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TND004: Data Structures
Lab 3: part 1

Goals

- To implement a priority queue using a binary heap.
- To use a priority queue to implement an event-driven simulation.

Getting started

This exercise is about improving the given implementation of a simulation system for particles collision.

To get started with the exercise, perform the steps indicated below.

- Create a folder for this lab named e.g. `Lab3-part1`.
- Download the zipped folder with the files for this exercise from the course website and unzip it into the lab folder.
- Execute the remaining instructions in the file `README.md` (can be opened with Notepad). The instructions given in `README.md` are similar to the ones given for the labs in TNM094.
- Compile, link, and execute the program (the `main` function is in `lab3.cpp`). When prompted for a particles file, enter e.g. `billiards10.txt` or `against-each-other.txt`. A particles collision simulation should then start.
- Read the remaining lab description and understand the given code. Compared to previous labs, a major part of this exercise is dedicated to understanding the given code[1].
- Implement both functions required for the exercise in this part 1. The concepts introduced in lecture 7 can be useful here, as well as sections 6.1 to 6.4 of the course book.

Note that you cannot modify the given code, except where explicitly indicated by the lab instructions.

If you have any specific question about the exercises, then send us an e-mail. Be short and concrete, otherwise you won't get a quick answer. You can write your e-mail in Swedish. Add the course code to the e-mail's subject, i.e. "`TND004: ...`".

Event-driven simulation: particles collision system

This exercise is about simulating the motion of $N > 0$ colliding particles according to the laws of elastic collision. Such simulations are widely used in molecular dynamics to understand and predict properties of physical systems at the particle level. This

[1] Code related to the rendering functionality can be safely ignored, though. It's not either required full understanding of the physics behind the particles' collisions, i.e. implementation of the functions declared in `particle.h`.

includes the motion of molecules in a gas, the dynamics of chemical reactions, and atomic diffusion. The same techniques apply to other domains that involve physical modeling of particle systems including computer graphics, computer games, and robotics.

The *hard sphere model* is used (or billiard ball model) which is an idealized model of the motion of atoms or molecules in a container. We focus on the two-dimensional version called the *hard disc model* which makes the following assumptions.

- N particles in motion, confined in a unit box.
- Particle i has position (rx_i, ry_i)[2], velocity (vx_i, vy_i), mass m_i, and radius σ_i.
- Particles interact via elastic collisions with each other and with the reflecting boundary (walls).
- No other forces are exerted. Thus, particles travel in straight lines at constant speed between collisions.

There are two natural approaches for simulating the system of particles.

- *Time-driven simulation*. Discretize time into time intervals of size *dt*. Update the position of each particle after every *dt* units of time and check for overlaps. If there is an overlap, roll back the clock to the time of the collision, update the velocities of the colliding particles, and continue the simulation. The major drawback of this approach is time efficiency. To ensure a reasonably accurate simulation, we must choose *dt* to be very small, and this slows down the simulation. On the other side, we may miss collisions if *dt* is too large.
- *Event-driven simulation*. Because it's possible to predict when collisions will occur (see section "Particles"), we focus only on those times at which interesting events[3] occur, when using event-driven simulation approach. Thus, our main challenge is to determine the ordered sequence of particle collisions. We address this challenge by maintaining a *priority queue* for future events, ordered by time.

In this exercise, we follow the event-driven simulation approach. Classes `Particle`, `Event`, `PriorityQueue`, and `CollisionSystem` implement the needed functionality. These classes are briefly described below.

The `main` function in `lab3.cpp` executes the simulation. The simulation duration is set to 10.000 seconds.

Data files

Several input files with particles are given in the folder `collisionsystem\data`. As illustrated below, the first line contains the number of particles $N > 0$. The remaining N lines contain six real values (a particle's center's position, velocity, mass, and radius) followed by three integers (particle's color in RGB). Particles do neither overlap with other particles nor with walls (the simulation box boundaries).

```
N
rx ry vx vy mass radius r g b
rx ry vx vy mass radius r g b
```

[2] Coordinates of the particle's center point. A particle can be idealized as a circle.
[3] e.g. collisions

…

Exercise: priority queue

The file `priorityqueue.h` contains a template class[4] representing a priority queue used by the simulation program. The priority queue is implemented as a heap. Your task in this exercise is to implement two member functions.

- A function `isMinHeap` to test whether the queue is a min-heap (i.e. the heap ordering property is satisfied). Then, uncomment the line "`//#define TEST_PRIORITY_QUEUE`" in the file file `priorityqueue.h`, execute the code, and check that no assertion fails.
- The heap-insert function. In the current implementation distributed with this lab, a lazy strategy is used to insert new elements (e.g. events representing collisions) in the heap through a function named `toss`. The function `toss` simply adds a new element to the last slot of the queue, though this may destroy the heap ordering property. Consequently, the heap ordering must be restored every time the min-element is removed from the heap.

  To test your implementation of the insert function, make sure the line "`#define TEST_PRIORITY_QUEUE`" remains uncommented, execute the code, and check that no assertion fails.

After having implemented and tested the functions indicated above, each call to function `toss` should be replaced with a call to the heap-insert function, in the file `collisionsystem.cpp` (see function `addEvent`). Then, it's time to check whether it's possible to run the simulation program. To this end, comment again the line "`#define TEST_PRIORITY_QUEUE`" in `priorityqueue.h` (`isMinHeap` is not called in this case) and then run the program with the given data files.

Note that it should still be possible to run the program by calling the function `toss`.

Finally, make sure you run the simulation with the input file `brownian.txt` (containing 1000 particles), first using the `toss` function and then again using the heap-insert function you have implemented. Notice the difference in the simulation "speed"[5].

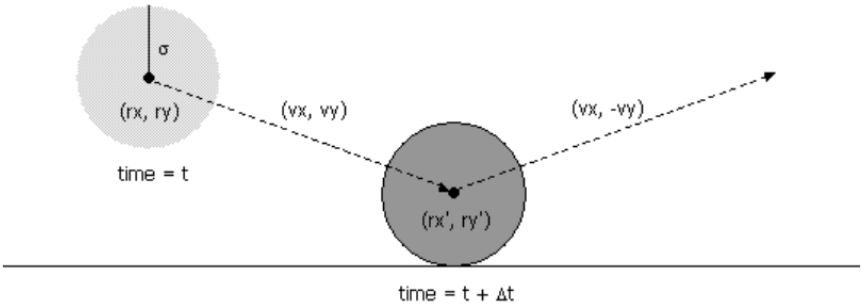
Classes

Particles

Class `Particle` represents particles and it has member functions to predict collisions of a particle with other particles and walls: `timeToHit`, `timeToHitVerticalWall`, and `timeToHitHorizontalWall`.

We illustrate below how to predict if and when a particle with position (*rx, ry*) at time *t* will collide with a horizontal wall.

[4] The implementation of member functions of a template class should be given in the header file.
[5] Of course, your computer's performance can also have an influence.



Since the coordinates are between 0 and 1, a particle comes into contact with an horizontal wall at time $t + \Delta t$, if the quantity $ry + \Delta t.vy$ equals either σ or (1 - σ). Solving for Δt yields:

$$\Delta t = \begin{cases} (1 - \sigma - ry) \,/\, vy & \text{if} \quad vy > 0, \\ (\sigma - ry) \,/\, vy & \text{if} \quad vy < 0, \\ \infty & \text{if} \quad vy = 0. \end{cases}$$

An event representing the collision of the particle with wall can then be added to the priority queue with priority given by the predicted time of the collision, i.e. $t + \Delta t$.

It's possible that the formula above predicts that no collision with a horizontal wall will occur ($\Delta t = \infty$) or that a collision occurs too far in the future, and consequently, outside the set simulation duration. In this case, an event is not added to the priority queue. Similar ideas apply to collisions with vertical walls and other particles.

When a collision occurs, then the velocity of the involved particle(s) needs to be updated. This is done by member functions `bounceOf`, `bounceOffVerticalWall`, and `bounceOffHorizontalWall`.

Events

Class `Event` represents either a collision or a rendering event. More concretely, there are four types of events: a rendering event; a collision with a vertical wall; a collision with a horizontal wall; or a collision between two particles.

Rendering events cater for the visualization of all particles in the system at a given point in time. Rendering events are automatically generated by the system with a given frequency (e.g. 10 times per time unit).

Each instance of this class stores the event's occurrence time and two pointers to particles (one or both pointers might be null, depending on whether the event represents a collision with a wall or is a rendering event, respectively).

Collision system

Class `collisionSystem` represents the system of particles and it has a member function to simulate (named `simulate`) the system for a given time period (i.e. the simulation duration).

Collisions modify the direction in which particles move. Since collisions events are not necessarily inserted in the queue by chronological order, it's possible that collision events already in the queue become invalid[6] when another event is inserted.

[6] For instance, a collision between two particles at a time t changes their velocity. Thus, some events already in the queue, and that have been predicted for some time $t' > t$, may not occur.

The main loop of function `simulate` executes the following steps:

1. Pull lowest-time event off event queue. Assume this event takes place at time t.
2. If the event corresponds to an invalidated collision, discard it. The event is invalid if one of the particles has participated in a collision since the time the event was inserted onto the priority queue.
3. If the event corresponds to a physical collision between particles i and j:
    a. Advance all particles to time t along a straight-line trajectory.
    b. Update the velocities of the two colliding particles i and j according to the laws of elastic collision.
    c. Determine all future collisions that would occur involving either i or j, assuming all particles move in straight line trajectories from time t onwards. Insert these events onto the priority queue.
4. If the event corresponds to a physical collision between particle i and a wall, do the analogous procedure (steps 3.a – 3.c) for particle i.

Presenting part 1 and deadlines

The exercises in this lab are compulsory and you should demonstrate your solutions during the lab session *Lab3 RE*. Read the instructions given in the labs webpage and consult the course schedule.

Necessary requirements for approving your lab are given below.

- Present the implementation of the functions required in exercise. Other modifications in the given code are not accepted.
- The code must be readable, well-indented, and use good programming practices.
- Be able to describe verbally the main steps of the code in the simulation function, i.e. `CollisionSystem::simulate`.

If your code for lab3/part1 has not been approved in the scheduled lab session *Lab3 RE* then lab 3 is considered a late lab. Late labs can be presented provided there is time in a another RE lab session. All groups have the possibility to present one late lab on the extra RE lab session scheduled in the end of the course.