Simulation of collective self-management by the movement of robotic vehicles using the method of molecular dynamics

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Abstract. The paper presents the results of computer modeling of traffic flows in a virtual city. The city has a local road, highway and road junction. The article proposes a system for autonomous driving of robotic vehicles in this virtual city. This system is based on the application of interaction rules taken from molecular dynamics modeling with kinetic energy dissipation. The proposed model uses the concept of a cellular automaton. The tests were carried out using computer simulations. The work has shown the efficiency of the proposed approach. The recommended rules of interaction allow you to organize traffic without traffic jams and without traffic lights in such a virtual city with the maximum possible traffic congestion.

1 Introduction

There are two approaches to the study of traffic flows. Each vehicle is viewed in interaction with each other—this is a micro-level approach. Transport streams are an object of study—this is a macro-level approach [1, 2]. Individual histories of the movement of vehicles are investigated depending on their characteristics and the structure of transport routes in the first case. Their integral characteristics are investigated in the second case. M.J. Lighthill and G.B. Whitham created in 1955 the first mathematical model designed to study traffic flows [3]. A hydrodynamic model was taken as a basis, which describes the dependence of the flow density on its intensity on a certain section of the road. The average speed of the traffic flow, its density and intensity were the main parameters of the model. The traffic flow is subject to phase transitions—sharp changes in speed and density, just like a liquid. This fact is shown within the framework of this model. The results made it possible to qualitatively describe the wave processes of the emergence and decay of plugs obtained in these works. However, specific recommendations are not given for managing traffic flows without congestion based on these models are not given in the discussed works.

2 Formulation of the problem

It is required to develop an autonomous system of self-government and find the rules of interaction for robotic vehicles. At the same time, traffic in the city should be organized without traffic jams, without traffic lights and without collisions, using these rules [4].

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The system should:

1. Provide the maximum possible traffic of the transport system.
2. The distance between two objects must not be less than a predetermined value.
3. Ensure that there are no traffic jams.

The task includes the formulation of recommendations for road users in a real city to improve safety and traffic optimization. The concept of *cellular* automaton was used as a modeling environment at the microlevel when solving the problem [5]. This approach has greatly simplified the computer simulation of traffic flows and made it possible to study a large number of implementations with different initial conditions [6–8].

3 Computer model

Research on the self-management system of robotic vehicles was carried out using computer simulation. The transport scheme of roads and junctions is set. Roads are arranged on two levels in the form of contiguous local ring roads, highways, and roundabouts. The quarters are located within the local ring road (figure 1). The traffic is one-way on all roads. There is a permanent parking place inside the quarters for each robotic vehicle. Vacant parking spaces are also available. All robotic vehicles have vision systems and can determine the coordinates of the nearest vehicles and road elements constantly. Traffic lights are not used. The constant movement of transport is organized so that the traffic flows do not cross. Each robotic vehicle has the ability to start moving at any time and to any vacant parking lot, stop there for the required time and return to the original parking lot.

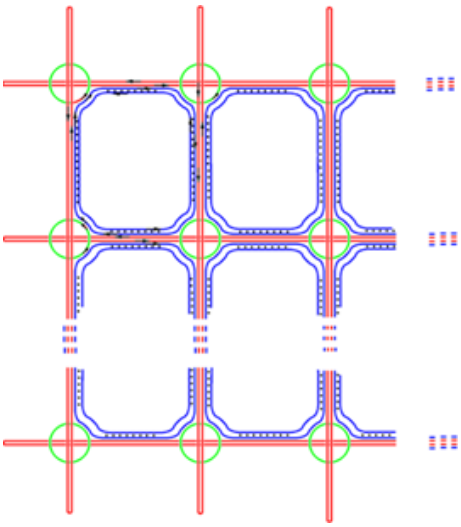

Figure 1. Transport scheme of the city

4 Transport Network Topology

The solution to the problem is divided into two parts. The topology of the network of roads and junctions is developed in the first part as follows:

- the arrangement of expressways is orthogonal and two-level;
- traffic streams do not cross.

Ring local roads exist next to each section of the highway. Travel speeds on these sections are lower than on highways. Roundabouts adjoin them. The speed of movement on them is even lower. This scheme of the organization of traffic flows is shown below in figure 1.

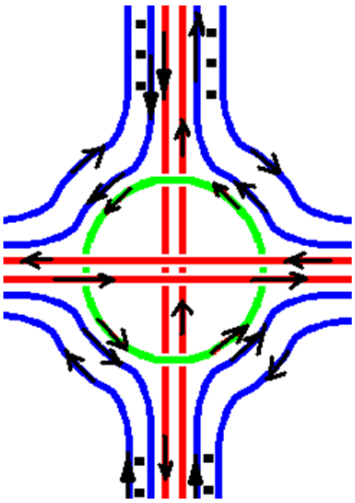

Figure 2. Two-level road junction scheme

Local roads—blue rings, roundabouts—green rings, long highways—red sections. The parking lots of the robotic vehicles are located between the blue roads. There are parking lots with even and odd numbers. Vehicles have an assigned parking space with odd numbers. Even numbered parking lots are shared property. Suppose a robotic vehicle chooses a destination. The optimal trajectory of movement is chosen from his own parking lot to any other, unoccupied parking lot with an even number. If this parking lot is occupied by another robot car, then the robotic vehicle selects the nearest unoccupied parking lot to it. The robotic vehicle can perform swaps in the following order: local road—roundabout—local road—highway—local road—roundabout—local road. It should be noted that the traffic order: roundabout—highway—roundabout is not provided. A diagram of a two-level movement with an indication of the direction of movement is shown in figure 2.

5 Interaction Rules

The second part of the assignment contains the organization of conflict-free movement. A system of rules for the interaction of moving robotic vehicles—intelligent agents—has been developed. Calculations of molecular dynamics are the basis. For each robotic vehicle, one-way traffic along the local road line and the roundabout is considered. In these calculations, the ring roads conditionally unfolds into a sequence of interconnected line segments. It is considered that only adjacent robotic vehicles affect the robotic vehicle. The quasi-cellular automaton implements the computer model of the city. A quasi-cellular automaton has two types of objects placed in cells.

The first type of objects is static—road elements and their types. The second type of objects—dynamic—imitates moving robotic vehicles. Each cell has a two-level link system. We will conventionally call local roads and ring intersections rings. Links of the first level provide an indication of the direction of movement between cells of one ring, and links of the second level provide transitions between rings.

The molecular dynamics method is the basis for the construction of a decentralized system of self-control of robotic vehicles. It is known that atoms are always located at distances not exceeding a certain value $r_{\min}$, during chaotic motion in various states of aggregation, as well as in cascades of atom-atom collisions [9]. Each robotic vehicle is conditionally represented by a macromolecule. The mass of this macromolecule is equal to the mass of the robotic vehicle, and the position of this macromolecule is related to the position of its center of mass. Force acts on a macromolecule, defined as the vector sum of all forces.

These forces act from the side of the nearest neighboring macromolecules and obstacles. The force is determined from the Lennard–Jones potential of the pairwise interaction known in molecular dynamics, acting on one macromolecule from the other [10]. The movement control of robotic vehicles does not allow the vehicles to collide with each other, built on the basis of such calculations. A special computational program was compiled and debugged to test the possibility of using the molecular dynamics method [9, 11, 12]. Computer simulation of the main modes of movement was carried out. Verification of the fulfillment of the law of conservation of energy in the system of macromolecules controlled the accuracy of the calculations.

The equations of motion have the form according to Newtonian mechanics:

$$\frac{d[\mathbf{r}_i]}{dt} = v_i, \quad m\frac{d[\mathbf{v}_i]}{dt} = f_i = \sum_{j=1, j\neq i}^{N} \mathbf{F}(\mathbf{r}_{i,j}).$$

Here t is the time, m is the mass of the macromolecule, f_i is the total force acting on the macromolecule with the number i from the side of other macromolecules of the system, $\mathbf{F}(\mathbf{r}_{i,j})$ is the force acting on the macromolecule with the number i from the side of the macromolecule with the number j.

The relationship between the force and energy of pair interaction is described by the equation

$$\mathbf{F}(\mathbf{r}_{i,j}) = -\nabla_i u(\mathbf{r}_{i,j}).$$

The equations are written as follows for the projections of the velocities along each coordinate axis:

$$V_{x(t+\Delta t)} = \frac{x(t+\Delta t) - x(t)}{\Delta t}, \quad V_{y(t+\Delta t)} = \frac{y(t+\Delta t) - y(t)}{\Delta t}.$$

Here Δt is the time step.

The forces acting in the system are described by Newton's II law:

$$\mathbf{F} = m\frac{d\mathbf{V}}{dt}.$$

The system of equations is obtained for the projections of the force acting on the macromolecule:

$$F_x = \frac{m}{\Delta t}(V_{x(t+\Delta t)} - V_{x(t)}), \quad F_y = \frac{m}{\Delta t}(V_{y(t+\Delta t)} - V_{y(t)}).$$

The equations are obtained after transformations for calculating the projections of the speeds of movement of robotic vehicles:

$$V_{x(t+\Delta t)} = V_{x(t)} + \frac{F_x \Delta t}{m}, \quad V_{y(t+\Delta t)} = V_{y(t)} + \frac{F_y \Delta t}{m}.$$

The Lennard–Jones potential was chosen to calculate the interactions in the work describing the Van der Waals interaction of neutral atoms. The Lennard--Jones potential has the form

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

where σ is the value of the interatomic distance at which $U(\sigma) = 0$, ε is the depth of the potential well located at a distance $\sigma\sqrt[6]{2}$. In this expression, the term r^{-6} dominates at large

distances and corresponds to dispersive dipole-dipole attraction. The term r^{-12} simulates a strong repulsion between a pair of atoms due to exchange interaction if they are very close to each other. The graph of this potential is shown in figure 3.

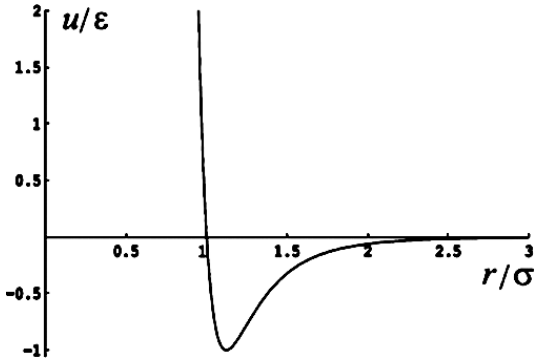

Figure 3. Lennard–Jones potential

The absolute value of the force is the first derivative of the potential energy of the pair interaction, taken with a minus sign:

$$F(r) = -\frac{d[U]}{dr}.$$

The so-called cutoff radius of the potential R_{ab} is introduced to speed up the calculations. In this case, the weak effect of distant macromolecules is not taken into account. Forces are calculated only within a sphere of this radius, acting on a given macromolecule. The issue of choosing the size of the time step Δt is important when carrying out calculations using schemes for the numerical integration of the equations of motion. As is known, a significant loss of calculation accuracy is observed when the value of Δt exceeds a certain threshold value, and the values of forces, coordinates, and velocities tend to infinity after some time.

Typically, researchers choose Δt by fit using molecular dynamics techniques. They increase the selected small time step value gradually. The procedure is carried out until a significant loss of accuracy occurs when repeatedly solving the same problem. Then the penultimate value Δt is chosen as the integration step. The change in the value of the integration step over time Δt can reach several orders of magnitude at the initial and final stages. The use of the traditional Δt selection scheme was an obstacle to computer simulation of the studied physical processes. An adaptive scheme for calculating Δt was proposed, which makes it possible to completely exclude the procedure of multiple empirical selection of this value. This allowed research [9, 11, 12]. The calculation scheme for Δt is constructed as follows. The minimum distance $r_{\min}$ is among all mutual distances between macromolecules. The potential of pair interaction is approximately replaced by a parabolic potential in the vicinity of this value. The second derivative of the potential energy of the pair interaction is equal to the constant of this parabolic potential

$$C = \left.\frac{d^2[U]}{dr^2}\right|_{r=r_{\min}}.$$

It is known that the period of harmonic oscillations of a macromolecule of mass m in such a field is

$$2\pi\sqrt{\frac{m}{C}}.$$

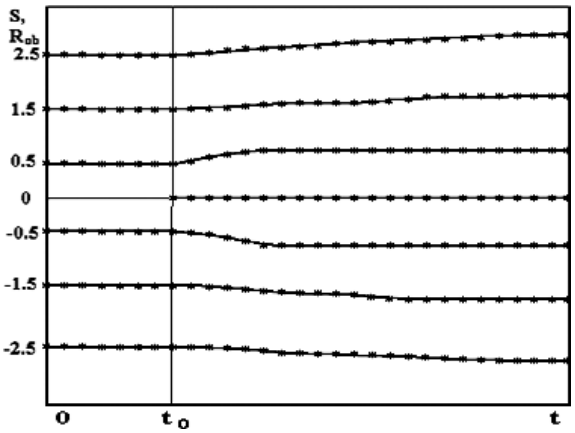

Figure 4. Transition of a tuple of robotic vehicles from a stressed state to a non-stressed state

We calculate the forces, coordinates and velocities of macromolecules only in a small vicinity of the potential acting on it. Therefore, we can take a rather small part of the vibrations of the macromolecule as the value of the time integration step. Experience shows that it is necessary to select this part in the range from 0.02 to 0.1 of the oscillation period. Then the divergence is not observed in the numerical scheme of calculations and there is no loss of the accuracy of calculations. The value of the time integration step is calculated in this work by the formula [9, 11]

$$\Delta t = 0.1\pi \sqrt{\frac{m}{\left.\frac{d^2[U]}{dr^2}\right|_{r=r_{\min}}}}.$$

Coefficient C is selected experimentally and introduced into the equations of motion. The coefficient is less than one and simulates the introduction of viscous forces into the system. These forces eliminate periodic oscillations of macro macromolecules near the positions of the potential minimum. In this case, all values of velocity projections are determined by integrating the motion of macroparticles. Projection values are multiplied by this factor. This leads to the dissipation of kinetic energy in the system. The values of the translational speed allowed for a given ring are subtracted from the velocities of all macromolecules. The interaction potential of a macromolecule is calculated as the sum of the interaction potentials of neighboring macromolecules. This potential can be zero. The road condition in this case is called unstressed. The interaction rules are formulated for the organization of accident-free movement of vehicles controlled by molecular dynamics calculations:

1. The robotic vehicle starts moving in accordance with the travel plan it has It can enter the road if a relaxed state is present at the moment. Suppose that a robotic vehicle has a need to rebuild to another road. He can enter it if the distance does not exceed the value $0.5R_{ab}$ to the nearest robotic vehicle.

2. The robotic vehicle can move around the ring at the speed allowed for that ring. The speed can only change according to the molecular dynamic's calculations when the point of the robotic vehicle on the ring is in a stressed state.

3. The robotic vehicle can change its speed from that allowed in a given place, if molecular dynamics calculations require it.

Suppose a robot vehicle enters another ring and puts the neighbors in a tense state. In this case, the process of calculating motion parameters begins with the use of molecular dynamics. This process clings until the entire cortege goes into a relaxed state. Let's say there are not enough ring sizes. Then the ring remains tense. Other vehicles cannot enter it. The unstressed state occurs when one or more robotic vehicles leave this ring. This process is shown in figure 4.

A tuple of six robotic vehicles travels along a certain ring during the time from 0 to t_0. The robotic vehicle enters from another ring between the third and fourth robotic vehicles at time t_0. The results of molecular dynamics calculations with kinetic energy dissipation show that the rearrangement processes proceed smoothly with oscillation damping.

6 Calculation results

Two groups of experiments were conducted. The city model consisted of $10 * 10$ local roads, and there were twenty thousand vehicles. The following values of the conditional velocities were chosen in the experiment: for the roundabouts—1, for the local roads—2, for the highway—4.

50 robotic vehicles and 50 vacancies were located along each side within the local road. The amount of traffic was measured in arbitrary units. $N_{\max}$ was the number of robotic vehicles that could simultaneously be at R_{ab} distance from each other. The total number of vehicles exceeded $N_{\max}$ by 3.2 times available in the city. Traffic congestion did not exist in all experiments with these parameters. The analysis of traffic flows was carried out in the case of the movement of robotic vehicles and in accordance with their individual travel histories in the situation of a virtual city model. Interaction rules were developed for car drivers based on this analysis. These rules were formulated as follows:

1. Drivers strive to always maintain a fixed distance between vehicles.
2. The distance must be greater than a fixed predetermined distance between his vehicle and vehicles already moving on the road. After that, the driver can start moving.
3. The driver can enter the local road only when the distance between his car and the cars already driving on the highway exceeds a fixed, predetermined value.
4. A car can go to another ring when changing lanes if the distance between cars is more than half of the fixed value.

The car tries to take a position in the middle between the front and rear vehicles until it moves away from them at a fixed distance.

Table 1. Results of computer experiments

	Cars			Robotic vehicles		
Traffic	0.14	0.28	0.44	0.18	0.34	0.58
Exceeding the time	1.22	1.28	1.47	1.08	1.15	1.35
Lengthening the Path	1.19	1.25	1.44	1.03	1.17	1.21

It should be noted that there is always a car located at the back and in front of each car in the case of a ring. The distances between them can be large. Traffic jams were not observed in the case of movement along the ring, subject to these rules. Therefore, rule 4 is universal. The results of computer experiments are shown in table 1 for robotic vehicles and cars.

The best movement parameters are observed in the case of robotic vehicles.

7 Conclusion

The obtained interaction rules allow organizing traffic without traffic jams, without traffic lights and without collisions of vehicles in the proposed city model. A large number of experiments have been carried out with different initial conditions. Traffic jams were not observed when the traffic intensity reached 58% of the theoretically possible in the case of robotic vehicles and 44% in the case of drivers driving cars while observing the rules of interaction. The molecular dynamics model has been proposed and tested in difficult traffic situations. The proposed model has shown its effectiveness. The methodical value of the work lies in this.

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