# Dynamic systems with quadratic integrals

PCA'2020

Ali Baddour, **Mikhail Malykh**, Leonid Sevastianov and Yu Ying

RUDN

9 okt. 2020, ver. October 10, 2020

# Dynamic systems

One of the main continuous models is a dynamic system described by an autonomous system of ordinary differential equations, that is, a system of equations of the form

$$\frac{dx_i}{dt} = f_i(x_1, \dots, x_n), \quad i = 1, 2, \dots n, \tag{1}$$

where $t$ is an independent variable commonly interpreted as time, $x_1, \dots, x_n$ are the coordinates of a moving point or several points. In practice, the right-hand sides $f_i$ are often rational or algebraic functions of coordinates $x_1, \dots, x_n$ or can be reduced to such form by a certain change of variables.

# Numerical integration

## Problem

The problem of numerical integration of the dynamical system (1) consists in finding its solution at the moment of time $t = T$ up to an error value that does not exceed the given boundary $\varepsilon > 0$.

Usually one tries to estimate the error, either by comparing the solutions obtained with different steps or by observing the change in quantities that should remain constant on the exact solution.
If the dynamical system under consideration has a considerable amount of conservation laws, then one usually monitors changes in the algebraic integrals of motion.
Ex.: AndrewSu, 2019. `habr.com/ru/post/437014`.

# Conservative schemes

The idea to construct difference schemes that precisely preserve the integrals of motion in dynamical systems arose in the late 1980s.

1. In the works of Cooper and Yu.B. Suris a large family of Runge-Kutta schemes was discovered that preserve all the polynomial first and second-order integrals of motion and also on the symplectic structure in Hamiltonian systems.
2. The first finite-difference scheme for the many-body problem, preserving all classical integrals of motion, was proposed in 1992 by D. Greenspan and by Simo and González.

**Example**

The symplectic schemes preserve all classical algebraic integrals of rigid body problem except for an additional integral in Kowalewski case.

# Usage for numerical integration

Against use of conservative schemes for numerical integration, two fundamental considerations come to mind:

- In the case of non-integrable systems, while remaining on the integral manifold, we can decline far from the exact solution. Thus conservation laws cease to be indexers of error but it is not guarantee of success.
- All conservative schemes are implicit thus at any step we have to solve a system of nonlinear algebraic equations. This is hard job, thus the methods is not effective.

**Note**

Buono and Mastroserio in 2002 proposed a construction which looks like explicit RK scheme and preserves integrals. Although it is not even difference scheme, this method is very effective for numerical integration. See: [Zhang, 2020].

# Newton's equations as difference equations

In the course of searching for numerical methods for integrating dynamical systems, a very interesting construction was found — a difference scheme of a dynamical system that preserves all algebraic integrals of motion.
Attempts have been made for a long time to consider Newton's equations as difference equations:

$$m\frac{d^2x}{dt^2} = F(x) \quad \to \quad m\frac{\Delta^2 x}{\Delta t^2} = F(x).$$

See, for ex., [Feynman, ch. 2, §3].
However with the standard discretization such a representation faces a violation of the fundamental conservation laws.

# Difference schemes as mathematical model

## Definition

Every difference scheme describes a transition from the value of $x$ taken at some time $t$ to the value of $x$ taken at the next moment in time $t + \Delta t$. Hereafter we denote these new values as $\hat{x}$. This relationship is described by an algebraic equation similar, in its form, to a differential equation.

## Question

When we recognize that the scheme is a difference mathematical model of the same phenomenon, the continuous model of which is the dynamical system?

# Difference model of the dynamical system

We recognize that the scheme is a difference model of the dynamical system, if

1. the schema has same discrete symmetries as the original problem, including $t$-symmetry

$$dt \to -dt, \quad x \to \hat{x}, \quad \hat{x} \to x$$

   and bodies permutations in many body problem.
2. the schema preserves all algebraic integral in some sense, for ex., like

$$g(x) = \text{const} \quad \to \quad g(\hat{x}) = g(x)$$

3. approximate solution inherits qualitative properties of exact solution like periodicity.

# Midpoint scheme vs. symmetric scheme

For ode $\dot{x} = f(x)$ there are two schemes with $t$-symmetry:

- midpoint scheme

$$\hat{x} - x = f\left(\frac{\hat{x} + x}{2}\right)\Delta t$$

- symmetric scheme

$$\hat{x} - x = \frac{f(\hat{x}) + f(x)}{2}\Delta t.$$

**Theorem (Cooper)**

The midpoint scheme preserves linear and quadratic integrals.

What about symmetric scheme?

# Ex. Elliptic oscillator

The autonomous system

$$\dot{p} = qr, \, \dot{q} = -pr, \, \dot{r} = -k^2 pq$$

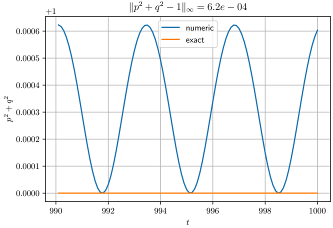
has two quadratic integrals of motion

$$p^2 + q^2 = \text{const}$$

and

$$k^2 p^2 + r^2 = \text{const}$$

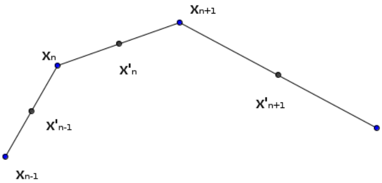
Numerical experiments with symmetric scheme was presented by Yu. A. Blinkov at PCA'2019.




The first integral variation fluctuates within the round-off error without a noticeable trend towards dissipation or anti-dissipation.

# Principle of duality

Let $x_0, x_1, x_2, \ldots$ be approximate solution calculated by midpoint scheme. Then midpoints $x'_0, x'_1, x'_2, \ldots$ of segments of broken line $x_0 x_1 x_2 \ldots$ are approximate solution calculated by symmetric scheme.




**Theorem (dual to Cooper's theorem)**

Symmetric scheme inherits linear and quadratic integrals of the dynamical system, difference analogue for the integral $g(x)$ will be

$$g\left(x - f(x)\frac{dt}{2}\right).$$

# Ex. Linear oscillator

The linear oscillator

$$\dot{x} = -y, \quad \dot{y} = x$$

has an integral $x^2 + y^2 = \text{const}$. Midpoint solution $(x_0, y_0), (x_1, y_1), \dots$ is a broken line, its vertexes lie at circle with radius $R$. Dual symmetric solution $(x'_0, y'_0), (x'_1, y'_1), \dots$ is a broken line, its vertexes lie at circle with radius $r$. They will be right polygon iff

$$r/R = \cos\frac{\pi}{N}, \quad N \in \mathbb{N}.$$

This approximate solution is periodic sequence with period $N$ iff the step $\Delta t$ is a root of the equation

$$1 + dt^2/4 = \cos^2\frac{\pi}{N}, \quad N \in \mathbb{N}.$$

See: [Gerdt V.P. et al., DCM & ACS, 2019]

# Ex. Elliptic oscillator

The integral

$$p^2 + q^2 = \text{const}$$

turning into the polynomial

$$(p^2 + q^2)\left(1 + \frac{r^2 dt^2}{4}\right).$$

If we follow the change of $p^2 + q^2$ on an approximate solution found by the symmetric scheme, then we will see a deviation from a constant value equal to

$$(p^2 + q^2)\frac{r^2 dt^2}{4}.$$

Exact solution is periodic thus these deviations look like periodic fluctuations.

# Hypothesis

In numerical experiments with periodical motion we have often that the scheme does not preserve exactly the integral $g(x)$ but its fluctuation is periodic, ex.:

- experiments with Kepler problem by Eugine Vorozhtsov at CASC'2020,
- experiments with line integral methods for conservative problems by Luigi Brugnano and Felice Iavernaro, 2016.

Hypothesis (Gerdt): in this situation, there is such a polynomial $G(x, \Delta t)$ that

$$G(\hat{x}, \Delta t) = G(x, \Delta t)$$

and

$$\lim_{\Delta t \to 0} G(x, \Delta t) = g(x).$$

# Many body problem

**Question**

How we can construct various such conservative difference schemes for the most famous family of dynamical systems, the many-body problem?

The classical problem of $n$ bodies consists in finding solutions to an autonomous system of ordinary differential equations

$$m_i \ddot{\vec{r}}_i = \sum_{j=1}^{n} \gamma \frac{m_i m_j}{r_{ij}^3} \left( \vec{r}_j - \vec{r}_i \right), \quad i = 1, \ldots, n \tag{2}$$

Here $\vec{r}_i$ is the radius vector of the $i$-th body, $m_i$ is its masses, $r_{ij}$ is the distance between the $i$-th and $j$-th bodies, and $\gamma$ is the gravitational constant.

# Algebraic integrals

Bruns [Whittaker, § 164] proved that every algebraic integral of motion in this system is expressed algebraically in terms of the 10 classical integrals.
The energy

$$\sum_{i=1}^{n} \frac{m_i}{2} |\vec{v}_i|^2 - \gamma \sum_{i,j} \frac{m_i m_j}{r_{ij}}$$

is not quadratic function thus midpoint scheme does not preserve energy integral.
For physicists the discrete model based on midpoint scheme is not interesting.

# Our idea

The simplest way to construct conservative schemes is to introduce additional variables with respect to which all algebraic integrals of the many-body problem are expressed in terms of linear and quadratic integrals.
The beginning of our study was laid by the description of a regularizing transformation, which was proposed by Burdet and Heggie, in the book by Marchal.
In other hand, the introduction of additional variables in the construction of difference schemes is known as the scalar auxiliary variable approach (SAV), proposed by Jie Shen et al.

# Rationalization of the $n$-body problem

First of all, let us eliminate irrationality by introducing new variables $r_{ij}$, distances between bodies.

## Theorem

System

$$\dot{\vec{r}}_i = \vec{v}_i, \quad m_i\dot{\vec{v}}_i = \sum_{j=1}^{n} \gamma \frac{m_i m_j}{r_{ij}^3} \left(\vec{r}_j - \vec{r}_i\right), \quad i = 1, \ldots, n$$

$$\dot{r}_{ij} = \frac{1}{r_{ij}} (\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j), \quad i, j = 1, \ldots, n; \, i \neq j$$

has 10 classical integrals and additionally the integrals

$$r_{ij}^2 - (x_i - x_j)^2 - (y_i - y_j)^2 - (z_i - z_j)^2 = \text{const}.$$

# System with quadratic polynomial integrals

## Theorem

The system

$$\dot{\vec{r}}_i = \vec{v}_i, \quad m_i \dot{\vec{v}}_i = \sum_{j=1}^{n} \gamma \frac{m_i m_j \rho_{ij}}{r_{ij}^2} \left( \vec{r}_j - \vec{r}_i \right), \quad i = 1, \ldots, n$$

$$\dot{r}_{ij} = \frac{1}{r_{ij}} (\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j), \quad i, j = 1, \ldots, n; \; i \neq j$$

$$\dot{\rho}_{ij} = -\frac{\rho_{ij}}{r_{ij}^2} (\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j), \quad i, j = 1, \ldots, n; \; i \neq j$$

has 10 classical integrals, which are linear or quadratic with respect new variables, and the additional integrals $r_{ij}\rho_{ij} =$ const and

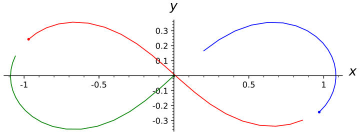
$$r_{ij}^2 - (x_i - x_j)^2 - (y_i - y_j)^2 - (z_i - z_j)^2 = \text{const}.$$

# Conservative schemes for $N$ body problem

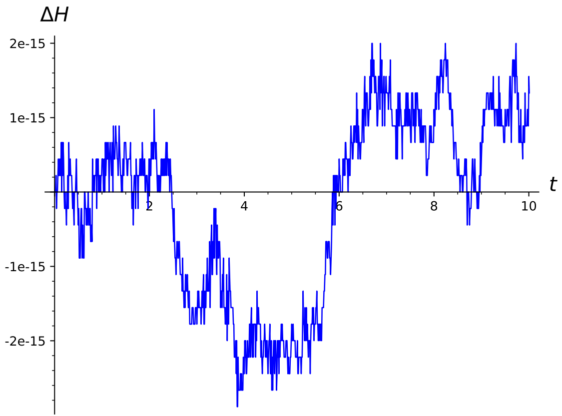
Since all classical integrals of the many-body problem, as well as the additional integrals, are quadratic in their variables, any symplectic Runge-Kutta difference scheme, including the simplest midpoint one, preserves all these integrals.
The midpoint scheme written for the system with additional variables, preserves all its algebraic integrals exactly and is invariant under permutations of bodies and time reversal.
It is not difficult to create high-order schemes which preserve all integrals of motion in the many-body problem, which is one of major advantages of the proposed approach to constructing conservative difference schemes.
Proves of Ths. see in: Gerdt V.P. et al. // ArXiv. 2007.01170.

# Choreographic test

Consider the dimensionless problem of the motion of three bodies of equal mass with $m_i = \gamma = 1$ on a plane.
In 1993, Chris Moore discovered a new periodic solution of the three-body problem, in which three bodies write out the eight; later in 2000 Chenciner and Montgomery gave a justification to this fact.
The initial conditions are known only approximately, we will use the values found numerically by Carles Simó.
We calculated the approximate solution by midpoint scheme. First at all, the figure-of-eight curve is really obtained even with a deliberately large step $\Delta t$.

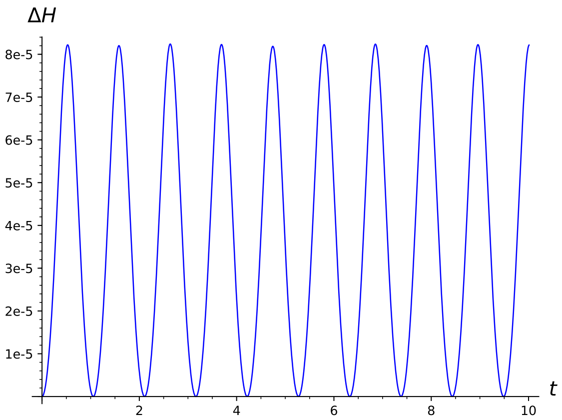


# Choreographic test, step $dt = 0.01$, 10 iterations.



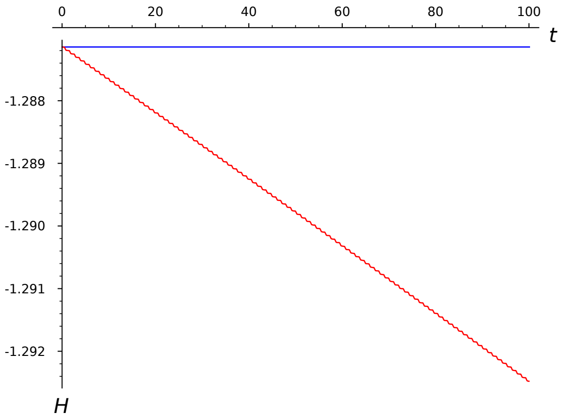

Dependence of energy increment $\Delta H$ on time for approximate solution founded by midpoint scheme **with** auxiliary variables.

# Choreographic test, step $dt = 0.01$, 10 iterations.




Dependence of energy increment $\Delta H$ on time for approximate solution founded by midpoint scheme **without** auxiliary variables.

# Choreographic test, step $dt = 0.01$.




Dependence of energy $H$ on time for approximate solutions found using our algorithm (blue) and the rk4 scheme (red).

## Comments

- For midpoint scheme **with** auxiliary variables the energy increment is within $\pm 2 \cdot 10^{-15}$ limit. At the same time, on the solution found by the midpoint scheme **without** introducing additional variables, the energy fluctuates in the limit from $0$ to $8 \cdot 10^{-5}$.
- On the solution found by the explicit fourth-order Runge-Kutta scheme, the energy changes monotonically.

# Iteration organization in further experiments

The midpoint scheme is implicit, so that at each step it is necessary to solve the system of algebraic equations. We are going to use the method of simple iterations: starting from $\hat{x}^{(0)} = x$ the sequence

$$\hat{x}^{(n+1)} = x + f\left(\frac{\hat{x}^{(n)} + x}{2}\right)\Delta t, \quad n = 0, 1, 2, \ldots, N$$

is constructed. Maximal number of iteration was equal $N = 100$.

## Note

1. We will monitor that the increment of the integrals of motion does not go beyond the given boundaries ($10^{-8}$ in our examples) rather than that $\|\hat{x}^{(n)} - \hat{x}\|$ is small.
2. When conducting numerical experiments, we often encountered divergence of the method. In this case we reduce the step $dt$. So our method has an adoptive step.

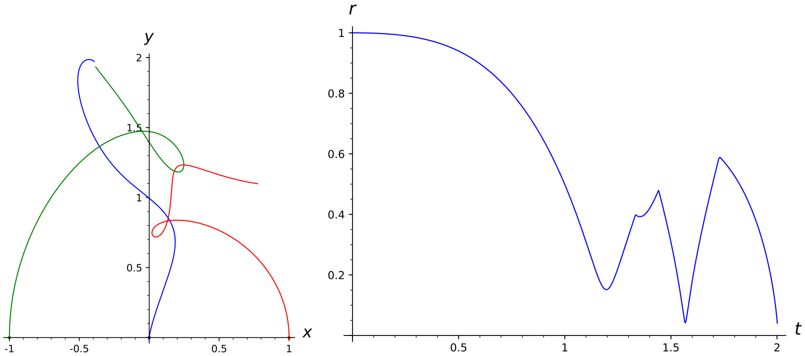
# Test with small distances

At the initial moment of time, the following conditions are taken: the bodies lie on the line $Ox$, the first body at the point $x = 0$, the second at $x = 1$, the third at $x = -1$. The first body is at rest, and the initial velocities of the other two bodies are directed along the $y$-axis and are equal to $1$ and $1.5$, respectively.
Then in the process of computation, it turns out that the bodies several times pass close to each other. Moreover, the applicability conditions of the iteration method make it necessary to reduce the step.

## Note

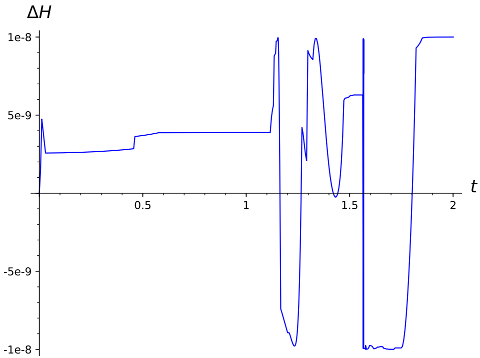
Of course, we cannot assume that at this moment a true collision occurs, since, according to the Weierstrass theorem, the collision in the many-body problem with arbitrary initial data is improbable.

# Test with small distances, initial step $dt = 6 \cdot 10^{-3}$.




Left: trajectories of the three bodies for $0 < t < 2$, initial positions marked by dots. Right: time dependence of the minimal distance between the bodies.

# Test with small distances




Several times the warning that the energy integral and the constraint integrals cannot be kept in a given corridor is triggered, but in the next steps it is possible to return to these corridors.

# Test with small distances: discussion

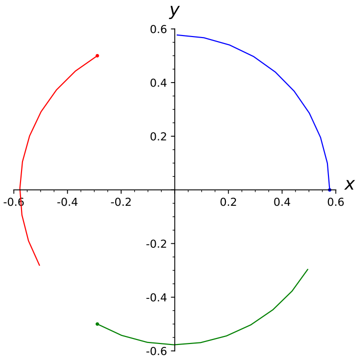
The test reveals a fundamental flaw in our algorithm: when the method of successive iterations is applied to the case when the bodies approach each other at distances that are only two orders of magnitude smaller than the initial ones, an excessive refinement of the step calculated occurs.
It is essential problem for usage of our method for numerical integration. However (thus?) non periodical case with small distances is not popular for numerical experiments.

# Test on Lagrange solutions

As is well known since Euler, the planar three-body problem has two families of particular solutions that can be described in elementary functions.

The first of them: the bodies form a regular triangle with sides of a fixed length $a$, which rotates around the center of mass with constant speed.

We took $a = 1$ and a quite noticeable step $dt = 1/10$, nevertheless, the nature of the movement remained the same, which is clearly visible along the trajectories.



# Algebraical problem about Lagrange solution

The distances between the points remain constant at the level of rounding error. — The error in calculating the distance between the center of gravity and the bodies, as well as in determining the energy and angular momentum, is much larger, at the level of the specified $10^{-8}$.

**Question**

Can we prove algebraically that distances $r_{ij}$ do not change on approximate solution in Lagrange case?

See also: Ayryan et al., CASC'2020.

# Algebraic form for Q.

Let be

$$T(\alpha) = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \quad \text{and} \quad A = T(2\pi/3).$$

We take initial conditions in the form

$$\vec{r}_i = A^i \vec{r}_1, \quad \vec{v}_i = A^i \vec{v}_1, \quad i = 2, 3,$$

so the bodies lie vertices of a regular triangle.

## Question

Is it possible to take the velocity $\vec{v}_1$ and the angle $\alpha$ so that hat variables are produced form initial one by the rotation $Q = T(\alpha)$:

$$\hat{\vec{r}}_i = Q\vec{r}_i, \quad \hat{\vec{v}}_i = Q\vec{v}_i, \quad \hat{r}_{ij} = r_{ij} = a, \quad \hat{\rho}_{ij} = \rho_{ij} = \frac{1}{a}?$$

# Eqs. of midpoint scheme

Eqs. for $r_{ij}$ и $\rho_{ij}$ give us

$$(\vec{r}_i - \vec{r}_j)^T (Q+E)^T (Q+E)(\vec{v}_i - \vec{v}_j) = 0$$

To satisfy these conditions we take such initial velocity $\vec{v}_1$ that

$$(\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j) = 0.$$

Eqs. for $\vec{r}_i$ и $\vec{v}_i$ give us

$$(Q-E)\vec{r}_i = \frac{dt}{2}(Q+E)\vec{v}_i, \quad (Q-E)\vec{v}_i = -\frac{3dt}{2a^3}(Q+E)\vec{r}_i$$

or

$$B^2 \vec{r}_i = -\frac{3dt^2}{a^3}(1+\cos\alpha)^2 \vec{r}_i,$$

where

$$B = (Q+E)^T(Q-E) = Q - Q^T = 2\begin{pmatrix} 0 & \sin\alpha \\ -\sin\alpha & 0 \end{pmatrix}$$

# Answer

Last eqs. can be rewritten as

$$4\begin{pmatrix}\sin^2\alpha & 0\\ 0 & \sin^2\alpha\end{pmatrix}\begin{pmatrix}x_i\\ y_i\end{pmatrix} = \frac{3dt^2}{a^3}(1+\cos\alpha)^2\begin{pmatrix}x_i\\ y_i\end{pmatrix}, \quad i = 1,2,3.$$

If

$$\tan\frac{\alpha}{2} = \frac{\sqrt{3}}{2}\frac{dt}{a^{3/2}}$$

these eqs. are satisfied identically. Thus we have only 3 nontrivial eqs. for velocities:

$$(Q+E)^T(Q-E)\vec{r}_i = (1+\cos\alpha)dt\vec{v}_i$$

Hence

$$\|\vec{v}_i\| = \frac{\sqrt{3}}{a}.$$

This is Lagrange case.

# Generalization: discrete Lagrange problem

## Problem

Using the midpoint scheme, find all approximate solutions of the planar three-body problem, in which the distances between the bodies are unchanged

$$\hat{r}_{ij} = r_{ij}, \quad i \neq j, \tag{3}$$

and the constraint integrals have their natural values

$$r_{ij}^2 - (x_i - x_j)^2 - (y_i - y_j)^2 = 0, \quad r_{ij}\rho_{ij} = 1. \tag{4}$$

In theory, this problem is algorithmically solvable; moreover, an algorithm for eliminating the unknowns based on the calculation of Gröbner bases and implemented in any computer algebra system is quite enough to solve it.

# Difficulties

Unfortunately, could not apply the standard computer algebra tools implemented in Sage. At CASC'2020 we proposed a solution in which part of the steps are done by the hands.
The midpoint scheme for the many-body problem is rich in discrete symmetries. The exclusion method implemented in Sage is based on the Gröbner bases with lex ordering and does not take the symmetry of the system into account, but sometimes the usage of such symmetries speeds up computing [Steidel, Faugère, 2013].

> *All computations have been made on a computer with 4 Intel(R) Xeon(R) CPU E5-4620 @ 2.20GHz with 387 GB of RAM. – Faugère, 2013.*

All our calculations were performed on a household computer (1 AMD A10-7800 @ 4 GHz with 4 GB of RAM) and processes interrupt after half an hour.

# Results presented in the talk

1. Symmetric scheme inherits linear and quadratic integrals of the dynamical system.
2. To construct such schemes we can introduce additional variables with respect to which all algebraic integrals of the many-body problem are expressed in terms of linear and quadratic integrals.
3. In Lagrange case solution found by midpoint scheme with additional variables inherits qualitative properties of an accurate solution.

# The End


Additional materials: `https://malykhmd.neocities.org`