Verified Computation as tools of analysis

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Introduction

I have been engaged in Verified Computation and always thought that

- Methods of verified computation should be tools of analysis of phenomena,

otherwise they have no future.

Today I will talk about a simple tool for analysis based on verified computation.

What is Verified Computation ?

Verification Computation, or **Numerical verification methods** are methods on numerical computation in order to prove existence of solutions of problems and to give error bounds of the solutions with rigorous estimation of truncation errors and rounding errors.

- Synonyms : "verified computation", "verified numerics", "verification methods", "numerical verification", "numerical methods with guaranteed accuracy", "computer assisted proof", "rigorous computation" , "rigorous numerics", ...
  The words "validation" or " validated methods" can be used but you should be careful since they are also used in other areas.

Interval arithmetic

Interval arithmetic is a basic tool in verified computation.

- For intervals of the form $[x] = [\underline{x}, \overline{x}] = \{x | \underline{x} \leq x \leq \overline{x}\}$,
  $[x] + [y] = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$,
  $[x] - [y] = [\underline{x} - \overline{y}, \overline{x} - \underline{y}]$,
  $[x] * [y] = [\underline{z}, \overline{z}]$,
  $\underline{z} = \min\{\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}\}$,
  $\underline{z} = \max\{\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}\}$,
  $[x]/[y] = [\underline{x}, \overline{x}] * [1/\overline{y}, 1/\underline{y}]$,
  where $0 \notin [y]$.
- Appropriate rounding operations are necessary in order to estimate rounding errors.
- Large amount of methods have been developed for interval arithmetic including methods to compute various functions.
- Unexpected expansion of resulting intervals may be caused by some reasons, e.g. Wrapping Effects.

Softwares

- INTLAB - INTerval LABoratory ：A multifunctional program package for interval arithmetic on MATLAB by S.M. Rump
  http://www.ti3.tu-harburg.de/rump/intlab/
- kv - a C++ Library for Verified Numerical Computation ：Programs with affine arithmetic on C++ presented by M. Kashiwagi
  http://verifiedby.me/kv/
- CAPD：A collection of flexible C++ modules with verified numerics for dynamical systems by the people of Jagiellonian University, Poland
  http://capd.ii.uj.edu.pl/
- MPFI：A library for multi-precision interval arithmetic based on MPFR by N.Revol, F.Rouillier
  http://perso.ens-lyon.fr/nathalie.revol/software.html.
- Arb ：A C library for rigorous arithmetic with arbitrary precision providing a wide range of mathematical functionality by F. Johansson et al.
  http://arblib.orgz

Verified Computation for Dynamical Systems

- Dynamical Systems are mathematical models to describe time development of systems.
- Theories and methods for Dynamical Systems can be considered as strong tools for analysis of phenomena.
- Concepts of Dynamical System includes Equilibria, Fix Points, Lyapunov functions, bifurcation, and so on...

It seems to follow that

- Application of Verified Computation to Dynamical Systems
  = Contribution of Verified Computation to analysis of phenomena,

and then I have conducted my research from this poin of view.

Indeed there are enormous applications of Verified Computation to Dynamical Systems[4]. Restricting them to what concern with the authors, there are

- Numerical verification of existence of closed orbits in Dynamical Systems[8, 9]
- Construction of local Lyapunov functions around hyperbolic equilibria with computer assistance[10, 11]
- Numerical verification method to specify homoclinic orbits as application of local Lyapunov functions [12]
- Numerical verification methods to construct local Lyapunov functions around non-hyperbolic equilibria [13, 14]

and so on.

But I have also another impression.

- People in Dynamical Systems applying Verified Computation to their own fields are scarcely interested in making tools for analysis of phenomena.

On the other hand, I have been interested in

- Numerical verification methods as tools based on Dynamical Systems for analysis of phenomena, not only for investigation of Dynamical Systems themselves.

In other words, I want to supply

- Mathematical tools easy to use for the People engaged in simulation of phenomena.

Numerical verification methods for ODE

Lohner method is the most representative among Numerical verification methods for ODE.

Lohner method

- A numerical verification method for ODE based on Taylor expansion and its error estimation, which verifies the solution on each time step point.
- It has various devices in order to reduce "Wrapping Effect" that causes expansion of interval radii during interval arithmetic.

On the other hand, Lohner method has no special device for ODEs with conserved quantities.

I have two ideas for this situation.

1. Using methods like Projection method together with Lohner method. The methods project the solutions to manifolds within which the conserved quantities are constant, and restrict the domain that Lohner method gives.
2. Calculating some quantities concerning conserved quantities in order to obtain the conditions for including or excluding specified solution orbits in the phase space.

The idea 1 is now under developing and will be demonstrated in the future.

The idea 2 is described today with simple examples. Note that this is not an improved version of Lohner method.

- Verified computation is used only for calculating the conserved quantities or the quantities concerned.
- The solution orbits are calculated approximately, not with verified computation.

1. Kepler problem

Kepler problem deals with motion of two mass points under universal gravitation in Newtonian mechanics.

- P_1, P_2: mass points with the mass m_1 and m_2, respectively
- $\mathbf{r}_1$, $\mathbf{r}_2$: the position vectors of each point
- $r = \|\mathbf{r}_2 - \mathbf{r}_1\|$ where the norm is the 2-norm

The equation of motion:

$$m_1\,\ddot{\mathbf{r}}_1 = -\frac{Gm_1m_2}{r^3}(\mathbf{r}_1 - \mathbf{r}_2),$$
$$m_2\,\ddot{\mathbf{r}}_2 = -\frac{Gm_1m_2}{r^3}(\mathbf{r}_2 - \mathbf{r}_1),$$

where G is the constant of universal gravitation and $\ddot{\mathbf{r}}$ etc. mean the second derivatives with respect to time.

We put

$$\mathbf{r} := \mathbf{r}_2 - \mathbf{r}_1,$$
$$r := \|\mathbf{r}\|,$$
$$M := m_1 + m_2,$$

and obtain

$$\ddot{\mathbf{r}} = -\frac{GM}{r^3}\mathbf{r}. \tag{1}$$

Conserved Quantities

The conserved quantities are as follows. For the simplicity, we take the mass of the mass point as $m = 1$.

- Total Energy:

$$E := \frac{1}{2}\|\dot{\mathbf{r}}\|^2 - \frac{GM}{r}$$

- Angular Momentum:

$$\mathbf{J} := \mathbf{r} \times \dot{\mathbf{r}}$$

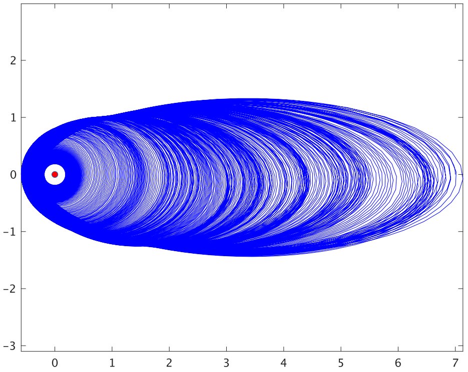
- Eccentricity vector

$$\mathbf{e} = \frac{(\dot{\mathbf{r}} \times \mathbf{J})}{GM} - \frac{\mathbf{r}}{r}$$

This is also called as Runge-Lenz vector.

We know that all the solutions of Kepler problem are quadratic curves. But rough computation may give orbits with drift as follows:

$GM = 1$, $t_0 = 0$, $t_{End} = 6400$, $x(0) = 7, y(0) = 0, \dot{x}(0) = 0, \dot{y}(0) = 0.1$, by ode45 of MATLAB with no option



We want to show that

- True solution corresponding to an approximate solution concerned remains within a finite domain
- and does not fall into a neighborhood of the origin $\mathbf{r} = \mathbf{0}$

without knowing that all the solutions are quadratic curves.

In other words, we want to obtain

- tools for analysis in order to help the People who are not so familiar to theoretical results about Kepler problem.

Including Orbits

Theorem 1

Take a radius $R_1 > 0$ arbitrarily and a sphere

$$S_{R_1} = \{\mathbf{r} \in \mathbb{R}^3 | r = R_1\}.$$

Consider a solution orbit of Kepler problem starting at a point inside the sphere.
If the total energy E of the solution satisfies

$$E < -\frac{GM}{R_1}, \tag{2}$$

then the whole solution orbit is included within the sphere S_{R_1}.

The proof comes from the fact that any solution orbit passes the sphere S_{R_1} has the energy

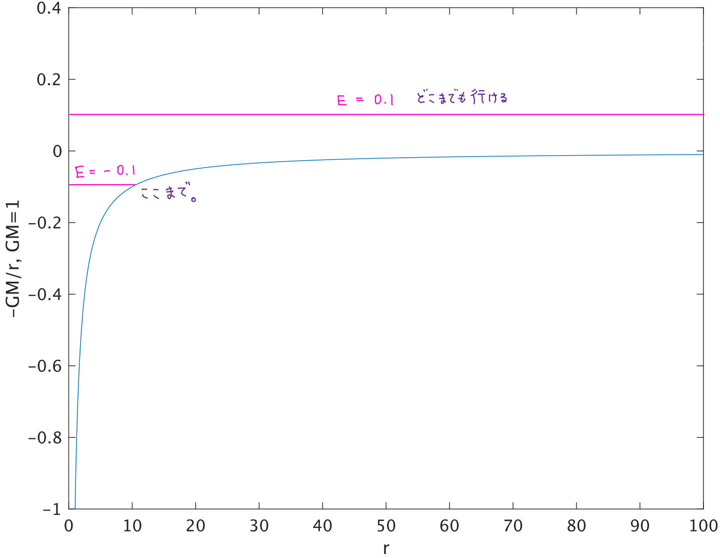
$$E = \frac{1}{2}\|\dot{\mathbf{r}}\|^2 - \frac{GM}{R_1} \geq -\frac{GM}{R_1}.$$

This means that if $E > 0$ then the solution may go to infinity. That is,

$$\|\dot{\mathbf{r}}\| = \sqrt{\frac{2GM}{\rho}}$$

implies the escape velocity.

考察



E = 0.1
どこまでも行ける
E = −0.1
ここまで。
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
-GM/r, GM=1
0
10
20
30
40
50
60
70
80
90
100
r

Note for Exclusion

Note that single use of total energy, or other conserved quantities, can not exclude solution orbits from a neighborhood of the origin.

Therefore we introduce a new conserved quantity using E and J in the following way.

A new conserved quantity

We represent $\dot{\mathbf{r}} = (u, v)$ where

- $v = \dot{r}$ is the element corresponding to the direction of the radius vector,
- u is the element corresponding to the direction orthogonal to the radius vector.

Consider the magnitude of Angular Momentum

$$J = \|\mathbf{J}\| = \|\mathbf{r} \times \dot{\mathbf{r}}\|$$

with

$$J = ru.$$

Now we define the conserved quantity F as

$$F := E - a\,J \tag{3}$$

with an arbitrary positive constant a.

A new conserved quantity

Using the definitions of E and J, we have

$$F = \frac{1}{2}(v^2 + u^2) - \frac{GM}{r} - a\,J = \frac{1}{2}\dot{r}^2 + \frac{1}{2r^2}\left(J^2 - 2a\,r^2 J\right) - \frac{GM}{r}$$
$$= \frac{1}{2}\dot{r}^2 + \frac{1}{2r^2}\left(J - a\,r^2\right)^2 - \left(\frac{1}{2}a^2 r^2 + \frac{GM}{r}\right),$$

which means

$$F \geq F_{min}(r; a) = -\left(\frac{1}{2}a^2 r^2 + \frac{GM}{r}\right). \qquad (4)$$

Note that $F = F_{min}(r; a)$ achieves when $\dot{r} = 0$ and $J = a\,r^2$.

Excluding Orbits

Theorem 2

Take a radius $R_0 > 0$ arbitrarily and a sphere

$$S_{R_0} = \{\mathbf{r} \in \mathbb{R}^3 | r = R_0\}.$$

Consider a solution orbit of Kepler problem starting at a point outside the sphere.
If the conserved quantity F of the solution satisfies

$$F < F_{min}(R_0; a) \tag{5}$$

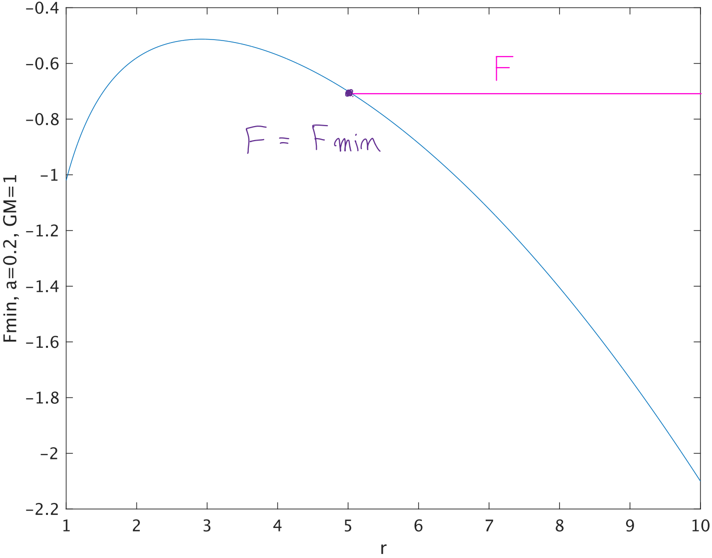
then whole the solution orbit is excluded from the sphere S_{R_0}.

Excluding Orbits

The proof comes from the fact that any solution orbit passes the sphere S_{R_0} has the conserved quantity satisfying

$$F \geq F_{min}(R_0; a)$$

考察



- From the above figure, we see that it is necessary for the existence of R_0 satisfying the theorem 2
  that the radius r giving $F = F_{min}(r; a)$ should be larger than the radius r_M giving the supremum of $F_{min}(r; a)$.
- This means that $F_{min}(r; a)$ should be decreasing at the radius r giving $F = F_{min}(r; a)$.

The condition of $F = F_{min}(r; a)$:

$$\dot{r} = 0 \quad \text{and} \quad J = a\,r^2$$

can be interpreted that the constant a should be the angular velocity ω when the solution orbit takes the closest approach to the origin.

Therefore the condition $r = \sqrt[3]{\frac{GM}{a^2}}$ to achieve the supremum of $F_{min}(r; a)$ gives

- $\omega^2 r = GM/r^2$

which means that the centrifugal force is equal to the gravity force.

The process of verified computation in order to show the exclusion of the solution orbit is as follows.

1. Calculate an approximate solution with the initial conditions $\mathbf{r}(0)$ and $\dot{\mathbf{r}}(0)$, and find the closest point to the origin. Let $\hat{R}_0$ be an approximation to the distance between the closest point and the origin. Chose a positive number R_0 satisfying

$$R_0 < \hat{R}_0.$$

2. Calculate the conserved quantities $\hat{E}$, $\hat{J}$ of the solution with respect to the initial values, using usual approximate arithmetic.

- $\hat{E} = \frac{1}{2}\|\dot{\mathbf{r}}(0)\|^2 - \dfrac{GM}{r(0)}$,
- $\hat{J} = r(0)u(0)$.

Calculate the constant a by

$$a = \frac{\hat{J}}{R_0^2}$$

with approximate arithmetic.

- Define the function

$$F_{min}(r; a) = -\left(\frac{1}{2}a^2r^2 + \frac{GM}{r}\right).$$

3. Take interval values $[\mathbf{r}(0)]$ and $[\dot{\mathbf{r}}(0)]$ that includes the initial values as the center with some small radii.
   Compute the conserved quantities $[\hat{E}]$, $[\hat{J}]$ and $[\hat{F}] = [\hat{E}] - a\,[\hat{J}]$ for the interval initial values by using interval arithmetic with verified computation.
4. Verify that

$$[\hat{F}] < F_{min}(R_0; a) \tag{6}$$

   holds by verified computation.

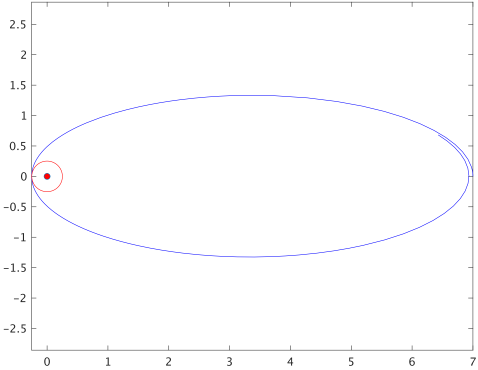
If the condition (6) holds, then it is proved that

- All the solution orbits with initial values within the intervals $[\mathbf{r}(0)]$ and $[\dot{\mathbf{r}}(0)]$ are excluded from the sphere centered at the origin with the radius R_0.

Numerical Example

Parameters for calculating an approximate solution and the closest point:

$GM = 1$, $t_0 = 0$, $t_{End} = 50$,
$x(0) = 7, y(0) = 0, \dot{x}(0) = 0, \dot{y}(0) = 0.1,$



Numerical Example

From the above figure, we take

$$\hat{R}_0 = 0.253875850544019, \quad R_0 = 0.251523281724059$$

and calculate the constant a as

$$a = 11.064751341482040.$$

The interval initial values are defined as

- $x(0) = \langle\, 7\,,\, 10^{-5}\,\rangle$, $y(0) = 0$, $\dot{x}(0) = 0$, $\dot{y}(0) = \langle\, 0.1\,,\, 10^{-5}\,\rangle$,

represented by the center-radius form of intervals.

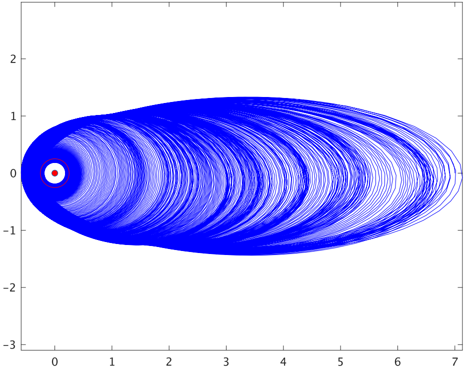
The results of verified computation are

- $[\hat{F}] = \langle\, -7.88318316263335\,,\, 0.00157239877214\,\rangle$,
- $F_{min}(R_0; a) = \langle\, -7.84843810773106\,,\, 0.00078559734526\,\rangle$,

which satisfy the condition (6) $[\hat{F}] < F_{min}(R_0; a)$.

The approximate orbit and the verified region

- The blue curve is the approximate orbit. It is drifting because of rough approximation.
- The inner region of the red circle excludes the true solution.
- Note that higher accurate approximation is not used in the process to specify the red circle.



Summary up to here

- We propose numerical verification methods to include and exclude the solution orbits of Kepler Problem and show an example.
- For exclusion, we derive a new conserved quantity, which reveals to be a simple tool for analysis of the calculated orbits of Kepler Problem.

By the way, what the quantity

$$F = E - a\,J$$

means in physical sense?

2. The circular restricted three-body problem[17]

The circular restricted three-body problem is a kind of three-body problems for 3 mass points P_1, P_2 and P_3 with their masses m_1, m_2 and m_3, respectively.

Assumptions of the circular restricted three-body problem are

- $m_1 >> m_3$ and $m_2 >> m_3$, that means the motion of P_3 has no influence to the motions of P_1 and P_2.
- The mass points P_1 and P_2 take uniform circular motion around their centroid with angular velocity ω.

Note that the total energy nor the angular momentum cannot be conserved quantities under these assumptions.

2. The circular restricted three-body problem[17]

The only conserved quantity of the circular restricted three-body problem is so called The Jacobi Integral, which has a similar form to

$$F = E - \omega J.$$

- We can also specify an excluding region for the solution orbits of the circular restricted three-body problem.
- The excluding region can be specified around equilibria of he circular restricted three-body problem, so called Lagrangian Equilibrium Points.
- Analysis using F by our method has strong relation to the method of Zero velocity curve which is a standard method of analysis in the dynamical astronomy field.
- There are very interesting stories about Trojan Asteroids, Tadpole and Horseshoe Orbits.

2. The circular restricted three-body problem[17]

- 質点 P_1, P_2, P_3 を考え、それぞれの質量を m_1, m_2, m_3 とする。
- $\mathbf{r}_1$： P_1 から P_3 への位置ベクトル。大きさ r_1
  $\mathbf{r}_2$：P_2 から P_3 への位置ベクトル。大きさ r_2
- 質点 P_1, P_2 の重心を原点にとり、ここからの質点 P_3 の位置ベクトルを $\mathbf{r}$ とすると、

$$\mathbf{r} = \frac{m_1}{m_1 + m_2}\mathbf{r}_1 + \frac{m_2}{m_1 + m_2}\mathbf{r}_2.$$

質点 P_3 の運動方程式：

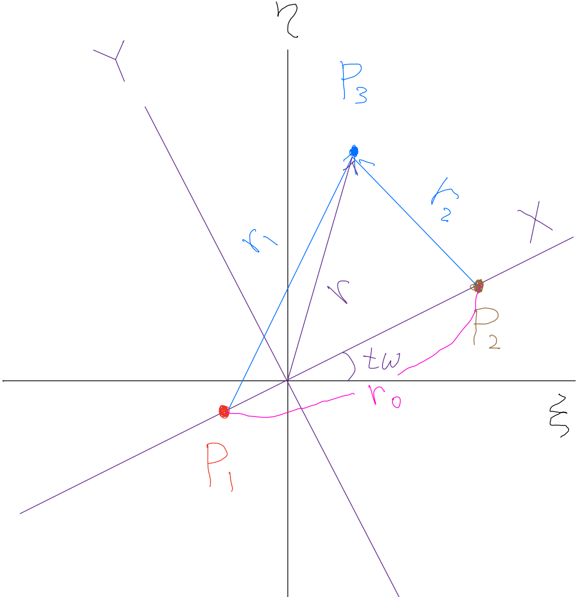
$$\ddot{\mathbf{r}} = -\left(\frac{\partial U}{\partial \mathbf{r}}\right)^T,$$

$$U = -\frac{Gm_1}{r_1} - \frac{Gm_2}{r_2}.$$

- ここで、$m_1 >> m_3$ かつ $m_2 >> m_3$ とし、質点 P_3 の運動は P_1, P_2 に影響を与えないものとする。
- この仮定により質点 P_3 のエネルギー、角運動量はともに保存量とはならないことに注意する。
- 質点 P_1 と P_2 はお互いの重心周りを等速円運動しているものとする (円制限３体問題)。その角速度を ω と置く。

- 慣性系 sidereal system での P_3 の位置ベクトル表現： $\mathbf{r} = (\xi, \eta, \zeta)^T$
- 質点 P_1, P_2 の回転に伴う回転座標系 synodic system での P_3 の位置ベクトル表現： $\mathbf{R} = (X, Y, Z)^T$

回転座標系：



回転座標系での運動方程式：

$$\ddot{\mathbf{R}} + 2\omega\left(-\dot{Y}, \dot{X}, 0\right)^T - \omega^2 (X, Y, 0)^T = -\left(\frac{\partial U}{\partial \mathbf{R}}\right)^T$$

左辺第２項はコリオリ力、第３項は遠心力に対応している [17]。

両辺に $\left(\frac{d\mathbf{R}}{dt}\right)^T$ を掛けて計算すると、

$$\frac{d}{dt}\left(\frac{1}{2}\|\dot{\mathbf{R}}\|^2 - \frac{1}{2}\omega^2\|\mathbf{R}\|^2\right) = -\frac{dU}{dt}$$

したがって、

$$\frac{1}{2}\|\dot{\mathbf{R}}\|^2 - \frac{1}{2}\omega^2\|\mathbf{R}\|^2 + U$$

は解軌道に沿って定数となる。

ヤコビ積分

$$\Omega = \frac{1}{2}\omega^2\|\mathbf{R}\|^2 - U$$

と置くと、

$$F = \frac{1}{2}\|\dot{\mathbf{R}}\|^2 - \Omega \tag{7}$$

が保存量となる。これをヤコビ積分と呼ぶ。

ヤコビ積分

ヤコビ積分の慣性系での表現は

$$F = \frac{1}{2}\|\dot{\mathbf{r}}\|^2 + U - \omega\left(\xi\dot{\eta} - \eta\dot{\xi}\right)$$

- これは P_1 と P_2 の距離を 0 に取る極限でケプラー問題の $F = E - \omega J$ に一致する。
- このとき ω は P_1 と P_2 が重なった質点の自転の角速度に相当し、極限では任意に取れる。

つまり、ケプラー問題における保存量 $F = E - a\,J$ は、円制限３体問題におけるヤコビ積分の極限と見做せることが分かる。

- 式 (7) から $F \geq -\Omega$ である。
- $\Omega = \frac{1}{2}\omega^2\|\mathbf{R}\|^2 - U(\mathbf{R}) \geq 0$ は動径の長さ $\|\mathbf{R}\|$ だけの関数ではないので原点中心の球を用いた軌道解析には馴染まない。

しかしながら次の定理は成り立つ。

Theorem 3

正数 Ω_0 を任意に選び、多様体

$$M_{\Omega_0} = \{\mathbf{R} \in \mathbb{R}^3 \,|\, \Omega(\mathbf{R}) = \Omega_0\,\}$$

を考える。

円制限３体問題の任意の解軌道の保存量 F が

$$F < \Omega_0 \tag{8}$$

を満たせば、この解軌道は多様体 M_{Ω_0} と共通点を持たない。

以下ではこの定理を用いた解析の例を示そう。

トロヤ群

ラグランジュの正三角形平衡解：

以下では $Z=0$ の平面で考える。

- r_0：質点 P_1 と P_2 の距離。円制限３体問題では定数である。
- L_4 : $X=\left(\frac{1}{2}-\frac{m_2}{m_1+m_2}\right)r_0,\ Y=\frac{\sqrt{3}}{2}r_0$
- L_5 : $X=\left(\frac{1}{2}-\frac{m_2}{m_1+m_2}\right)r_0,\ Y=-\frac{\sqrt{3}}{2}r_0$

L_4, L_5 は円制限３体問題の平衡点であり、$\triangle P_1P_2L_4$, $\triangle P_1P_2L_5$ はともに正三角形をなす。

トロヤ群

木星の離心率は約 0.0485 であり、太陽を P_1, 木星を P_2, 軽い天体を P_3 とすると円制限３体問題による近似が可能である。

- L_4 付近の小惑星にはトロイア戦争のギリシャ側の英雄の名前が付けられている。
- L_5 付近の小惑星にはトロイア戦争のトロイア側の英雄の名前が付けられている。
- これらの小惑星はまとめて「トロヤ群」と呼ばれ、2012 年 11 月現在で 5425 個が確認されている。

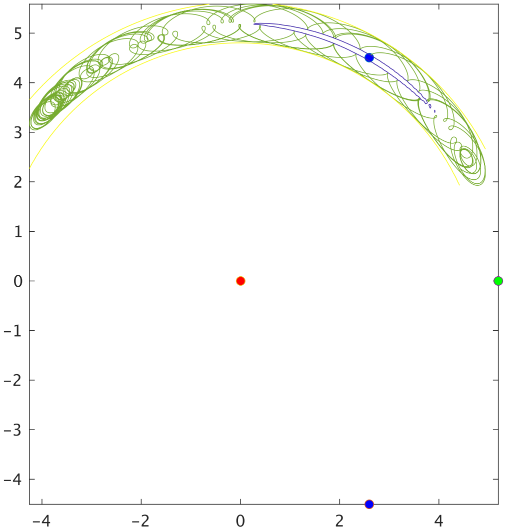
トロヤ群の小天体のシミュレーション

次の図は、$L_4 = (X_4, Y_4)$ 近傍の小天体の軌道のシミュレーションである。
長さの単位は天文単位、時間の単位は年である。

- $m_1 = 1.9891 \times 10^{30}$ kg.　$m_2 = 1.898 \times 10^{27}$ kg.
- $\omega = 2\pi/11.862,\quad r_0 = 5.2026$
- 初期点 $X = 1.011 \cdot X_4$, $Y = 1.011 \cdot Y_4$
- 初期速度　0
- 計算時間範囲 $0 \le t \le 1000$
- L_4 における $\Omega = 11.38776$
- 解軌道の $\Omega_0 = 11.3891$：青のラインの閉曲線

計算は MATLAB の ode45 を用い、オプションは
opts = odeset('abstol',1e-10,'reltol', 1e-10)
とした。なお計算精度を上げても図はほとんど変わらないことは確認している。

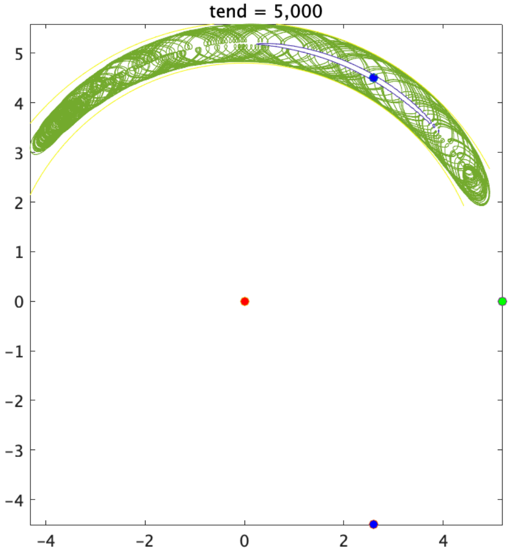
トロヤ群の小天体のシミュレーション



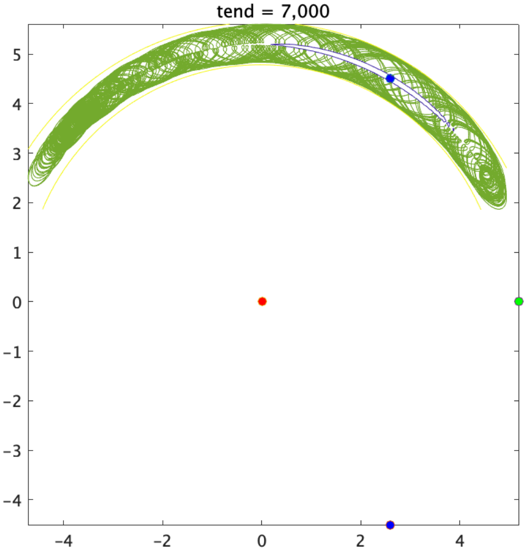
トロヤ群の小天体のシミュレーション

- このような軌道は Tadpole orbit （おたまじゃくし軌道）と呼ばれている。
- L_4 における力学系の線形近似による安定性解析の結果は、ヤコビ行列の固有値の実部が 0 である。したがって L_4 は局所安定とも局所不安定とも言えない。
- 青のラインの内側に、L_4 を囲む閉曲線上に連結する小区間を取って Ω の値を精度保証計算すれば、実際にこの解軌道が L_4 に近づかないことが証明できるはず。
- これは野人研の 4 年生が計算中。
- おたまじゃくし軌道全体の存在範囲を特定することは、この方法では出来ない。
- 実際、計算終了時刻を大きく取ると存在範囲が広がっていく。
  計算時間範囲 $0 \le t \le t_{end}$,
  $t_{end} = 5000, 7000, 8000, 8680, 10000, 100000$ の図を次に示す。

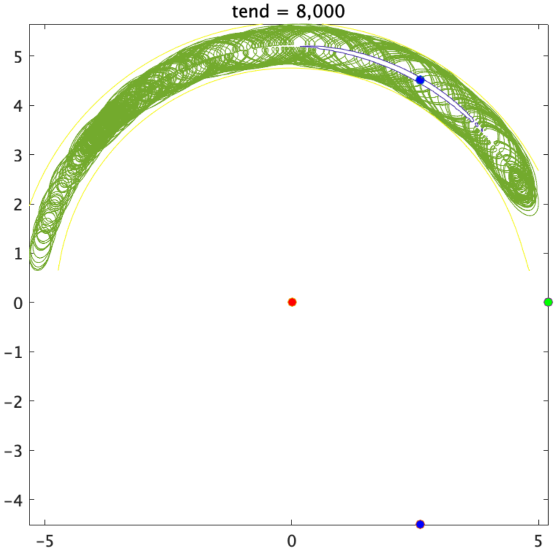
トロヤ群の小天体のシミュレーション (長時間)



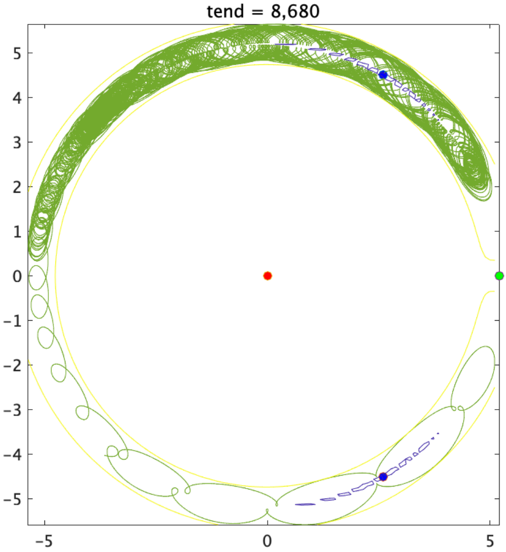
トロヤ群の小天体のシミュレーション (長時間)



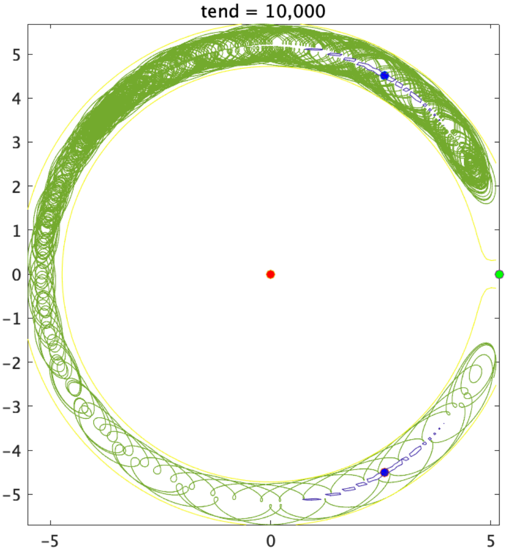
トロヤ群の小天体のシミュレーション (長時間)



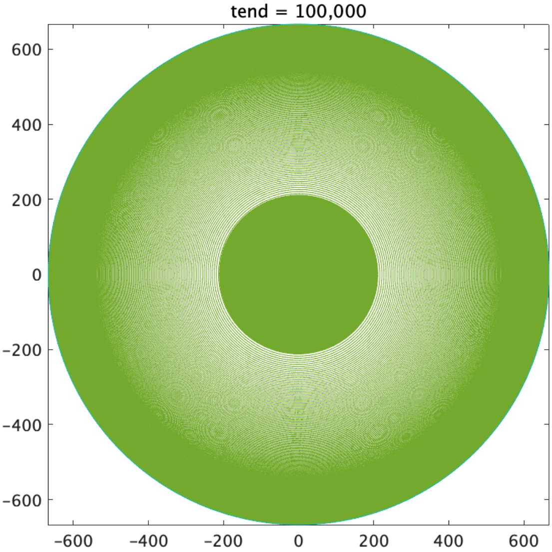
トロヤ群の小天体のシミュレーション (長時間)



トロヤ群の小天体のシミュレーション (長時間)



トロヤ群の小天体のシミュレーション (長時間)



ここまでのまとめ

- ケプラー問題の保存量 F は、円制限３体問題のヤコビ積分に対応することがわかった。
- ヤコビ積分を用いて解軌道の様子を解析することが可能。
- 特に、平衡点の近傍で「落ちない」ことが示せると思われる。
- 保存量が一つしかないので、解軌道の閉じ込めはこの方法では出来ない。

以上の解析手法は、天体力学で用いられる「ゼロ速度曲線」による解析手法と本質的に同じであると思われる。

3. Motion in Schwarzchild Metric

Consider a Schwartzchild Black Hole and let us analyze motion around it [18].

- This part is a cooperative research together with H. Hoshino (Waseda Univ.) and K. Nitta (TDSE Inc.).

Schwarzchild Metric:

$$ds^2 = -\left(1 - \frac{r_s}{r}\right)dt^2 + \frac{dr^2}{1 - r_s/r} + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2.$$

Since the spacetime in Schwarzchild Metric is spherical symmetry, we take $\theta = \pi/2$ without loss of generality. Hereafter we treat the following.

$$ds^2 = -\left(1 - \frac{r_s}{r}\right)dt^2 + \frac{dr^2}{1 - r_s/r} + r^2 d\phi^2.$$

- The Event Horizon is a sphere with the radius $r_s = 2GM/c^2$ from the center of the Black Hole, where M is the mass of the Black Hole.
- We assume that $r > r_s$.

- Lagrangian :

$$L = \frac{1}{2} m g_{\mu\nu} \dot{x}^\mu \dot{x}^\nu = \frac{1}{2} m \left[-\left(1 - \frac{r_s}{r}\right) (c\dot{t})^2 + \frac{\dot{r}^2}{1 - r_s/r} + r^2 \dot{\phi}^2 \right]. \quad (9)$$

- $x^\mu = (ct, r, \theta, \phi)$
- The dot symbol $\dot{}$ denotes the differential with respect to the proper time τ for a mass point, or the affine parameter λ for a photon.

We derive two conserved quantities from the Lagrangian:

$$\mathcal{E} = -mc^2 \left(1 - \frac{r_s}{r}\right) \dot{t},$$
$$\mathcal{J} = m r^2 \dot{\phi}.$$

Moreover from $g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu = -kc^2$ we have

$$-\left(1-\frac{r_s}{r}\right)(c\dot{t})^2+\frac{\dot{r}^2}{1-r_s/r}+r^2\dot{\phi}^2=-kc^2,$$

where $k=1$ for a mass point and $k=0$ for a photon.
From these above we obtain

$$m^2\dot{r}^2=\frac{\mathcal{E}^2}{c^2}-km^2c^2-\frac{\mathcal{J}^2}{r^2}+km^2\frac{r_s}{r}c^2+\frac{r_s\mathcal{J}^2}{r^3}. \tag{10}$$

Hereafter we consider a mass point and take $k=1$. Using $r_s=2GM/c^2$ and divide the both side by $1/(2m)$, then we have

$$\frac{1}{2}m\dot{r}^2=\underbrace{\frac{\mathcal{E}^2}{2mc^2}-\frac{1}{2}mc^2}_{\equiv E_S}\underbrace{-\frac{\mathcal{J}^2}{2mr^2}+\frac{GMm}{r}+\frac{G\mathcal{J}^2M}{c^2r^3m}}_{\equiv -V_S}.$$

Namely,

$$\frac{1}{2}m\dot{r}^2=E_S-V_S. \tag{11}$$

Note that

$$E_S = \frac{1}{2}m\dot{r}^2 + V_S \geq V_S$$

and

$$V_S = \frac{\mathcal{J}^2}{2mr^2}\left(1 - \frac{r_s}{r}\right) - \frac{GMm}{r}$$

Therefore it follows that

$$E_S \geq -\frac{GMm}{r}$$

on the sphere with the radius $r > r_s$.

Consider a sphere with the radius $r = R_1$. If an orbit has its conserved quantity $E_S = \hat{E}_S$, which starts from an inner point of the sphere, and

$$\hat{E}_S < -\frac{GMm}{R_1}$$

holds, then the orbit does not go out of the sphere.

This means The Inclusion of solution orbits.

Conserved Quantity F

Now we consider a conserved quantity $\mathcal{F} = E_S - a\,\mathcal{J}$ by a similar manner in Kepler Problem, and derive its non-dimensional form.

Let

$$\rho = \frac{r}{r_s}, \quad v = \frac{\dot{r}}{c}, \quad u = \frac{r\dot{\phi}}{c}.$$

Note that $|v| < 1$, $|u| < 1$ as $k = 1$.

Define J by

$$J = \frac{r}{r_s}\frac{r\dot{\phi}}{c} = \rho u,$$

which has no dimension and $\mathcal{J} = r_s mc\, J$ holds.

Note that E_S can be represented by

$$\begin{aligned} E_S &= \frac{1}{2}mc^2\left(v^2 + (1+u^2)(1-\frac{1}{\rho}) - 1\right) \\ &= \frac{1}{2}mc^2\left(v^2 + (1-\frac{1}{\rho}) + J^2\frac{1}{\rho^2}(1-\frac{1}{\rho}) - 1\right) \end{aligned} \tag{12}$$

with respect to each point (ρ, v, u) on the orbit considered.

On the analogy of Kepler problem, we suppose that $a = \dot{\phi}(1 - \frac{r_s}{\tilde{r}_0})$ and calculate it by the following process.

1. Take a set of initial values $\rho(0)$, $v(0)$, $u(0)$ for an orbit, and define
$$\hat{J} = \rho(0)u(0).$$
2. From approximate computation of the orbit, find the closest point to the Black Hole, and let the value ρ of the point $\rho = \hat{\varrho}_0$. Take a little bit smaller value $\varrho_0 < \hat{\varrho}_0$, and set $R_0 = r_S \varrho_0$.
3. As we have
$$\dot{\phi} = \frac{1}{\rho^2} \frac{c}{r_s} J,$$
we calculate the constant a by
$$a = \frac{c}{r_s} \frac{1}{\varrho_0^2} \left(1 - \frac{1}{\varrho_0}\right) \hat{J}. \tag{13}$$

Conserved Quantity F

From (12), (13) and $\mathcal{J} = r_s mcJ$, we have

$$\begin{aligned}\mathcal{F} &= \frac{1}{2}mc^2\left(v^2 + (1-\frac{1}{\rho}) + J^2\frac{1}{\rho^2}(1-\frac{1}{\rho}) - 1 - 2a\,\frac{r_s}{c}J\right)\\ &= \frac{1}{2}mc^2\left(v^2 + (1-\frac{1}{\rho}) + J^2\frac{1}{\rho^2}(1-\frac{1}{\rho}) - 1 - 2\frac{1}{\varrho_0^2}\left(1-\frac{1}{\varrho_0}\right)\hat{J}\,J\right).\end{aligned}$$

Then define F with no dimension by

$$F = v^2 + (1-\frac{1}{\rho}) + J^2\frac{1}{\rho^2}(1-\frac{1}{\rho}) - 2\frac{1}{\varrho_0^2}\left(1-\frac{1}{\varrho_0}\right)\hat{J}\,J. \qquad (14)$$

Conserved Quantity F

For $\rho > 1$,

$$F = v^2 + \frac{1}{\rho^2}(1 - \frac{1}{\rho}) \left(J - \frac{\rho^2}{1 - \frac{1}{\rho}} \frac{1 - \frac{1}{\varrho_0}}{\varrho_0^2} \hat{J} \right)^2$$
$$+ (1 - \frac{1}{\rho}) - \frac{\rho^2}{1 - \frac{1}{\rho}} \frac{(1 - \frac{1}{\varrho_0})^2}{\varrho_0^4} \hat{J}^2$$
$$\geq (1 - \frac{1}{\rho}) - \frac{\rho^2}{1 - \frac{1}{\rho}} \frac{(1 - \frac{1}{\varrho_0})^2}{\varrho_0^4} \hat{J}^2. \quad (15)$$

Conserved Quantity F

Define

$$A_0 = \frac{(1 - \frac{1}{\varrho_0})^2}{\varrho_0^4} \hat{J}^2$$

and write the right hand side of (15) by

$$f(\rho) = (1 - \frac{1}{\rho}) - \frac{\rho^2}{1 - \frac{1}{\rho}} A_0,$$

then $f(\rho)$ is constant on a sphere with its radius ρ.

Therefore

- If an orbit has its conserved quantity F and an intersection point with the sphere with the radius ρ, then

$$F \geq f(\rho) \tag{16}$$

  holds.

Conserved Quantity F

On the other hand

$$F < f(\rho)$$

holds, then the orbit has no intersection with the sphere.

In case of $\rho = \varrho_0$, if the condition

$$F < f(\varrho_0) = (1 - \frac{1}{\varrho_0})(1 - \frac{\hat{J}^2}{\varrho_0^2})$$

holds, then the orbit with the quantity F remains out side of the sphere, namely it is excluded by the area with the distance $R_0 = r_S \varrho_0$ from the center of the Black Hole.

Time evolution Equation

The motion equation from the Lagrangian is as follows.

t-direction:

$$-\frac{r_s}{r^2}\dot{r}\dot{t} + \left(1 - \frac{r_s}{r}\right)\ddot{t} = 0$$

r-direction:

$$\frac{mr_s}{(1 - r_s/r)^2 r^2}\dot{r}^2 + \frac{m}{1 - r_s/r}\ddot{r} - \frac{1}{2}m\left[-\frac{c^2 r_s \dot{t}^2}{r^2} - \frac{r_s \dot{r}^2}{r^2(1 - r_s/r)^2} + 2r\dot{\phi}^2\right] = 0$$

ϕ-direction:

$$mr\ddot{\phi} + 2m\dot{r}\dot{\phi} = 0$$

Time evolution Equation

In order to solve the motion equation with respect to time, we define $\rho_1 = r/r_s$, $t_1 = \frac{c}{r_s}t$.
Then we have a time evolution equation with no dimension as

$$
\begin{aligned}
\dot{t}_1 &= t_2, \\
\dot{\rho}_1 &= \rho_2, \\
\dot{\phi}_1 &= \phi_2, \\
\dot{t}_2 &= \frac{\rho_2}{\rho_1(\rho_1 - 1)} t_2, \\
\dot{\rho}_2 &= (\rho_1 - 1)\phi_2^2 - \frac{3}{2}\frac{\rho_2^2}{(\rho_1 - 1)\rho_1} - \frac{1}{2}\frac{\rho_1 - 1}{\rho_1^3} t_2^2, \\
\dot{\phi}_2 &= -2\frac{\rho_2}{\rho_1}\phi_2.
\end{aligned}
$$

Time evolution Equation

The initial values of coordinate time t is supposed to be $t(0) = 0$, $\dot{t}(0) = 1$, then we take our set of initial values as

$$
\begin{aligned}
&t_1(0) = 0, \quad t_2(0) = \frac{c}{r_s}, \\
&\rho_1(0) = \rho(0), \quad \rho_2(0) = \frac{c}{r_s} v(0), \\
&\phi_1(0) = 0, \quad \phi_2(0) = \frac{c}{r_s} \frac{u(0)}{\rho(0)}
\end{aligned}
$$

Note that c/r_s can be regarded as a scale parameter with respect to the proper time.

Derivation of Binet Equation

Our problem can be solved by another way. That is, so called Binet Equation is derived from (10). Define

$$b = \frac{1}{r}$$

and differentiate b by ϕ, then we have

$$\frac{db}{d\phi} = -\frac{m}{\mathcal{J}}\dot{r},$$

which implies $m^2\dot{r}^2 = \mathcal{J}^2(\frac{db}{d\phi})^2$.

Substituting this to (10),

$$\mathcal{J}^2(\frac{db}{d\phi})^2 = \frac{\mathcal{E}^2}{c^2} - m^2c^2 - \mathcal{J}^2b^2 + m^2c^2r_sb + r_s\mathcal{J}^2b^3$$

is obtained. Differentiate this again by ϕ and divide the both side by $2\mathcal{J}^2\frac{db}{d\phi}$, then the Binet Equation

$$\frac{d^2b}{d\phi^2} = \frac{3}{2}r_sb^2 - b + \frac{m^2c^2}{2\mathcal{J}^2}r_s$$

is derived.

Moreover we introduce

$$s = \frac{r_s}{r} = r_s b$$

and then the Binet Equation becomes

$$\frac{d^2 s}{d\phi^2} = \frac{3}{2}s^2 - s + \frac{1}{2J^2}. \tag{17}$$

with no dimension. From (17) we have ODE system:

$$\frac{ds_1}{d\phi} = s_2,$$
$$\frac{ds_2}{d\phi} = \frac{3}{2}s_1^2 - s_1 + \frac{1}{2J^2}.$$

The initial values are given by

$$s_1(0) = \frac{1}{\rho(0)}, \quad s_2(0) = -\frac{1}{\rho(0)}\frac{v(0)}{u(0)}.$$

Process :

1. As is described above, calculate a solution orbit of the Time Evolution Equation or Bine Equation using the set of initial values $\rho(0), v(0), u(0)$ or corresponding set of $s_1(0)$ and $s_2(0)$, and find the closest point to the Black Hole. Set $\hat{\varrho}_0$ from the position of the point, and chose $\varrho_0 > 1$ satisfying

$$\varrho_0 < \hat{\varrho}_0$$

   and define $R_0 = r_S \varrho_0$.

2. From the initial values calculate approximately

- $\hat{J} = \rho(0)u(0)$,
- A_0,
- and define

$$f(\rho) = (1 - \frac{1}{\rho}) - \frac{\rho^2}{1 - \frac{1}{\rho}} A_0.$$

3. Consider intervals $[\rho(0)], [v(0)], [u(0)]$ whose radii are small and

$$\rho \in [\rho(0)], \quad v(0) \in [v(0)], \quad u(0) \in [u(0)]$$

   as the centers.
   Compute $[J]$ and $[F]$ corresponding $[\rho(0)], [v(0)], [u(0)]$ by interval arithmetic with verified computation.
4. Check whether

$$[F] < f(\varrho_0) \tag{18}$$

   holds or not using verified computation.

If the condition (18) holds, then we have proven that

- All the solution orbits starting from the initial values including the intervals $[\rho(0)], [v(0)], [u(0)]$ do not attain the sphere centered at the Black Hole center with radius R_0.

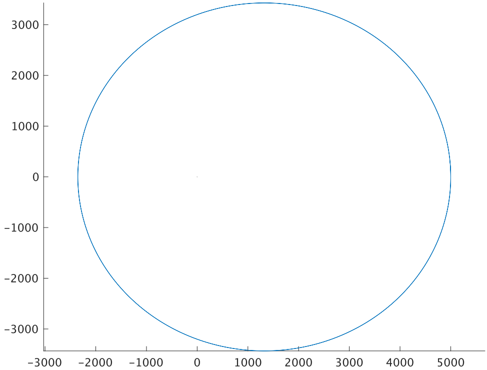
Example 1

First we confirm that results of Time Evolution Equation and Binet Equation coincide in an area far from the Black Hole.

- $\phi(0) = 0$, $\phi(End) = 4\pi$
- $\rho(0) = 5000$, $v(0) = 0$, $u(0) = 0.008$
- $c/r_s = 100$, $\tau_{end} = 40000$

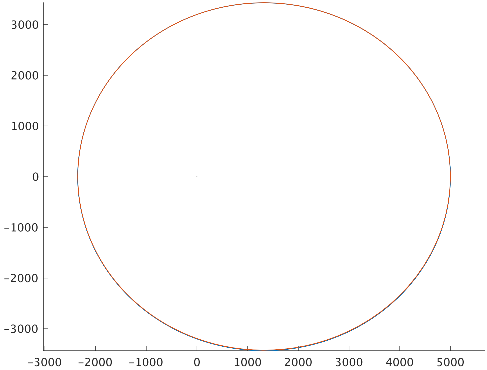
The options of ode45 in MATLAB are
Binet： opts = odeset('abstol',1e-10,'reltol',1e-10);
Time Evolution: opts = odeset('abstol',1e-20,'reltol',1e-20);

Time Evolution :



Example1

Binet：



Example 2

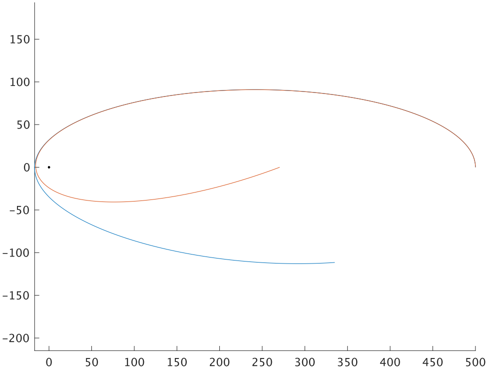
However the two Equations show different results for an area near the Black Hole.

- $\phi(0) = 0$, $\phi(End) = 2\pi$
- $\rho(0) = 500$, $v(0) = 0$, $u(0) = 0.008$
- $c/r_s = 100$, $\tau_{end} = 250$

Example 2

Blue line: Time Evolution   Red line: Binet:

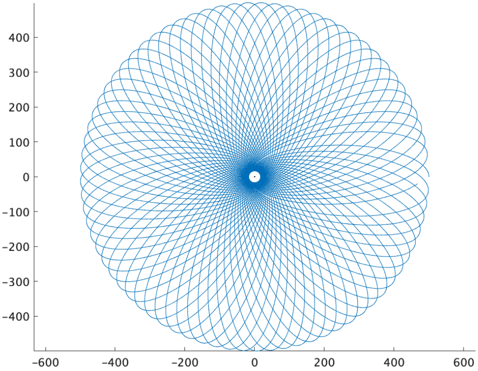
Initially they coincide each other but become different after the turning point.



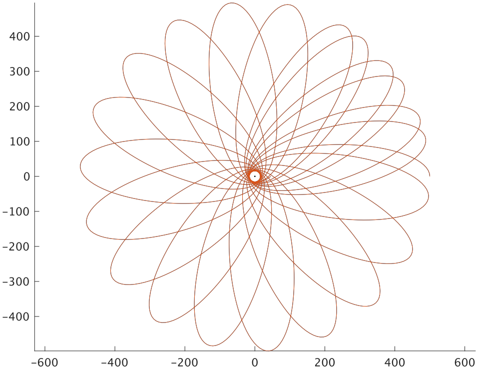
Example 3

Longer time computation gives the following.

Time Evolution:



Binet：



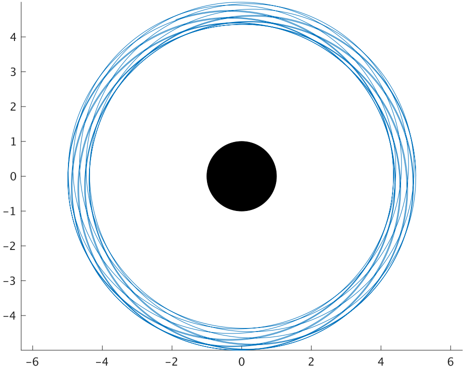
Example 4

More closer area to the Black Hole:

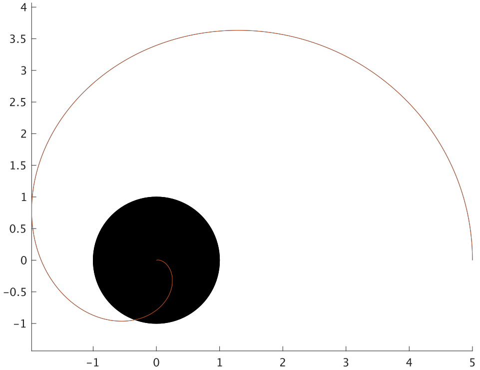
- $\phi(0) = 0$, $\phi(End) = 46\pi$
- $\rho(0) = 5$, $v(0) = 0$, $u(0) = 0.3$
- $c/r_s = 50$, $\tau_{end} = 28$

Example 4

Time Evolution:



Binet：



Example 5

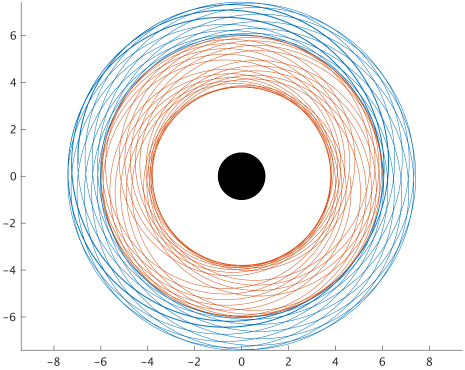
Which is reliable Time Evolution or Binet ?

In order to check this, we consider the following example:

- $\phi(0) = 0$, $\phi(End) = 48\pi$
- $\rho(0) = 6$, $v(0) = 0$, $u(0) = 0.31$
- $c/r_s = 50$, $\tau_{end} = 50$

Example 5

Blue line: Time Evolution   Red line: Binet:



Verification

From the result of Binet Equation, we take $\hat{\varrho}_0 = 3.792646015975992$.

Initial value intervals represented by center-radius form:

- $\rho(0) = \langle\, 6\,,\, 10^{-5}\,\rangle$, $v(0) = 0$, $u(0) = \langle\, 0.31\,,\, 10^{-5}\,\rangle$

- We have verified that the exact solution orbits do not come into the sphere with the radius corresponding to $\varrho_0 = 3.79$.
- On the other hand, we cannot success in verification of the condition (18) for $\varrho_0 = 3.8$.

This implies indirectly that Binet Equation is reliable rather than Time Evolution Equation.

Consideration

Maybe

- Nonlinearity of the computation gets larger and larger as the orbit comes to the Black Hole near and near.
- As Time Evolution Equation has 3 variables, the nonlinearity influence its computation rather than Binet Equation who has only 1 variable.
- Actually computation of E_s in Time Evolution Equation w.r.t. the proper time may have fluctuation.

I feel that we have to use Structure-Preserving Numerical Methods in order to reduce the fluctuation of E_s.

- Our method has strong relation to so called Effective Potential, which serves as a standard analytical method for analyzing geodesic orbits.

精度保証の必要条件

必要条件：

- 式 (16) で $\rho = \hat{\varrho}_0$ とすれば $f(\hat{\varrho}_0) \leq \hat{F}$ が成り立つ。
- これと、「落ちない」条件 $F < f(\varrho_0)$ から、必要条件として

$$f(\hat{\varrho}_0) < f(\varrho_0)$$

　が得られる。

理論上は、ϱ_0 は $\hat{\varrho}_0$ にいくらでも近い値に取ることができる。したがって軌道が半径 $\hat{\varrho}_0$ の球面から「落ちない」ための必要条件は

- $f(\rho)$ が $\rho = \hat{\varrho}_0$ において減少すること

すなわち

$$f'(\rho)\Big|_{\rho=\hat{\varrho}_0} < 0$$

である。

精度保証の必要条件

そこで f' を算定すると、

$$f'(\rho) = \frac{1}{(\rho - 1)^2}\left(1 - \frac{2}{\rho} + \frac{1}{\rho^2} - \rho^2(2\rho - 3)A_0\right)$$

であるから、 $f'(\rho) < 0$ は

$$\frac{(\rho - 1)^2}{\rho^4(2\rho - 3)} < A_0$$

と同値である。

精度保証の必要条件

ただし、不等式変形では

$$2\rho > 3$$

を仮定している。

- このことは物理的には、$3r_s/2$ 以下の半径の球の内部では、たとえ事象の地平線に落ち込んでいなくても、周回軌道に乗ることはできず必ず「落ちる」ことを意味する。
- ただし、脱出速度は光速未満なので動径方向の初期速度が十分大きければ脱出できる。

精度保証の必要条件

さて、ここで $\varrho_0 = \hat{\varrho}_0$ とした上で A_0 の定義式を代入し、さらに $\rho = \hat{\varrho}_0$ に取れば、

$$\frac{\hat{\varrho}_0^2}{2\hat{\varrho}_0 - 3} < \hat{J}^2 \tag{19}$$

を得る。

条件 (19) は、

- 半径 $\hat{\varrho}_0$ の球の外側から出発した解軌道がこの球の外に留まる

ための必要条件を与える。

考察

この問題に関しては　Innermost stable circular orbit (ISCO) と呼ばれる軌道が知られている。これは条件

$$c^2\mathcal{J}^2 - 12G^2m^2M^2 > 0 \tag{20}$$

を満たす軌道で、これが初期時刻で半径 $3r_s$ の球の外側にあり動径方向速度が 0 であれば、時間発展後も外側に留まる。

ここで

$$\mathcal{J} = r_s mc\,J,$$
$$r_s = \frac{2GM}{c^2}$$

を用いて変形すれば (20) は

$$J^2 > 3$$

を意味する。

考察

一方で、「初期時刻で半径 $3r_s$ の球の外側にある」ためには $\hat{\varrho}_0 = 3$ と取ればよい。すると条件 (19) から

$$\hat{J}^2 > 3$$

を得る。これは ISCO の条件に符合する。

考察

さらに条件 (19) からは、与えられた $\hat{J}$ に対し、軌道が通過しない球面の半径の候補は

$$\hat{J}^2\left(1-\sqrt{\hat{J}^2-3}\right) < \hat{\varrho}_0 < \hat{J}^2\left(1+\sqrt{\hat{J}^2-3}\right)$$

にあることがわかる。同時にこれが実数値であるためには

$$\hat{J}^2 \geq 3$$

でなければならない。

つまり

- 「落ちない」ための角速度の下限は $\hat{J}=\sqrt{3}$ である。
- また、このとき $\hat{\varrho}_0=3$ となる。
- 実は数値例４では $\hat{J}=1.5<\sqrt{3}$ であった。したがって軌道が「落ちる」Binet が正しい。

以上を鑑みれば、(19) の導出過程は ISCO 条件の導出過程（有効ポテンシャルを用いた議論）と理論的な対応があるものと思われる。

Conclusion

- We consider a method of verified computation as a simple example of tool for analysis of phenomena.
- Our method is based on a conserved quantity which has a common form for Kepler Problem, Circular restricted three-body problem, and Motion in Schwarzchild Metric as

$$F = E - a\,J$$

- Using our conserved quantity with verified computation, we have shown this simple tool is useful in analysis of solutions and checking reliability of approximate computation concerning.
- Moreover we can derive some theoretical results from consideration of conditions of verification, as well as standard analytical methods in each fields.

I hope that future research of verified computation will develop tools easy to use for people engaged in analysis of phenomena.

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