Power of the interaction particles

Minzorov Oleksandr

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Typically in the MD calculation used the Verlet algorithm, when the position of the point can be calculated without knowing the speed. This algorithm is a compromise between the accuracy of the calculation procedure and the speed of its implementation.

The calculation sequence has the form:

First calculate the speed-up.

$$a_i(t) = \frac{f_i(x)}{m_i} \tag{1}$$

a_i – speed-up;

m_i – mass of the particle;

$f_i(x)$ – the value of the interaction power for two particles, calculated by the formula (3).

Next step calculate the speed.

$$v_i(t + \Delta t) = v_i(\Delta t) + a_i(t)\Delta t \tag{2}$$

$v_i(\Delta t)$ – current value of speed of movement;

Δt – time step for system;

a_i – the value of the speed-up, calculated by the formula (1).

In a software implementation, this function is called "Speed" and has four input parameters [t_step v_current m_ball LJpow]:

t_step – time step for system;

v_current - current value of speed;

m_ball - particle mass we are working with;

LJpow – particle interaction force calculated using Lennard-Jones potential.

And now we can calculate coordinate of particles.

$$x_i(t + \Delta t) = x_i(\Delta t) + v_i(t)\Delta t + a_i(t) * \frac{\Delta t^2}{2}$$

$x_i(\Delta t)$ – the current coordinate along one of the axes (x y);

v_i – the speed value, calculated by the formula (2);

a_i – speed-up value, calculated by the formula (1).

In a software implementation, this function is called "newParticleCoordinate" and has five input parameters [t_step cord_current m_ball speed LJpow]:

t_step – time step for system;

cord_current - current coordinate;

m_ball – mass of the particle;

speed - particle velocity;

LJpow – particle interaction force calculated using Lennard-Jones potential.

To obtain the force of interaction it is necessary to use the potential. From all existing selected Lennard-Jones potential:

$$U(r) = 4\sigma[(\frac{\sigma}{\varepsilon})^{12} - (\frac{\sigma}{\varepsilon})^{6}]$$

r- the distance between the centers of the particles.
ε- the depth of potential well.
σ- the distance at which the interaction energy becomes to zero.
After conversion we have the next formula:

$$f(r) = \frac{12\varepsilon}{\sigma}[(\frac{\sigma}{\varepsilon})^{13} - (\frac{\sigma}{\varepsilon})^{7}] \tag{3}$$

In a software implementation, this function is called "LennardJonesPower" and has three input parameters [e q r]:
e - the depth of potential well;
q - the distance at which the interaction energy becomes zero;
r - the distance between the centers of the particles;

There are also functions setup, draw and funk.
setup - contains a vector with information about particles. vector structure: coord - particle coordinate by XYZ axis; mass - particle mass; curLJPower - current value of the interaction force; curSpeed - current value of the particle speed.

draw - this function performs the task of visualizing particles by their coordinates.

funk - a function that, as a result of its execution, recalculates the coordinates of all particles. Verbal description of the funk function algorithm:
-first, we calculate the value of the force of interaction of the particles with each other and summarize these values , by the formula(3);
-next, we calculate the speed of each particle;
-now we can calculate the new coordinates of each particle based on the results from previous steps.

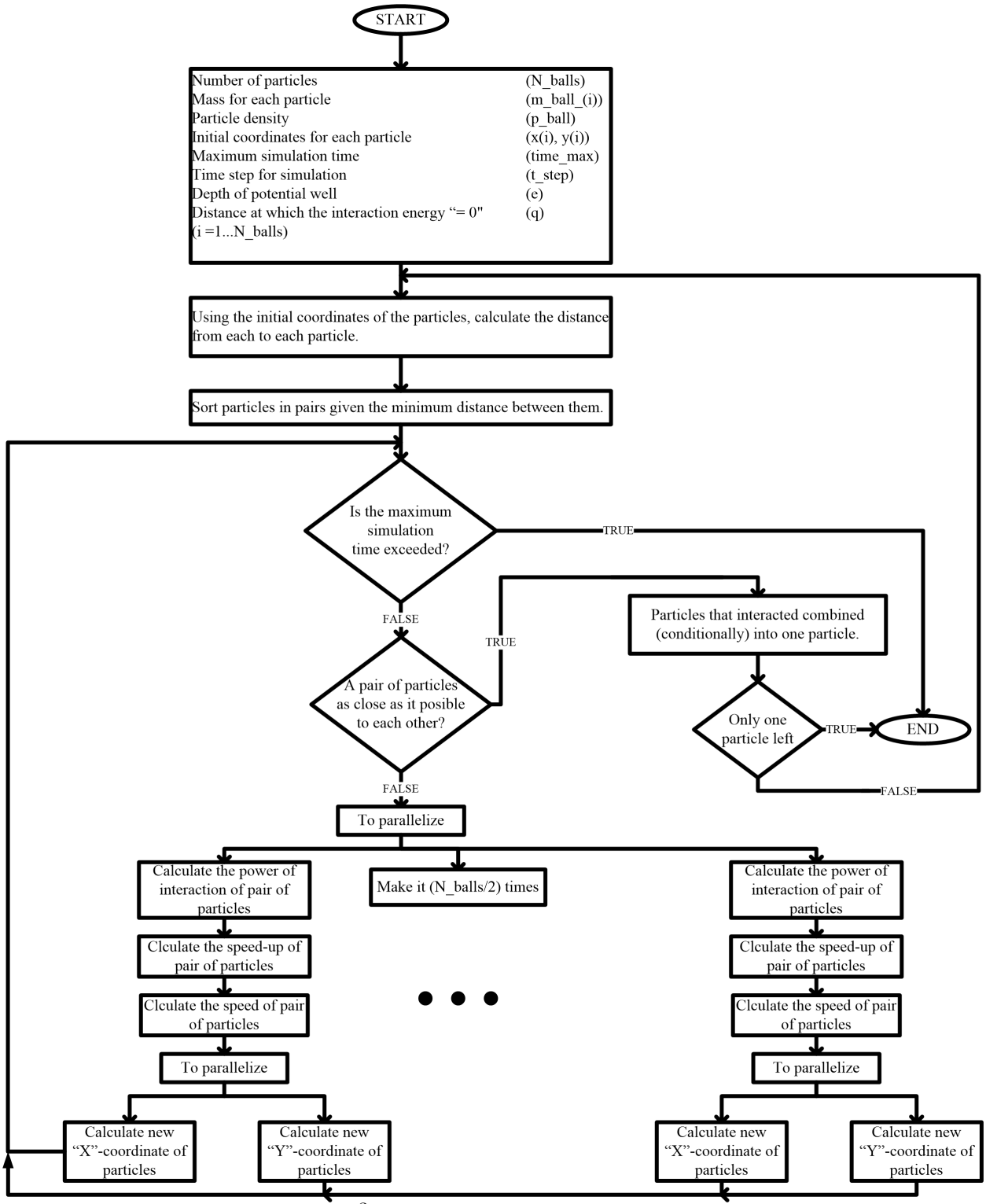

Figure 1: General algorithm.