Nbr particles :

200 :

```
 Enter ND, the spatial dimension (2 or 3).
3

 Enter NP, the number of particles (500, for instance).
200

 Enter ND, the number of time steps (500 or 1000, for instance).
400

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

 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

 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   19849.695286       0.000000   0.000000e+00
       40   19846.956991     178.246259   8.841847e-03
       80   19865.946981     232.967422   1.255531e-02
      120   19897.139253     224.920070   1.372132e-02
      160   19898.424578     229.032558   1.399326e-02
      200   19898.879796     229.573455   1.404344e-02
      240   19899.186447     230.129433   1.408690e-02
      280   19900.000000     229.655424   1.410400e-02
      320   19900.000000     229.655424   1.410400e-02
      360   19900.000000     229.655424   1.410400e-02
      400   19900.000000     229.655424   1.410400e-02

 Elapsed cpu time: 1.147777 seconds.
```

500:

```
 Enter ND, the spatial dimension (2 or 3).
3

 Enter NP, the number of particles (500, for instance).
500

 Enter ND, the number of time steps (500 or 1000, for instance).
400

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

 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

 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  124513.468873    1381.709422   1.174384e-02
       80  124711.023112    1372.944029   1.326102e-02
      120  124744.513012    1368.496853   1.349442e-02
      160  124747.269266    1370.882468   1.353574e-02
      200  124749.545621    1371.804833   1.356145e-02
      240  124749.126649    1372.816443   1.356621e-02
      280  124749.812181    1372.726643   1.357100e-02
      320  124749.499166    1373.163167   1.357199e-02
      360  124749.994472    1372.962561   1.357436e-02
      400  124750.000000    1373.210025   1.357639e-02

 Elapsed cpu time: 7.136647 seconds.

MD
```

1000:

```
C version
A molecular dynamics program.

Enter ND, the spatial dimension (2 or 3).
3

Enter NP, the number of particles (500, for instance).
1000

Enter ND, the number of time steps (500 or 1000, for instance
400

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

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

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  498159.395148       0.000000   0.000000e+00
      40  499012.893416    5569.677662   1.289382e-02
      80  499472.370640    5369.521901   1.341438e-02
     120  499491.063099    5374.812291   1.346252e-02
     160  499497.902064    5373.475997   1.347356e-02
     200  499498.537753    5374.799705   1.347750e-02
     240  499499.495596    5375.379444   1.348058e-02
     280  499500.000000    5375.480339   1.348180e-02
     320  499500.000000    5375.703093   1.348225e-02
     360  499500.000000    5375.703093   1.348225e-02
     400  499500.000000    5375.703093   1.348225e-02

Elapsed cpu time: 28.681789 seconds.

MD
Normal end of execution.
```