

A set of tools developed based on the Calogero system for testing numerical methods for solving many-body problems
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Wang Shiwei, Mikhail Malykh and Yu Ying

Peoples' Friendship University of Russia, Moscow, Russia

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Introduction

- An original package for investigating numerical solutions of ordinary differential equations, which is built in the Sage computer algebra system is being developed in RUDN.
- This project is focused on a closer integration of numerical and symbolic methods while primarily aiming to create a convenient tool for working with numerical solutions in Sage.
- Based on the completely integrable Calogero dynamical system, a tool for testing difference schemes will be presented in the talk.

Geometric integrators in CAS

Our goal

is to create a convenient tool for the numerical and analytical study of difference schemes that is well integrated with algebraic tools.

- Tools required to design and investigate the algebraic properties of geometric integrators are presently available in CAS.
- CAS provide a rather poor toolset for working with approximate solutions, because this question is traditionally related to numerical methods.

Example

```
sage: var('x, y, t')
sage: desolve_system_rk4([x*(1-y), -y*(1-x)], [x,y],
ics=[0,0.5,2], ivar=t, end_points=20)
```

FDM for Sage

We present an original fdm package built in the Sage computer algebra system.

Our general principles:

- The implementations of the methods do not depend on the field ($\mathbb{R}, \mathbb{C}, \mathbb{Q}, \mathbb{F}_p$) and especially on the number of bits allocated to a number.
- The actions that can be performed analytically are performed analytically. The initial problems are regarded as elements of the new class, which enables symbolic computations.
- The numerical solutions are regarded as elements of the new class, which enables interpolation and visualization.

Ref.: <https://github.com/malykhmd/fdm>

Classes in FDM

Standard approach does not provide clear separation between a well-posed mathematical problem and a method for its solution. In package FDM for Sage, there are two classes:

- initial problem,
- numerical solve.

Any method of integration is map from one to other.

Implemented numerical methods:

- explicit Runge-Kutta methods up to 14 order (Butcher's tables, calculated in Maple by Peter Stone, were implemented in FDM by Pavlyuchenkov).
- symplectic Runge-Kutta methods.
- Methods using Cremona transformations (Kahan method).

Tools for analyze of numerical don't depend on methods of integration and thus described in class NumSol.

Initial problems class

Description of the initial problem

$$\dot{x}_1 = x_2, \quad \dot{x}_2 = -x_1, \quad x_1(0) = 0, \quad x_2(0) = 1$$

on the segment $0 < t < 10$:

```
sage: var("x1,x2,t")
```

```
sage: pr=Initial_problem([x1,x2],[x2,-x1],[0,1],10)
```

An example of methods of initial problem class:

```
sage: pr.latex()
```

```
\left \{ \begin{aligned}
```

```
& \frac{d}{dt} x_{1} = x_{2} ,
```

```
\quad \frac{d}{dt} x_{2} = -x_{1} , \ \&
```

```
x_{1} (0)= 0 , \quad x_{2} (0)= 1
```

```
\end{aligned} \right.
```

Numsols class

Explicit Runge-Kutta method with N points:

```
sage: sol=erk(pr, N=20)
```

Examples of Numsols class methods:

```
sage: sol.value(x1,pi)
```

```
0.00142448822043750
```

```
sage: sol.zeros(x1)
```

```
[3.1430180411731743, 6.286036263964258, 9.429057230259955]
```

```
sage: sol.plot(x1,x2)
```

```
graphic object
```

Many-body problems suitable for testing

In order to test numerical methods for integral dynamic systems in FDM for Sage, a suitable dynamic system needs to be found. Among many Hamiltonian systems, the selected system named Calogero has the following three advantages:

- The many-body problem has theoretical solutions for any number of particles.
- The many-body problem is completely integrable, i.e. a number of algebraic integrals of motion is equal to the number of particles.
- The theoretical solution of the many-body problem contains singularities (collision points).

Ref.: J. Moser, Integrable Hamiltonian systems and spectral theory. Edizioni della Normale, 1983.

Calogero system

Calogero system is a one-dimensional system of many particles of the same mass. Let particles be numbered starting from 0 and q_i be the position of i -th particle, then

$$\ddot{q}_i = -\frac{\partial U}{\partial q_i}, \quad i = 0, \dots, n-1,$$

where

$$U = \sum_{i < j} V(q_i - q_j), \quad V(x) = \frac{b}{x^2}, \quad -1 \leq b \leq 1$$

where b is potential constant. When b is positive, particles repel each other, otherwise they attract each other.

The Hamiltonian of this system is:

$$H = \frac{1}{2} \sum_{i=0}^{n-1} p_i^2 + U$$

Lax pair

The theoretical solution and integral of motions of the Calogero system is described with the help of Lax pairs. A Lax pair is a pair of time-related matrices or operators that satisfy the following relationship:

$$\frac{d\hat{L}}{dt} = \hat{A}\hat{L} - \hat{L}\hat{A}.$$

In the Calogero system there are the following Lax pairs:

$$\hat{L} = \text{diag}(p_0, p_1, \dots, p_{n-1}) + \sqrt{-b} \left(\frac{1 - \delta_{jk}}{q_j - q_k} \right)$$

and

$$\hat{A} = \sqrt{-b} \text{diag}(d_0, d_1, \dots, d_{n-1}) - \sqrt{-b} \left(\frac{1 - \delta_{jk}}{(q_j - q_k)^2} \right),$$

where $d_k = \sum_{j=0}^{n-1} \frac{1 - \delta_{jk}}{(q_j - q_k)^2}$.

Spectrum of the matrix \hat{L}

Theorem

In Calogero system, the spectrum of the matrix \hat{L} doesn't depend on t .

Cauchy problem

$$\frac{d}{dt}\hat{U} = \hat{A}\hat{U}, \quad \hat{U}(0) = E,$$

has a solution \hat{U} , which is an orthogonal matrix. From the eq.

$$\frac{d\hat{L}}{dt} = \hat{A}\hat{L} - \hat{L}\hat{A}$$

follows that

$$\frac{d}{dt}(\hat{U}^{-1}\hat{L}\hat{U}) = 0,$$

and therefore

$$\hat{U}^{-1}\hat{L}\hat{U} = \hat{L}|_{t=0}.$$

Integrals of motion in the Calogero system

Theorem

In Calogero system of n particles, there are n integrals of motion

$$F_k = \text{Sp } \hat{L}^k,$$

where $k = 0, 1, \dots, n - 1$.

From the eq.

$$\frac{d\hat{L}}{dt} = \hat{A}\hat{L} - \hat{L}\hat{A}$$

follows that the spectrum of the matrix \hat{L} doesn't depend on t . Thus the sum of eigenvalues of matrix \hat{L} is independent of time, that is, there are n integrals of motion

$$\text{Sp } \hat{L}^k = \lambda_1^k + \dots + \lambda_n^k,$$

where λ_1, \dots are eigenvalues of \hat{L} .

Theoretical solution of Calogero system

Theorem

The theoretical solution q_0, q_1, \dots, q_{n-1} of the Calogero system is the eigenvalues of the following matrix

$$\hat{M} = \hat{Q}|_{t=0} + t\hat{L}|_{t=0}.$$

Let

$$\hat{Q} = \text{diag}(q_0, q_1, \dots, q_{n-1}),$$

then

$$\frac{d}{dt}\hat{U}^*\hat{Q}\hat{U} = \hat{U}^*\hat{L}\hat{U} = \hat{L}|_{t=0}.$$

So there is:

$$\hat{U}^*\hat{Q}\hat{U} = \hat{Q}|_{t=0} + \hat{L}|_{t=0} \cdot t.$$

Algebrodynamics

The positions of n bodies are the roots of a polynomial

$$F(q, t) = \det(\hat{M} - q\hat{E}),$$

coefficients of which are rational functions of t and the initial position of the system. Thus:

- any symmetric function of q_1, \dots, q_n is rational with respect of t , but q_i itself has movable branch points,
- we can analytically calculate the positions on bodies at any time, but we can't understand which from they is for 1st body,
- analytical continuation of $q_1(t)$ give us q_2, \dots, q_n , i.e. there are no n bodies, but there are n exemplars of one body at sheets of Riemann surface.

Ref.: Kassandraov et al.// Gravit. Cosmol. 29, 50–56 (2023).

Moment of collision in Calogero system

Because the Cauchy problem is transformed into an algebraic problem, the collision moment can be easily obtained. The collision point is the solution to the following system of equations:

$$F = 0, \quad \frac{\partial F}{\partial q} = 0.$$

Compared with the collision position, the collision moment is easier to obtain. The collision moment can be obtained by solving the Gröbner basis of these polynomials only with respect to time.

Counterexample to Golubev conjecture

Golubev conjecture, 1953

If the dynamical system has unambiguous first integrals then it can be integrated in meromorphic functions.

Calogero system has n rational first integrals

$$F_k = \text{Sp } \hat{L}^k$$

in involution, but q_i are algebraic multiple-valued functions of t . Furthermore, symmetric functions of q_0, \dots, q_{n-1} are rational functions of t , and thus Calogero system has Painlevé property only after the change of variables:

$$s_k = \sum_{j=0}^{n-1} q_j^k, \quad k = 1, \dots, n.$$

Implementation of Calogero system in Sage

In Sage the following tools have been added to FDM for Sage:

- Function `calogero_problem` is used to specify the Calogero system in Sage.
- Function `calogero_q` returns the positions of particles at a fixed time t in Calogero system.
- Function `calogero_curve` returns the equation F used to plot the motion of the particles in Calogero system.
- Function `calogero_solution_crash` returns the moment of collision in Calogero system.
- Function `calogero_integral` returns the integral of motion in Calogero system.

Specifying Calogero system in Sage

The function `calogero_problem` has four optional parameters:

- `ics` is the list of initial values, with the positions of the bodies coming first, and then their momenta,
- `n` is the number of bodies,
- `T` is the final time; we always take $t = 0$ for the initial time,
- `b` is the value of parameter b , default $b = -1$.

For example, define a five-body problem in which the initial positions of the particles as follows: $q_i(0) = i$, $i = 0, \dots, n - 1$. Let the initial momentum be close to zero, the final time $T = 0.5$ and the potential constant $b = -1$. Then this problem can be specified as follows:

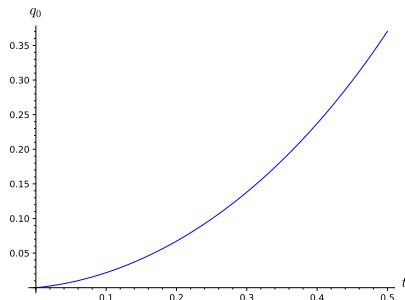
```
sage: n=5
sage: ics=list(range(n))+[0.1,0.2,-0.1,0,0]
sage: problem_calogero=calogero_problem(ics,n=n,T=0.5,
b=-1)
```

Specifying the Calogero system in Sage

This problem can be solved numerically using the tools in FDM. It is solved using the 4th order explicit Runge-Kutta method with one hundred steps as follows:

```
sage: sol=erk(problem_calogero,N=100)
```

The figure on the right shows the trajectory of the first particle



Computation of theoretical solution

To compare exact and numerical solutions the function `calogero_q` was added to FDM to calculate the positions of particles at a fixed time. This function has four optional parameters:

- `ics` is the list of initial values, with the positions of the bodies coming first, and then their momenta,
- `n` is the number of bodies,
- `t` is the fixed time, default `t = 1`,
- `b` is the value of parameter `b`, default `b = -1`.

Computation of theoretical solution

For example, use this function to compare the theoretical solution and the numerical solution of the fourth-order Runge-Kutta method in the previous five-body problem. The positions of the particles at time $t=0.1$ are shown in the left part below. The numerical solution obtained is shown in the right part below.

Theoretical solution

```
sage: calogero_q(ics,n,b=-1,t=0.1)
[0.02174568377617522?,
1.022008478256518?,
1.989567507785786?,
2.998508164438269?,
3.988170165743252?]
```

Numerical solution

```
sage: Q=[SR('q'+str(i))
for i in range (n)]
sage: [sol.value(q,0.1)
for q in Q]
[0.0217456837809339,
1.02200847823443,
1.98956750781722,
2.99850816441585,
3.98817016575156]
```

Calculation of F

Function `calogero_curve` is added in FDM to return the polynomial

$$F(q, t) = \det(\hat{M} - q\hat{E}).$$

This function has three optional parameters:

- `ics` is the list of initial values, with the positions of the bodies coming first, and then their momenta,
- `n` is the number of bodies,
- `b` is the value of parameter `b`, default `b = -1`.

Draw particle trajectory diagrams in Sage

For example, the polynomial F of the previous five-body problem is obtained as follows:

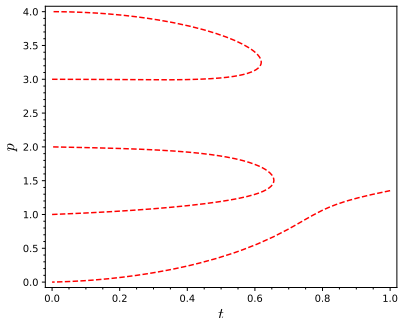
```
sage: calogero_curve(ics,n,b=-1)
-q^5 + 1/5*q^4*t - 18089/3600*q^3*t^2
+ 23053/36000*q^2*t^3 - 526651/129600*q*t^4
+ 104483/1296000*t^5 + 10*q^4 - 2*q^3*t
+ 18101/600*q^2*t^2 - 5347/2000*q*t^3
+ 266021/32400*t^4 - 35*q^3 + 34/5*q^2*t
- 196199/3600*q*t^2 + 6829/4000*t^3 + 50*q^2
- 43/5*q*t + 51523/1800*t^2 - 24*q + 12/5*t
```

Drawing of trajectories of bodies

In Sage the function `implicit_plot` is used to draw the curve, defining be equation with two variables.

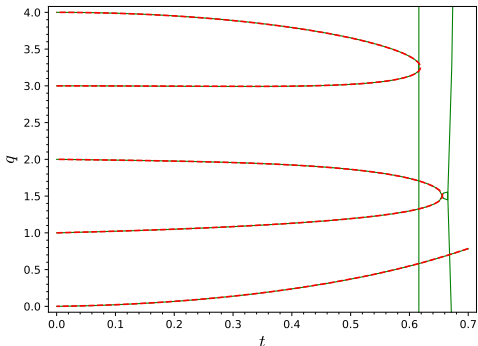
For example, the trajectory diagram of the previous five-body problem can be drawn as follows:

```
sage: implicit_plot(calogero_curve(ics,n),(t,0,1),(q,0,4),
color='red', linestyle='--', axes_labels=['$t$', '$p$'], as
pect_ratio=1/5)
```



Comparison of exact and approximate trajectories

The figure below shows the exact trajectories (dashed line) and numerical solution (solid line) of the previous five-body problem.



Of course, calculations according to the scheme of Runge-Kutta break after the collision of bodies.

Calculating the moment of collision

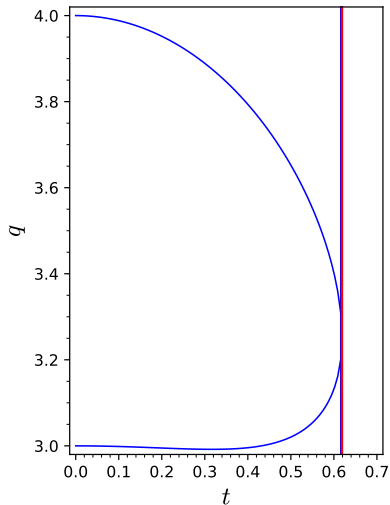
The function

`calogero_solution_crash` has two optional parameters: `ics` and `n`.

For example, the moment of collision of the previous five-body problem is calculated as follows:

```
sage: calogero_solution_crash(ics,n)
0.618840603733536?
```

In the right picture the blue line is the numerical solution, and the red line is the theoretical collision moment.



Integrals of motion in the Calogero system

The function `calogero_integral` has two optional parameters: `n` and `k`. `n` is the number of bodies, `k` is the number of the integral. It should be noted that when `b` is positive, the matrix `L` is complex but its trace is real. This function is appropriately simplified and returns a real function with real coefficients.

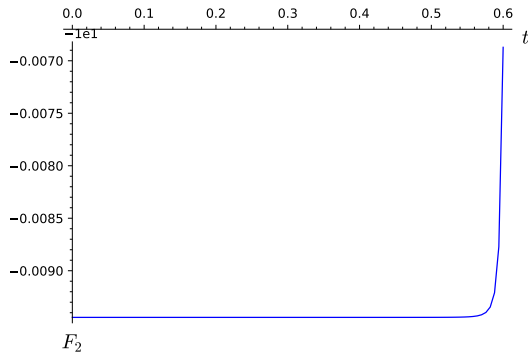
For example, the integral F_1 in the previous five-body problem can be obtained as follows:

```
sage: calogero_integral(1,n)
p0 + p1 + p2 + p3 + p4
```

This tool is very useful to check conservativity of difference scheme. Linear problems with quadratic integrals create vain expectations.

Integrals of motion in the Calogero system

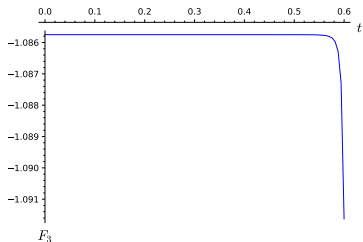
The integral of energy in the Calogero system is not quadratic, so even the symplectic Runge-Kutta method does not conserve it. The picture on the right shows the dependence of F_2 for the previous five-body problem.



Observation

Although there is a case where these integrals increase monotonically near the collision point, there is no sharp jump like when the explicit Runge-Kutta method is applied to classic three-dimensional many-body problems.

This implies that the system Calogero is simple and does not fully exhibit the characteristics of the explicit Runge-Kutta method.



The problem of determining the singularity

In 2003 G.I. Marchuk asked the following question:

Problem of G.I. Marchuk, 2003

For a given Cauchy problem and interval $a < x < b$ determine the position of moving singular points in this interval and their orders by analyzing one or several approximate solutions of the Cauchy problem.

In 2005, E. A. Al'shina suggested to use the complex Rosenbrock scheme of the first order (CROS), for which the approximate solution tends to a finite value, when the exact solution has a pole.
Ref.: E. A. Al'shina et al. // Computational Mathematics and Mathematical Physics, vol. 45, no. 10, pp. 1769–1779, 2005.

Regular points

At regular points the approximate solution $x(t_n, \Delta t)$ can be expanded in an asymptotic series

$$x(t_n, \Delta t) = \varphi(t_n) + r(t_n)\Delta t^p,$$

where $x = \varphi(t)$ is the exact solution and p is the order of approximation or effective accuracy order. Therefore, at regular points the ratio

$$\frac{x(t_n, \Delta t) - x(t_n, \Delta t/2)}{x(t_n, \Delta t/2) - x(t_n, \Delta t/2^2)} \approx \frac{1 - \frac{1}{2^p}}{\frac{1}{2^p} - \frac{1}{2^{2p}}} = 2^p$$

Singular points

Theorem (Painlevé, 1897)

A moving singular point of a nonsingular system is always algebraic, i.e., in its vicinity the solution can be expanded in a Puiseux series:

$$x = C_1(t - a)^r + \dots, \quad r \in \mathbb{Q}$$

The smallest r in the sequence is defined as the order of singularity in this singularity. This order can be used to determine the type of singularity.

Assuming that

$$x(t_n, \Delta t) \simeq C_1(t - a)^r + \dots$$

at in the vicinity of the point $t = a$, then

$$\frac{x(t_n, \Delta t) - x(t_n, \Delta t/2)}{x(t_n, \Delta t/2) - x(t_n, \Delta t/2^2)} \approx 2^r$$

It is the special property of CROS scheme.

Apply Alshina's method to determine the order of singularity in the Calogero system in Sage

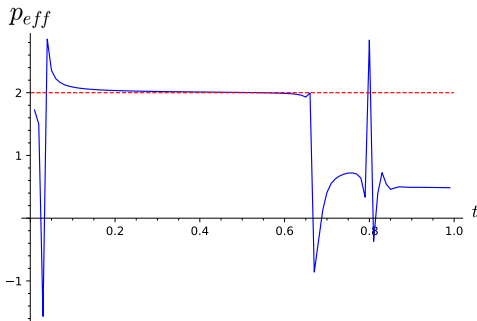
In FDM, the function `eff_order` can return the time-related p_{eff} based on the CROS scheme. This function has three optional parameters:

- `problem` is a Cauchy problem,
- `u` is initial moment,
- `N` is the number of points.

Use this method to numerically determine the order of singularity of the previous five-body problem as follows:

```
sage: eff_order(problem_calogero, q0, N=100)
```

Apply Alshina's method to determine the order of singularity in the Calogero system in Sage



From the implicit function theorem it follows that in the previous five-body problem at the collision point the coordinates of the bodies have an algebraic singularity of the order of $\frac{1}{2}$. There is no theoretical explanation for the sharp jumps near the starting and collision point.

Kahan method

Since 1990s the difference scheme, defining birational map between layers, investigated, see talk of Lapshenkova at PCA'2024.

For Hamiltonian system with

$$H = T(p) + U(q),$$

we can write such a scheme:

$$\hat{p} - p = -\frac{\partial U}{\partial q}(q)\Delta t, \quad \hat{q} - q = +\frac{\partial T}{\partial p}(\hat{p})\Delta t.$$

It is a birational map:

$$(p, q) \rightarrow (\hat{p}, \hat{q}) :$$

$$\hat{p} = p - \frac{\partial U}{\partial q}(q)\Delta t,$$

$$\hat{q} = q + \frac{\partial T}{\partial p}(\hat{p})\Delta t,$$

$$(\hat{p}, \hat{q}) \rightarrow (p, q) :$$

$$q = \hat{q} - \frac{\partial T}{\partial p}(\hat{p})\Delta t,$$

$$p = \hat{p} + \frac{\partial U}{\partial q}(q)\Delta t,$$

Kahan method and Calogero system

The Calogero system define algebraic, but non rational correspondence between initial and final data. Thus Kahan method is not natural for this problem.

We believe that the Calogero system is the example when Kahan method is bad choice among numerical methods.

We want to investigate this bad case in future.

Conclusion

The completely integrable dynamical Calogero system, which describes the one-dimensional many-body problem, allows creating a convenient tool for testing difference schemes by means that do not go beyond the algebraic framework.

We tested:

- preservation of the integrals by symplectic Runge-Kutta schemes,
- Alshina's method for the determination of movable singular points (here we found the strange point where p_{eff} has a jump),
- Kahan method, for which the Calogero system is convenient, but not natural.

Thank you for the attention!