AMERICAN UNIVERSITY OF ARMENIA
College of Science and Engineering
CS 226 Math Modeling Applications

PROJECT 2B

PRELIMINARY SUBMISSION DEADLINE: Thursday, December 13, 2018, before 18:00 sharp
FINALSUBMISSION DEADLINE: Thursday, December 20, 2018, before 22:00 sharp

Reading: H. Gould, J. Tobochnik, W. Christian, "*An Introduction to Computer Simulation Methods: Applications to Physical Systems*", 3rd ed.
(Gould_Tobochnik_Christian_Intro_to_Comp_Simulation_Methods_3rd_ed_2011.pdf in References.zip)
Chapter 8. **The Dynamics of Many Particle Systems**

Consider a simple version of the floor-planning problem: on the 2D plain given N spherical bodies of different sizes, arrange them within the given rectangular area A. It is one of the common combinatorial problems that requires heavy computing resources. Represent the bodies as a 2D many-particle system. All particles have unit mass and the interaction between any pair of particles depends only on the distance between them.

The particles outside the area A are subject to a long-range attracting force $\boldsymbol{C}(\boldsymbol{r}) = (C_x(\boldsymbol{r}), C_y(\boldsymbol{r}))$, where $\boldsymbol{r}$ defines the distance and orientation between the particle and the center of mass of other particles currently inside the area A.

Within each pair of particles inside the area A, they mutually impose a long-range attracting force $\boldsymbol{F}(\boldsymbol{r}) = (F_x(\boldsymbol{r}), F_y(\boldsymbol{r}))$ and a short-range repulsive force $\boldsymbol{G}(\boldsymbol{r}) = (G_x(\boldsymbol{r}), G_y(\boldsymbol{r}))$, where the vector $\boldsymbol{r}$ defines the distance and orientation between the particles in the pair. For this type of interactions use the periodic boundary conditions within the area A (chapter **8**, section **8.5**).

Assume the following forms of the forces:

$$C(\boldsymbol{r}) \sim -Mr^c,\ F(\boldsymbol{r}) \sim -r^f,\ G(\boldsymbol{r}) \sim r^{-g},$$

where $f > 0$, $g > 0$ and M is the number of particles currently residing in the area A.

The state of the n^{th} particle at the k^{th} time moment is specified by the horizontal and vertical components of its position and velocity respectively – $(x_{nk}, y_{nk}, u_{nk}, v_{nk})$. The horizontal and vertical components of the acceleration $a_{x\,nk}$ and $a_{y\,nk}$ are the sum of all the forces acting on the particle n^{th} particle at the k^{th} time moment. Implement the *Verlet algorithm* to determine the state at the k^{th} moment:

$$x_{nk} = x_{nk-1} + u_{nk-1}\,\Delta t + a_{x\,nk-1}\,\Delta t^2 / 2$$
$$u_{nk} = u_{nk-1} + (a_{x\,nk-1} + a_{x\,nk})\,\Delta t / 2$$
$$y_{nk} = y_{nk-1} + v_{nk-1}\,\Delta t + a_{y\,nk-1}\,\Delta t^2 / 2$$
$$v_{nk} = v_{nk-1} + (a_{y\,nk-1} + a_{y\,nk})\,\Delta t / 2$$

Task 1: Write a program that does the following:

1. Inputs the problem parameters c, f, g, Δt and others, if necessary, and the number of iterations T.
2. Inputs the amount of particles N. Randomly generates the initial values of x and y coordinates and sizes of all N particles within the area A. Set the initial values of the velocities to 0.
3. Applies the *Verlet algorithm* T times and saves and / or prints particles' coordinates.

Task 2: Run the **Task 1** for different values of the problem parameters to measure when a steady state is achieved.

Task 3: Repeat the **Task 1** using a modified *Verlet algorithm*, where the velocities are artificially kept 0:

$$x_{nk} = x_{nk-1} + a_{x\,nk-1}\,\Delta t^2 / 2$$
$$u_{nk} = (a_{x\,nk-1} + a_{x\,nk})\,\Delta t / 2$$
$$y_{nk} = y_{nk-1} + a_{y\,nk-1}\,\Delta t^2 / 2$$
$$v_{nk} = (a_{y\,nk-1} + a_{y\,nk})\,\Delta t / 2$$
$$x_{nk+1} = x_{nk} + u_{nk}\,\Delta t + a_{x\,nk}\,\Delta t^2 / 2$$
$$u_{nk+1} = 0$$
$$y_{nk+1} = y_{nk} + v_{nk}\,\Delta t + a_{y\,nk}\,\Delta t^2 / 2$$
$$v_{nk+1} = 0$$

Task 4: Compare the results from the previous tasks and check, if the suggested approach can be used for the packing problem.