Università degli Studi di Trento – Dipartimento di Fisica

Computational Physics 1

Recitation class, March 17, 2021

The Lennard-Jones fluid

Write a program to perform numerical simulations of a Lennard-Jones fluid for a given reduced density $\rho^* = \rho\sigma^3$ and reduced temperature $T^* = k_\mathrm{B}T/\varepsilon$.

Compare your results with the reference values published in the Lennard-Jones benchmark page at NIST.

1 Structure of the program

It might be convenient to define some common variables and arrays such as

```
#define N 108

double rho;     /* density - reduced units */
double T;       /* temperature - reduced units */

double X[N][3]; /* positions */
double V[N][3]; /* velocities */
double a[N][3]; /* accelerations = forces */
double L;       /* box length */
double cutoff;  /* cutoff for the pair interaction calculation */
double dt;      /* time step */

#define S 100
double g[S];
```

and write some functions that operate on these variables, such as

```
void calculate_forces();
/* zeroes out a[N][3], loop on all the pairs, calculates the distance,
   checks the cutoff, update forces */

void velocity_Verlet();
/* performs one step of the velocity Verlet algorithm, calling the previous
function to calculate the forces */

void rescale_velocities();
```

```
/* rescale velocities to match the assigned temperatures */

/* and so on */
```

2 Equilibration

Start from a face-centered cubic configuration generated using the provided routine, using $N = 108$ particles to develop the program and $N = 256$ to perform the final simulation runs.

Equilibrate the system by regularly rescaling the kinetic energy to match the assigned temperature; equilibration is attained when the potential energy begins to fluctuate around its average value. A good starting point for the integration time step is $dt = 0.005$.

3 Measurements

From this point on perform constant-energy molecular dynamics and measure the average potential and kinetic energies. Calculate and plot the pair distribution function $g(r)$.