Comparative analysis of Euler, Verlet and Runge-Kutta methods. Applications in science

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1 Introduction

Nowadays there exists a plethora of tasks in neuroscience, geography, biology, physics, chemistry, sociology and many more sciences, that require definite descriptive illustrations, complex multistep calculations and analysis.

For the last several decades computer simulation serves to resolve that problem. It is used as a method of portraying objective reality and consists in replication of real-world processes and phenomenons, employing other objects or abstract descriptions as images, equations, algorithms and programs. The main benefit of modelling is the ability to study non-repetitive events, objects that are impossible to depict under any laboratory conditions, visualise theoretical bodies, control time in the process and perform an unlimited amount of experiments. Because of these matters, it was decided to analyse Euler, Verlet and Runge-Kutta methods and consider definite examples of their application in science.

Euler, Verlet and Runge-Kutta methods are all numerical methods of solving differential equations. They are used for theoretical investigations of differential equations, finding the trajectory of a moving body and a variety of other purposes. One of the goals of this work is to determine which method best suits models to which it is applied.

And so, the goals of the research:

1. Develop a testing model for the comparative analysis of numerical methods of solving differential equations.
2. Test selected methods using developed model.
3. Characterize given methods on the basis of the testing results.
4. Verify the correctness of our choice on the basis of actual models used in science.

That happens to be necessary, therefore serves for explaining the originality of the research due to the following reasons:

1. No such characteristics has been given to the numerical methods before.
2. No such model was applied for the comparative analysis before.

2 Development of the method of comparative analysis of numerical methods of solving differential equations

The study of various methods of solving differential equations leads to a question of evaluation of their efficiency. A method based on a physical law, specifically, the law of conservation of energy, was developed.

It is known, that total mechanical energy of a system is conserved in absence of non-conservative forces, and that concept was applied in an idealisation. Thus, let us a construct a simulation: a pendulum consisting of a mass $m = 1$, attached to a weightless rod of length $L = 3$, deflected at an angle of $\theta_0 = 30^o$. Then, total mechanical energy of a system equates to:

$$E_0 = mgL(1 - cos\ \theta_0)$$

Due to errors arising from an approximating nature of the method, total mechanical energy will dissipate from its initial value. In each discrete moment of time, knowing velocity and coordinates of a mass, total mechanical energy will be calculated. Introducing relative error function:

$$\delta(t) = \frac{|E - E_0|}{E_0},$$

whereas

$$E = mgL(1 - cos\ \theta) + \tfrac{mv^2}{2}$$

It is also necessary to determine the variable parameters of the pendulum. There are three of them in the model: angle θ between $x = 0$ and line, connecting a mass and point (0;0); angular velocity of a mass $\frac{d\theta}{dt}$ and time t.
With such simulation, $\delta(t)$ will increase, and so, that $\delta(t)$ will be possible to represent as a linear function (excluding Verlet method), what will be shown in further experiments. The efficiency of a method will be determined based on the slope of that line. Approximation of $\delta(t)$ will be conducted using linear regression.

3 Comparative analysis

3.1 Euler method [1]

Euler method is fundamental. In the abstract, it constitutes a construction of a fractured line, approximating a function.
Let a differential equation:

$$\frac{dy}{dx} = f(x)$$

With initial condition:

$$f(0) = x_0$$

Next, we approximate a derivative by a small finite difference Δx:

$$\frac{y(x + \Delta x) - y(x)}{\Delta x} = f(x)$$

Then, Euler method:

$$y(x + \Delta x) = y(x) + f(x)\Delta x$$

And so, we apply the method of comparative analysis.

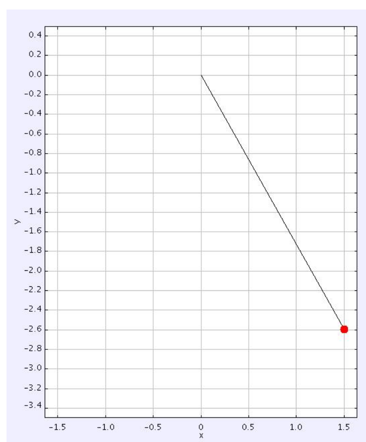
For the pendulum, Euler method takes a form:

$$\theta(t + \Delta t) = \theta(t) + \frac{d\theta(t)}{dt}\Delta t$$

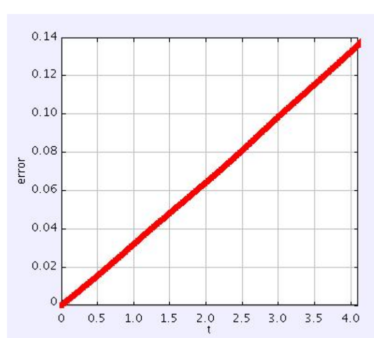
$$\frac{d\theta(t + \Delta t)}{dt} = \frac{d\theta(t)}{dt} - \frac{g}{L}\sin\theta(t)\Delta t$$

Let $\Delta t = 0.01$

Initializing and starting a simulation:



After 4 seconds of simulation, plot of $\delta(t)$:



It is trivial, that $\delta(t)$ is a linear function. Analysing discrete data (first column - time, second column - error):

```
3.8799999999999613 0.12834726543846783
3.889999999999961 0.12869079199953265
3.899999999999961 0.1290347141540609
3.9099999999999606 0.1293790517852555
3.9199999999999604 0.12972382501392238
3.92999999999996 0.13006905412301645
3.93999999999996 0.13041475947876757
3.9499999999999598 0.13076096144871846
3.9599999999999596 0.13110768031700046
3.9699999999999593 0.13145493619722404
3.979999999999959 0.1318027489433776
3.989999999999959 0.13215113805911793
3.9999999999999587 0.13250012260589347
4.009999999999959 0.13284972111032226
4.019999999999959 0.13319995147128147
4.0299999999999585 0.13355083086716556
4.039999999999958 0.1339023756637721
4.049999999999958 0.13425460132330647
4.059999999999958 0.1346075223149
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Then, for Euler method $\delta(t) = kt$, where $k = 3.3125 * 10^{-2}$. A case, when $k = 0$ (assuming $b = 0$), shows an absolute efficiency of the method, and we will conduct further comparisons on the basis of a slope of a linear function.

3.2 Euler-Richardson method [1]

That method is a modification of Euler method. It consists in a construction of a tangent to a function that is being approximated at the point $t = t_n + \frac{1}{2}\Delta t$, using Euler method. Then, a ray, parallel to a tangent, is drawn from t_n. Then, the next point is an intersection of the ray and a line $x = t_{n+1}$.
For the pendulum, method look as follows:

$$\theta_{mid} = \theta(t) + \frac{1}{2}\frac{d\theta(t)}{dt}\Delta t$$

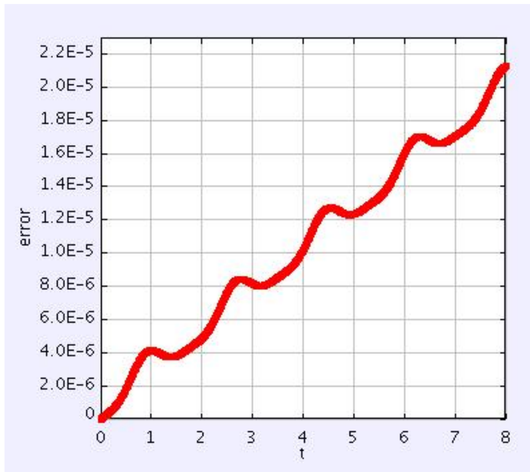
$$\frac{d\theta_{mid}}{dt} = \frac{d\theta(t)}{dt} - \frac{1}{2}\frac{g}{L}\sin\theta(t)\Delta t$$

$$\frac{d^2\theta_{mid}}{dt^2} = -\frac{g}{L}\sin\theta_{mid}$$

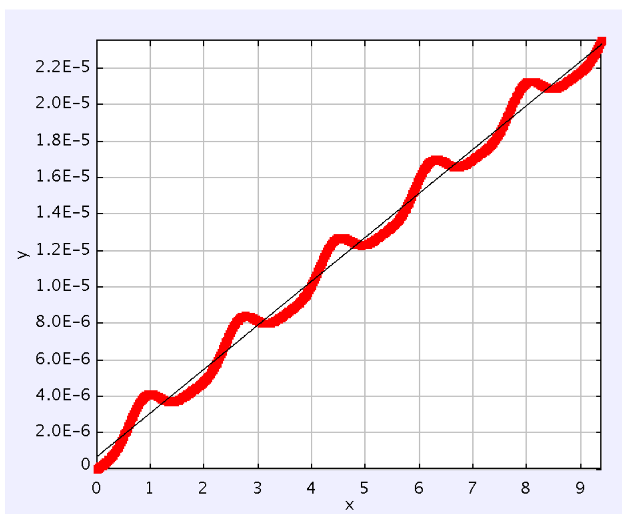
$$\theta(t + \Delta t) = \theta(t) + \frac{d\theta_{mid}}{dt}\Delta t$$

$$\frac{d\theta(t + \Delta t)}{dt} = \frac{d\theta(t)}{dt} + \frac{d^2\theta_{mid}}{dt^2}\Delta t$$

Starting a simulation, let $\Delta t = 0.01$.
After 8 seconds, the plot of $\delta(t)$:



As seen from the plot, it is reasonable to apply the linear regression model to represent $\delta(t)$ as a linear function:



Then, for Euler-Richardson method $\delta(t) = kt$, where $k = 2.43 * 10^{-6}$.

In spite of lack of any radical changes to the Euler method, the efficiency was augmented by a factor of 13632.

These changes happen, supposedly, due to the fact, that, if the function is monotonous between t_n and t_{n+1}, then, in case of employing Euler method, a fractured line that is being constructed precipitously dissipates, whereas constructing a tangent line at $t_n + \frac{1}{2}\Delta t$ gives a more accurate approximation.

3.3 Runge-Kutta fourth-order method [1]

The following method is, perhaps, the most used one. In spite of great calculation complexity (in comparison with Euler method), Runge-Kutta fourth-order method produces extremely accurate results when applied in most models.

The method consists in following: let k_1 is the value of the function at the beginning of the interval $x = x_n$. Then, employing Euler method, calculate the value of the function at $x_n + \frac{1}{2}\Delta x$, let k_2 be that value. Then, substituting k_2, instead of k_1, employing Euler method, calculate the value of the function at $x_n + \frac{1}{2}\Delta x$. And now substituting k_3, calculate k_4 at $x_n + \Delta x$. Compute the target value, giving more weight to the points at the middle of the interval:

$$y(x + \Delta x) = y(x) + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\Delta t.$$

Applying the method to the model,

For the angle:

$$n_1 = \frac{d\theta(t)}{dt}$$

$$n_2 = \frac{d\theta(t)}{dt} + \frac{1}{2}\frac{dn_1}{dt}\Delta t$$

$$n_3 = \frac{d\theta(t)}{dt} + \frac{1}{2}\frac{dn_2}{dt}\Delta t$$

$$n_4 = \frac{d\theta(t)}{dt} + \frac{dn_3}{dt}\Delta t$$

$$\theta(t + \Delta t) = \theta(t) + \frac{1}{6}(n_1 + 2n_2 + 2n_3 + n_4)\Delta t$$

For the angular velocity:

$$m_1 = \frac{d^2\theta(t)}{dt^2} = -\frac{g}{L}\sin\theta(t)$$

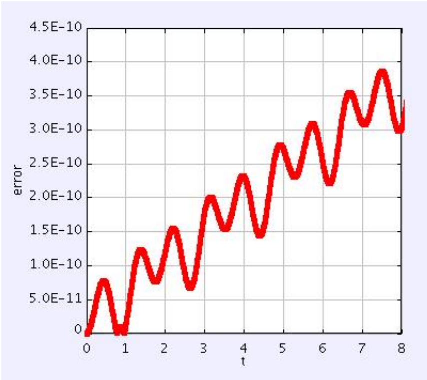
$$m_2 = -\frac{g}{L}\sin\theta(t) + \frac{1}{2}\frac{dm_1}{dt}\Delta t$$

$$m_3 = -\frac{g}{L}\sin\theta(t) + \frac{1}{2}\frac{dm_2}{dt}\Delta t$$

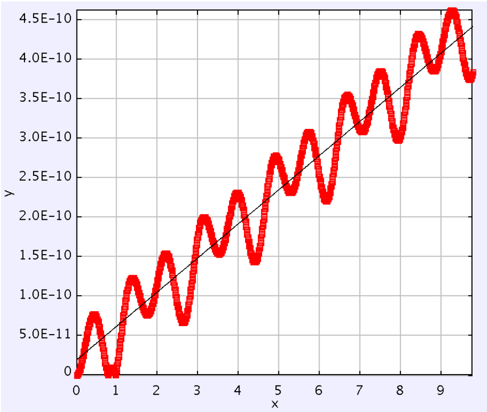
$$m_4 = -\frac{g}{L}\sin\theta(t) + \frac{dm_3}{dt}\Delta t$$

$$\frac{d\theta(t+\Delta t)}{dt} = \frac{d\theta(t)}{dt} + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4)\Delta t$$

Initiating the simulation, $\Delta t = 0.01$. Plot $\delta(t)$ after 8 seconds of simulation:



Linear regression is also reasonable in case of Runge-Kutta method:



Then for the Runge-Kutta fourth-order method, $\delta(t) = kt, \;\; k = 4.38 * 10^{-11}$.

The fourth-order Runge-Kutta method is 55480 times more efficient than the Euler-Richardson method.

3.4 Verlet method [1]

The Verlet method is most often used in a variety of computer games, but looking only at the mathematical description of the method described below, this fact does not seem obvious. Using the developed method of comparative analysis, the reason for this usage becomes clearly visible. Applying the method to the model:

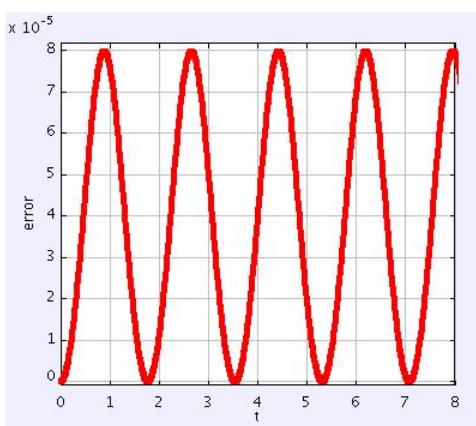
$$\theta(t+\Delta t) = \theta(t) + \frac{d\theta(t)}{dt}\Delta t - \frac{1}{2}\frac{g}{L}\sin\theta(t)(\Delta t)^2$$

$$\frac{d^2\theta(t+\Delta t)}{dt^2} = -\frac{g}{L}\sin\theta(t+\Delta t)$$

$$\frac{d\theta(t+\Delta t)}{dt} = \frac{d\theta(t)}{dt} + \frac{\frac{d^2\theta(t)}{dt^2} + \frac{d^2\theta(t+\Delta t)}{dt^2}}{2}$$

$$\frac{d\theta(t+\Delta t)}{dt} = \frac{d\theta(t)}{dt} - \frac{g}{L}\frac{\sin\theta(t) + \sin\theta(t+\Delta t)}{2}$$

Starting the simulation, $\Delta t = 0.01$. Plot of $\delta(t)$ after 8 seconds:



As we can see, $\delta(t)$ is a sine function, so using linear regression is not reasonable. Therefore, taking discrete data into account, sine period is $T = 1.83$, and amplitude is $A = 4 * 10^{-5}$. Then

$$\delta(t) = A \sin(\frac{2\pi}{T} t - \frac{\pi}{2}) + A$$

The application of the algorithm becomes clear. Runge-Kutta method is quite resource intensive for computer games, and Euler method is imprecise. Howevwer, the problem of Euler-Richardson method is that $\delta(t)$ is constantly increasing over time and after $\frac{k_{richardson}}{A} = 16.46$ seconds of simulation, $\delta_{richardson}(t)$ becomes equal to the average value of $\delta_{verlet}(t)$.

For all these methods, one can find a correspondence: the number of sections of monotony of $\delta(t)$ is equal to the number of steps taken in the method. So Euler method is a one-step method, so $\delta_{Euler}(t)$ has only one section of monotony, meaning that the sign of $\frac{\delta(t)}{dt}$ is constant; Euler-Richardson method is a two-step method, and $\delta_{Richardson}(t)$ has two recuring sections of monotony (fig.1); Runge-Kutta method is a four-step method, and $\delta_{Runge-Kutta}(t)$ has four recuring sections of monotony (fig.2); Verlet method is a two-step method, and has two recuring sections of monotony (fig.3).

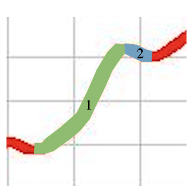


fig.1

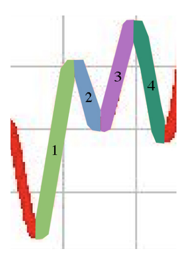


fig.2

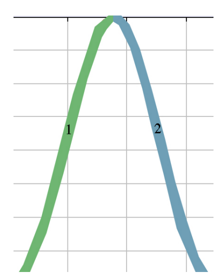


fig.3

4 The final comparative characteristic of the methods and the guide for usage in models

The Euler method is extremely inaccurate and the system parameters dissipate quickly, but it is necessary for the functioning of more efficient methods.
The Euler-Richardson method produces noticeable improvements and does not significantly increase computational complexity, but with continuous simulations the error becomes noticeable. It serves as the best alternative to Verlet method in case of impossibility of its application (differential equation of the form other than $\frac{d^2x(t)}{dt^2} = A(x(t))$).
The fourth-order Runge-Kutta method is the most effective, but it can not always be applied due to computational complexity.
The Verlet method is the best option for continuous simulations of the motion of particles, if low computational cost is required.

One of the goals of the work is to draw attention to the practical application of these methods. To familiarize the reader with the concept of computer modeling, in the next section a simple earthquake model is analyzed that does not include the methods described above. We will apply the methods in two models: the three-body problem and the Hodgkin-Huxley biophysical model. For both models, the fourth-order Runge-Kutta method is the best option, however, due to the high computational costs, for the three-body problem we will use the Verlet method (movement of particles), and for the Hodgkin-Huxley model, the Euler-Richardson method (system of differential equations of the form other than $\frac{d^2x(t)}{dt^2} = A(x(t))$).

5 Models

5.1 Cellular automata. Simple model of an earthquake

5.1.1 Introduction

In the end of 1940, J. von Neumann and C. Zuse formulated the idea of cellular automata. It was considered as a universal computing environment for constructing methods. The initial state of all cells and the rule of their transition from one state to another determine the development of events in the models

5.1.2 Earthquake model

The model is the dependence of the number of pushes $n_p$and earthquakes of a given size N_e on the limit value of force $F_c$and the change in the tension of blocks ΔF, having coordinates $(i; j)$, after each discrete time moment t. The lattice length L, F_c, ΔF and N are specified, which determinesN_e, numerically equal to the number of pushes at a discrete-time instant.

5.1.3 Rules of cell update

—1—. Value of F in each cell is increased by ΔF, and t by 1. This increment is a moving force effect due to the slow movement of the tectonic plate.

—2—. $F(i, j)$ is compared with F_c. If $F(i, j)$ ¡ F_c, Then the system is stable and —1— is repeated. Otherwise, $(F(i, j) \geq F_c)$, —2—→—3—.

—3—. The release of tension due to block slippage is indicated by assigning $F(i, j) = F(i, j) - F_c$. The transmission of tension is indicated by updating tension in positions that are four adjacent to the current – $(i, j \pm 1)$ $(i \pm 1, j)$ – according to the following rule: $F \rightarrow F + 0.25F_c$.

—4—. Periodic boundary conditions are not used.

Initialize and run the simulation:

$$L = 20;\ \Delta F = 0.01;\ F_c = 4;\ N = 5.$$

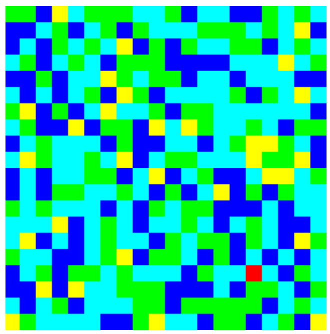


Figure 1: The state of the model at time $t = 23$.

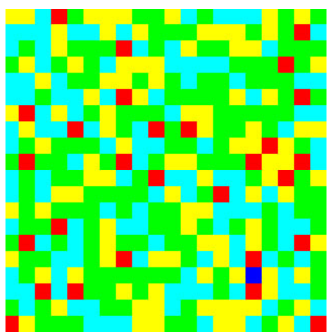


Figure 2: The state of the model at time $t = 93$.

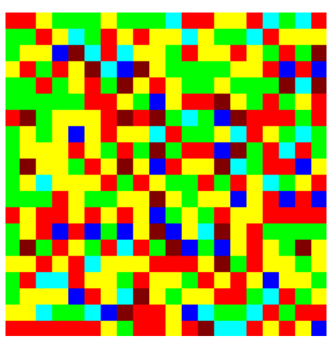


Figure 3: The state of the model at time $t = 158$.

5.2 Three-body problem [1]

5.2.1 Introduction

The problem is to determine the relative motion of the three particles that gravitationally interact with each other. In the years 1892-1899, Henri Poincare proved that the system of differential equations of the problem cannot be reduced to integrable.

5.2.2 Modeling

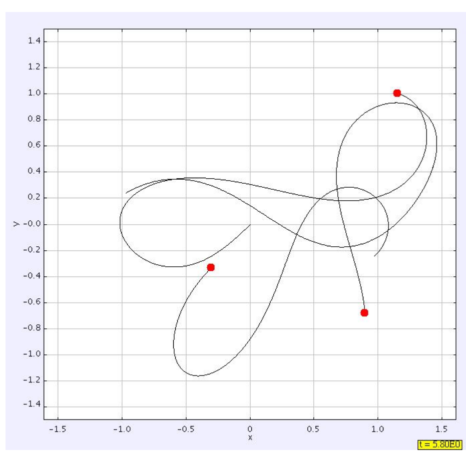
The system of differential equations describing the movement of three bodies:

$$\begin{cases} \frac{d^2\vec{r_1}}{dt^2} = Gm_2\frac{\vec{r_2}-\vec{r_1}}{|\vec{r_2}-\vec{r_1}|^3} + Gm_3\frac{\vec{r_3}-\vec{r_1}}{|\vec{r_3}-\vec{r_1}|^3} \\ \frac{d^2\vec{r_2}}{dt^2} = Gm_1\frac{\vec{r_1}-\vec{r_2}}{|\vec{r_1}-\vec{r_2}|^3} + Gm_3\frac{\vec{r_3}-\vec{r_2}}{|\vec{r_3}-\vec{r_2}|^3} \\ \frac{d^2\vec{r_3}}{dt^2} = Gm_1\frac{\vec{r_1}-\vec{r_3}}{|\vec{r_1}-\vec{r_3}|^3} + Gm_2\frac{\vec{r_2}-\vec{r_3}}{|\vec{r_2}-\vec{r_3}|^3} \end{cases}$$

where $G$is a gravitational constant, m_i respectively are the masses,

r_i respectively are the radius vectors

All three equations are of the form $\frac{d^2x(t)}{dt^2} = A(x(t))$, so we use the Verlet method for them. We initialize the simulation, assign random values ranging from -1 to 1 to the initial coordinates and velocities of the bodies.



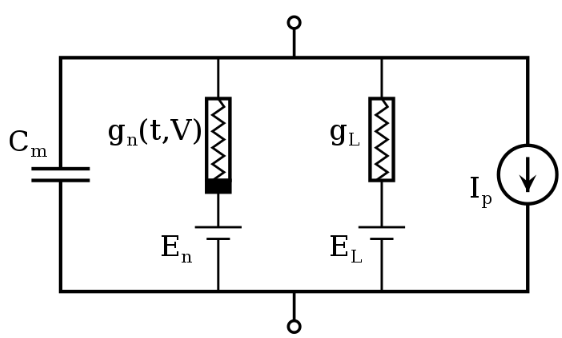
5.3 Hodgkin-Huxley [2]

5.3.1

The one under consideration is a biophysical model that describes the action potential in neurons. It was described by A. Hodgkin and E. Huxley in 1952, for which they received the Nobel Prize in Physiology or Medicine in 1963. The action potential or nerve impulse is a rapid increase, and then a decrease in the potential of the cell membrane. It occurs when, with an increase in the cell membrane potential due to external factors, a certain threshold is reached. Then, for example, in the axon of a neuron, when a threshold is reached (in our model we will consider the threshold of -55 mV), voltage-dependent channels of sodium ions open. Sodium ions quickly enter the cell, thereby causing membrane depolarization, then the sodium channels are deactivated, the channels of potassium ions open, the potential decreases again, repolarization occurs, and gradually, the potential returns to its initial resting position (-70 mV in our model).

5.3.2 Modeling

The electrical circuit described by Hodgkin and Huxley:



C_m - cell membrane, E_n - electrochemical gradient of ions,

$g_n(t, V)$ - voltage-dependent channel,

E_L - electrochemical gradient of passively moving elements,

g_L - channels of passively moving elements

The system of differential equations describing the system (V is potential):

$$\begin{cases} C_m \frac{dV}{dt} = -g_K n^4 (V - V_k) - g_{Na} m^3 h (V - V_{Na}) - g_L (V - V_L) + I_{ext}(t) \\ \frac{dn}{dt} = \alpha_n (1-n) - \beta_n n \\ \frac{dm}{dt} = \alpha_m (1-m) - \beta_m m \\ \frac{dh}{dt} = \alpha_h (1-h) - \beta_h h \end{cases}$$

Hodgkin and Huxley empirically determined the coefficients:

$$\alpha_n = 0.01 \frac{V+55}{1 - e^{-\frac{V+55}{10}}}$$

$$\beta_n = 0.125 e^{-\frac{V+65}{80}}$$

$$\alpha_m = 0.1 \frac{V+40}{1 - e^{-\frac{V+40}{10}}}$$

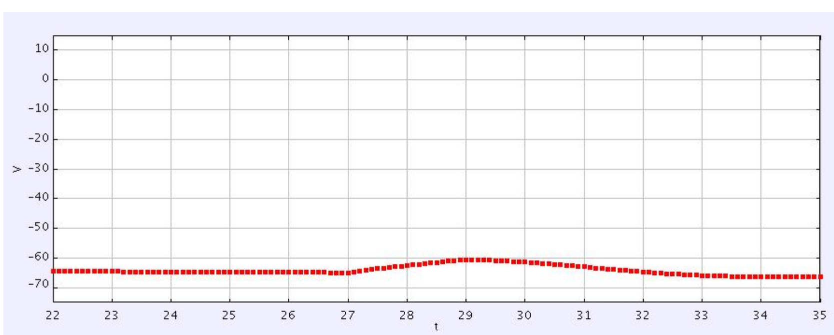
$$\beta_m = 4 e^{-\frac{V+65}{18}}$$

$$\alpha_h = 0.07 e^{-\frac{V+65}{20}}$$

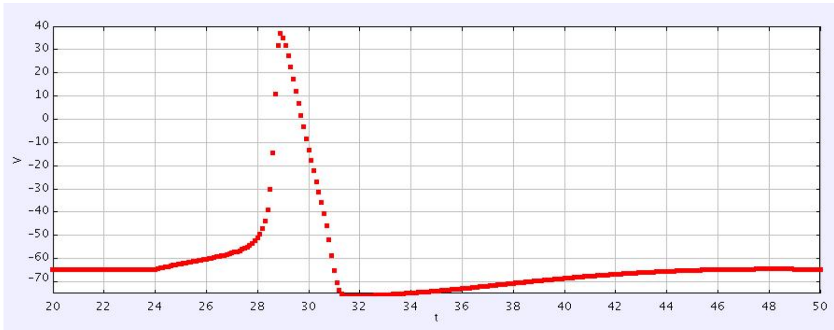
$$\beta_h = 1/[1 + e^{-\frac{V+35}{10}}]$$

Thus, we introduce into the model the solution of equations by the Euler-Richardson method. When a button is pressed, an electric current is applied to the simulation dendrites.

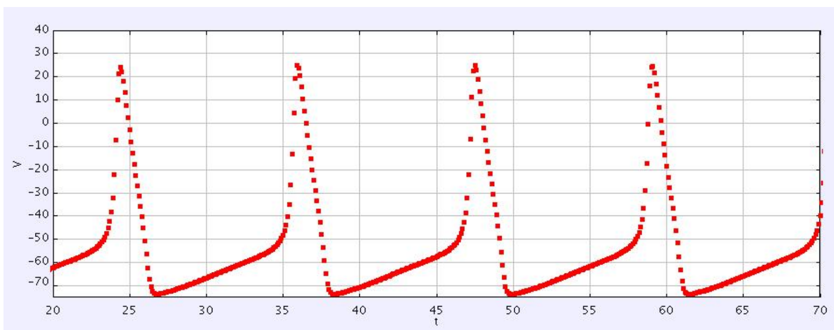
A current of 3 mA is supplied for a short time so that the potential does not exceed the threshold of -55 mV:



A current of 3 mA is supplied for a time sufficient to overcome the threshold of -55 mV:



A current of 20 mA is supplied continuously:



6 Conclusion

1. The developed model turned out to be suitable for a comparative analysis of numerical methods for solving differential equations.

2. As a result of testing, specific numerical characteristics of the methods were obtained.

3. As a result of the analysis of the characteristics, the specificity of each method was revealed, which made it possible to make a conscious choice of a method for usage in the models.

4. Based on testing of specific models used in science, the legitimacy of the obtained characteristics was confirmed.

References

[1] Christian W. Harvey G., Tobochnik J. *An introduction to computer simulation methods: applications to physical systems.* – 2016.

[2] Thomas Trappenberg. *Fundamentals of Computational Neuroscience.* – 2010.