e+00 |
| 40 | 19792.693106 | 174.560544 | 5.922427e-03 |
| 80 | 19841.466234 | 182.256028 | 8.767237e-03 |
| 120 | 19870.213058 | 188.827633 | 1.054653e-02 |
| 160 | 19889.444106 | 189.256856 | 1.153699e-02 |
| 200 | 19894.904829 | 190.400827 | 1.186972e-02 |
| 240 | 19897.226369 | 190.618816 | 1.199766e-02 |
| 280 | 19899.479046 | 189.178079 | 1.203856e-02 |
| 320 | 19899.992946 | 189.011261 | 1.205605e-02 |
| 360 | 19899.996664 | 189.368894 | 1.207425e-02 |
| 400 | 19899.393284 | 190.368438 | 1.209421e-02 |

Elapsed time for main computation:

1.345414 seconds.

Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 500

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 4

ND, the spatial dimension, is 3

NP, the number of particles in the simulation, is 500

STEP_NUM, the number of time steps, is 400

DT, the size of each time step, is 0.100000

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.

The sum of these energies should be a constant.

As an accuracy check, we also print the relative error
in the total energy.

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 124433.847243 | 0.000000 | 0.000000e+00 |
| 40 | 124244.521135 | 1261.977812 | 8.620257e-03 |
| 80 | 124589.861837 | 1261.409496 | 1.139099e-02 |
| 120 | 124712.954747 | 1215.629632 | 1.201230e-02 |
| 160 | 124737.617850 | 1209.146002 | 1.215840e-02 |
| 200 | 124743.793304 | 1210.432323 | 1.221837e-02 |
| 240 | 124747.806292 | 1208.848522 | 1.223789e-02 |
| 280 | 124749.448048 | 1207.553512 | 1.224068e-02 |
| 320 | 124748.834586 | 1209.154327 | 1.224861e-02 |
| 360 | 124749.794722 | 1209.341428 | 1.225783e-02 |
| 400 | 124749.999367 | 1209.093603 | 1.225748e-02 |

Elapsed time for main computation:

7.384180 seconds.


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Enter ND, the spatial dimension : 3

Enter NP, the number of particles : 1000

Enter step_num, the number of time steps : 400

Enter DT, the size of the time step (0.1, for instance) : 0.1

Enter nbrThreads, the number of threads to use : 4

```

```

ND, the spatial dimension, is 3
NP, the number of particles in the simulation, is 1000
STEP_NUM, the number of time steps, is 400
DT, the size of each time step, is 0.100000

```

Initializing positions, velocities, and accelerations.

Computing initial forces and energies.

At each step, we report the potential and kinetic energies.
The sum of these energies should be a constant.
As an accuracy check, we also print the relative error
in the total energy.

| Step | Potential Energy P | Kinetic Energy K | (P+K-E0)/E0 Relative Energy Error |
|------|-----------------------|---------------------|--------------------------------------|
| 0 | 498159.395148 | 0.000000 | 0.000000e+00 |
| 40 | 497938.061734 | 5564.472483 | 1.072576e-02 |
| 80 | 499298.289524 | 5046.970762 | 1.241744e-02 |
| 120 | 499461.763696 | 4979.830517 | 1.261082e-02 |
| 160 | 499486.607188 | 4975.818833 | 1.265264e-02 |
| 200 | 499494.166781 | 4973.664134 | 1.266349e-02 |
| 240 | 499498.370122 | 4971.844320 | 1.266827e-02 |
| 280 | 499498.813404 | 4972.176829 | 1.266983e-02 |
| 320 | 499499.209733 | 4972.321851 | 1.267092e-02 |
| 360 | 499499.990024 | 4971.894047 | 1.267162e-02 |
| 400 | 499499.116976 | 4972.943401 | 1.267198e-02 |

```

Elapsed time for main computation:
30.716481 seconds.

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