How the Taylor Center may assist in teaching mathematics

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ABSTRACT. This article introduces a powerful ODE solver called the Taylor Center for PCs [1] as a tool for teaching and performing numeric experiments with ODEs. The Taylor Center is an All-in-One GUI-style application integrating ODEs by applying the modern Taylor Method (Automatic Differentiation), and offering powerful dynamic graphics (including 3D stereo vision). After a brief review of the features of the Taylor Center, we consider instructive examples of ODEs in various applications and also several particular samples illustrating intricacies of numeric integration. The article therefore continues the thesis of Borrelli and Coleman [2] that awareness and caution are needed while interpreting the results of numeric integration. We offer practical ideas and advice on how to use the Taylor Center for teaching ODEs, and to increase the motivation and interest of students.

1. Preface

In this article we are dealing with *holomorphic*[1] Ordinary Differential Equations (ODEs) and their holomorphic solutions in accordance with the Theorem of Cauchy-Kovalevskaya on existence and uniqueness of the solution.

The goals of the article are:

- To introduce a powerful ODE solver, called the Taylor Center for PCs [1] as a tool for teaching and numeric experiments with ODEs (Introduction);
- To illustrate its usefulness by demonstration of problems from simple (Section 3) to the more advanced (Sections 4-6);
- To show that awareness is always prudent in dealing with and interpretation of computer-generated results (Section 7). In doing this we are continuing the discussion started by Borrelli and Coleman [2].

2. Introduction

It seems there have been no sophisticated Taylor Solvers designed for PCs since 1994 (ATOMFT [3, 4]). We expect an application with advanced interactive visualization to provide:

Key words and phrases. ODE, Automatic differentiation, dynamic graphics, intricacies of numeric integration, 3D stereo.

[1]A complex function is called holomorphic in a neighborhood of a point if its Taylor expansion at this point exists and has nonzero convergence radius.

- User interface with style, controls, and handlers fit the specific model and operational tasks;
- Realistic visualization of the modeled processes employing all appropriate faculties of the human perception, achievable with advanced hardware and multimedia.

With that in mind we introduce a powerful ODE solver the Taylor Center [5] - an All-in-One system for integration of ODEs by applying the modern Taylor Method (Automatic Differentiation), and offering powerful dynamic graphics (including 3D stereo vision with conventional monitors and anaglyph Red/Blue glasses).

The Modern Taylor Method is a descendant of its classical counterpart. It is an efficient method for numerical integration of the Initial Value Problems (IVP) for ODEs (presuming that no singularities occur on the integration path). What distinguishes the Taylor Method from all other numerical methods for ODEs is the ability to compute the approximation to the solution with principally unlimited order of approximation (the number of terms in the Taylor expansion). With no singularities on the integration path, the step *does not* approach zero regardless of how high accuracy is specified (presuming the order of approximation may increase to infinity and the length of mantissa is unlimited). It is the distance to the singularities which bounds the finite integration step.

An unlimited order of approximation is possible because the method performs the *Automatic Differentiation* (i.e. exact computing of the derivatives up to any desired order n by optimized formulas for n-order differentiation) providing the Taylor series of a desired length for the solution components.

Automatic Differentiation is applicable to a subclass of holomorphic ODEs whose right hand sides are the so called generalized elementary vector-functions. The generalized elementary functions widen the class of the traditional (Liouville) elementary functions. The generalization was suggested by R. Moore [6] in the 1960s and further developed by Gofen [7]. Moore defined *generalized elementary functions as those that may be represented as solutions of explicit (nonlinear) ODEs whose right hand sides are rational in all variables.* For brevity, we will call them simply "elementary" functions.

It appears that practically all ODEs used in applications are comprised of (generalized) elementary functions. At the moment, only the Gamma function and Gamma integral are proved to be non-elementary [7]. Other candidates suspected (but not yet proved) to be non-elementary are general solutions of elementary ODEs *as functions of their parameters* or *of their initial values.* However, the solutions of elementary ODEs as functions of the variable of integration are always elementary (the theorem of closeness of the class of elementary functions [7]). The composition of elementary functions and their inverse are elementary too [7]. *Therefore, the subclass of elementary ODEs covers mostly all problems emerging in applications and courses of Mathematics and Physics taught in universities, making this Taylor solver widely applicable.* In fact, the Taylor Center applies to any normal first-order system whose right hand sides are commonly known analytic functions of the state variables.

In the most straightforward way this software may be used to illustrate dynamics in every initial value problem taught in universities, and we will point out many such examples further on. However, the Taylor Center also gives an opportunity to explain and demonstrate particularities of numerical integration. In so doing, it raises the awareness of the students when they interpret the computed numerical solutions. All the examples discussed in the article or illustrated here with a *static* picture may be run *animated* via the free demonstration version of the Taylor Center[2] available at the Taylor Center web page [5].

For every illustration in the article, the path via the Main menu's *Demo* item, or the name of the respective script file for loading via File/Open script is given. (After the installation, the sub-folder *Samples* contains all pre-loaded *scr* files and *ode* files). In this article, all illustrations on a black background are stereo images which should be viewed through Red/Blue glasses available here or with the author. (See Appendix 1 for the complete list of features of the Taylor Center).

3. A powerful tool for dynamic drawing

The Taylor Center is beneficial whenever drawing of curves is required: planar – but especially non-planar (viewed in stereo), with the source of the curves being either an initial value problem for ODEs, or merely parametric equations.

Example 1. *Here is the "Wine glass" solution (Fig. 1) for the ODEs of autocatalitic reaction (from the book of Borrelli and Coleman [8]) graphed as a planar curve:*

[2]To obtain the license for the full version, the contacts of the author are available under Help/Registration.

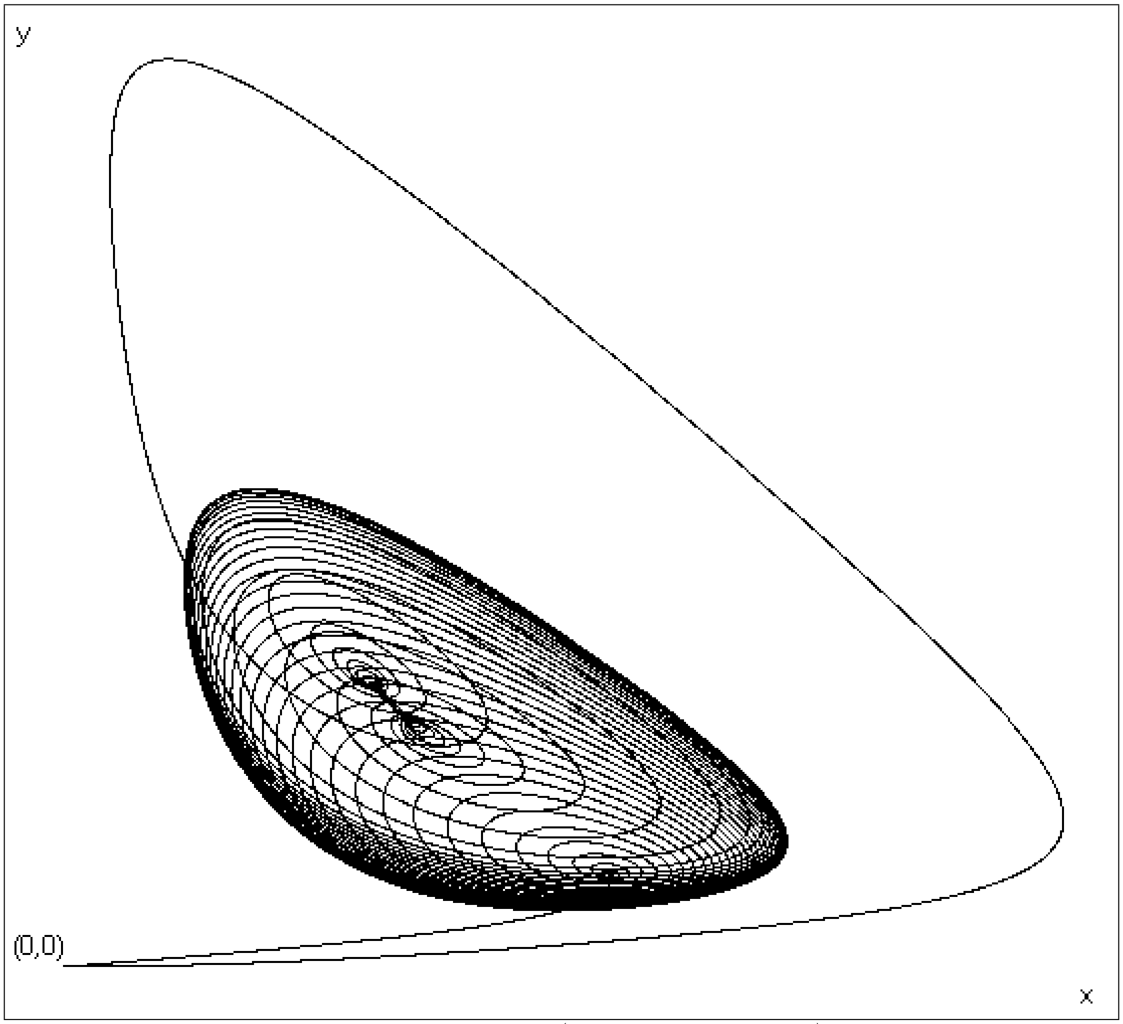

Fig. 1. The "Wine glass solution" (script file Borrelli.scr*)*

The corresponding ODEs as loaded in the Taylor Center are:

$t = 0$	$t' = 1$ [3]
$x = 0$	$x' = exp(-0.002 * t) - 0.08 * x - x * y\hat{}2$
$y = 0$	$y' = 0.08 * x - y + x * y\hat{}2$

Generally the entry format for an IVP in the Taylor Center is:

Constants	Auxiliary variables
Initial values	ODEs

[3] Generally a trivial equation for the independent variable (like $t' = 1$) may be omitted. However it is necessary in order that dynamic Play be possible. Also, it is necessary if the user plans switching from one independent variable to another.

(see the program's front panel). The names of the variables may be multi-character identifiers, and the arithmetic expressions must obey the syntax of Pascal (the multiplication sign * cannot be omitted).

And here is an example[4] of a field of direction for the singular ODE

$$t^2x' + (t-1)x + 1 = 0$$

in the area $[-1, 1;\ 0, 2]$.

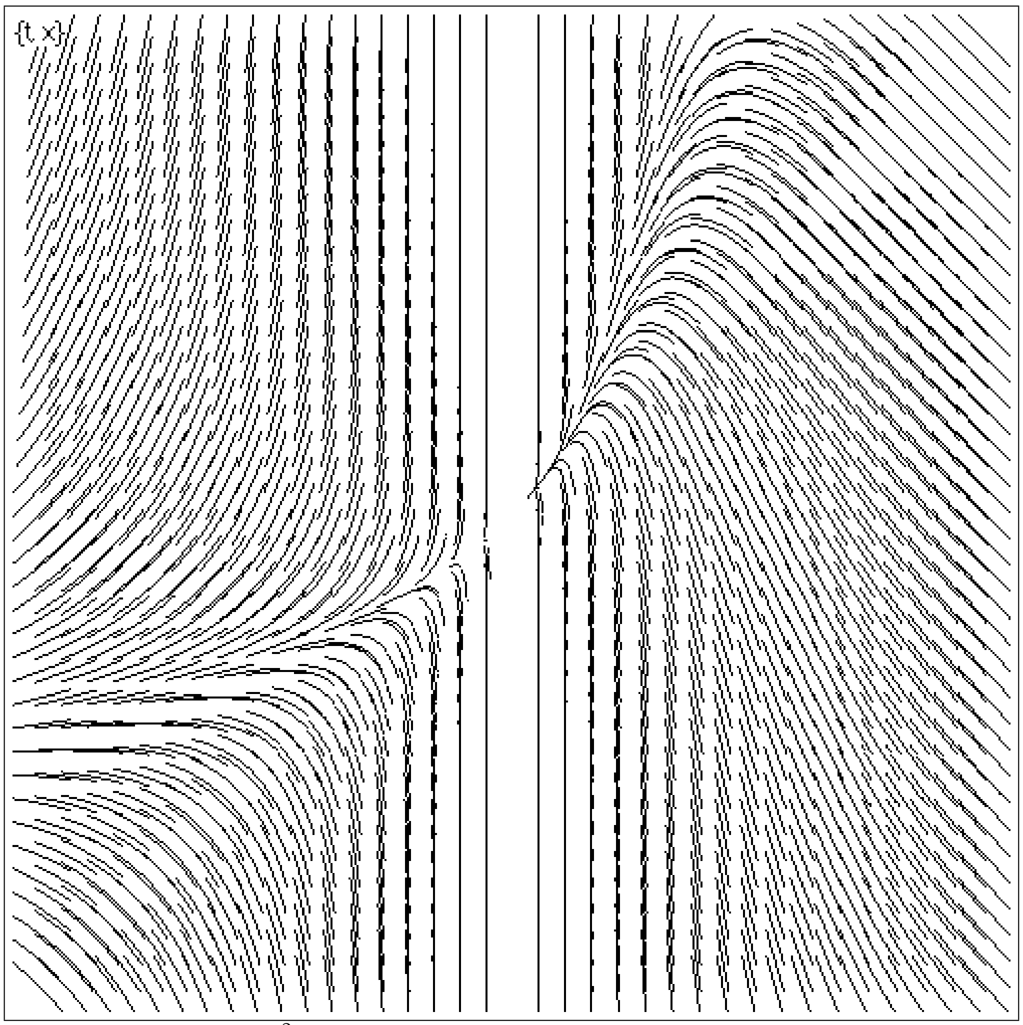

Fig. 2. Singular ODE $t^2x' + (t-1)x + 1 = 0$ in the area $[-1, 1;\ 0, 2]$. The curvy elements (whose length depend on the heuristic radius) are obtained at points of regular grid 36×36, some elements connected. For $t = 0$ evaluation fails so the median vertical is missed.

[4]This example is borrowed from the textbook "The methods of integration of Ordinary Differential Equations" by N.Matveev.

(This is an example of a singular ODE for which evaluation of coefficients a_n of its formal Taylor expansion at the point of singularity $(0,1)$ is possible, but $a_n = n!$ so that the convergence radius is zero).

However the Taylor Center is really indispensable for visualizing dynamics. There is a huge difference between a static picture of a trajectory (say in a book) vs. the real time animation of the motion along the trajectories in the Taylor Center. In it not only can the viewer watch the near real time evolution of the motion, but also observe its acceleration and decelerations, examine the ODEs, and vary the parameters.

Example 2. *Here you can see only the final shot of the motion of the double pendulum described with the ODEs*

$$\theta_1'' = -\frac{L_2\{m_2\cos(\theta_1-\theta_2)[L_1\theta_1'^2\sin(\theta_1-\theta_2)-g\sin(\theta_2)]+gm\sin(\theta_1)+m_2L_2\theta_2'^2\sin(\theta_1-\theta_2)\}}{L_1L_2(m_1+m_2\sin^2(\theta_1-\theta_2)}$$

$$\theta_2'' = \frac{L_1\{gm[\sin(\theta_1)\cos(\theta_1-\theta_2)-\sin(\theta_1-\theta_2)]+\sin(\theta_1-\theta_2)(m_2L_2\cos(\theta_1-\theta_2)\theta_2'^2+mL_1\theta_1'^2)\}}{L_1L_2(m_1+m_2\sin^2(\theta_1-\theta_2)}$$

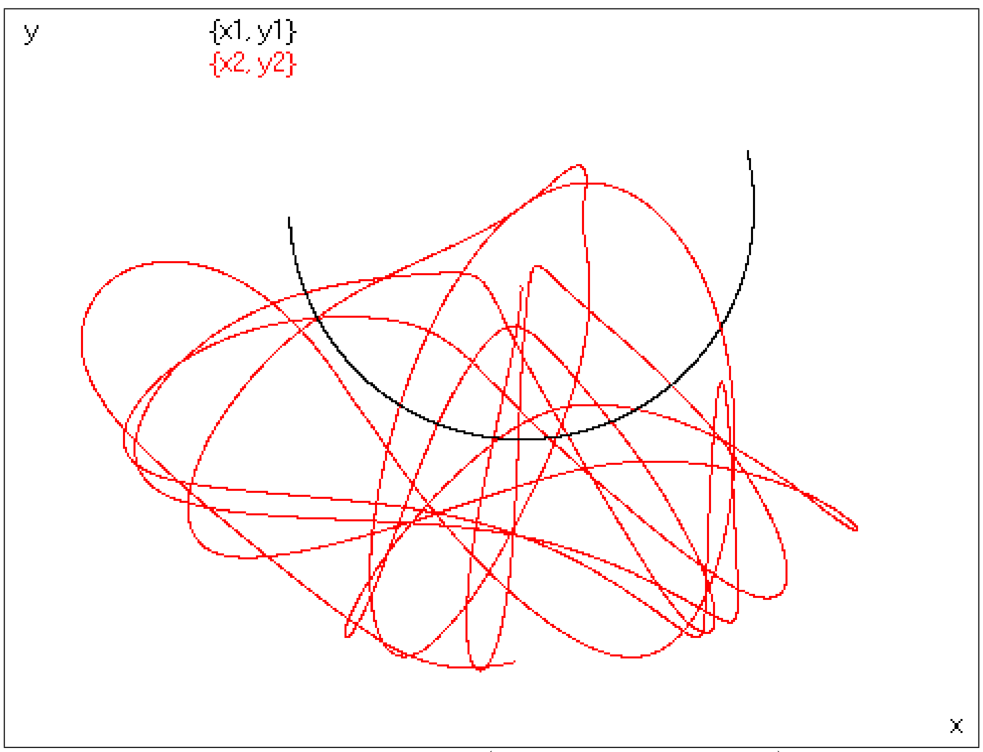

Fig. 3. Double pendulum (file *DoublePendulum.scr*)

(Run the program to watch the motion).

And here is how the ODEs for the double pendulum look like in the Taylor Center (the auxiliary variables are displayed first - just in order to fit the page):

Auxiliary variables in the *DoublePendulumODEs*

$$y1 = -L1 * cos(Te1)$$
$$x1 = L1 * sin(Te1)$$
$$y2 = -L2 * cos(Te2) + y1$$
$$x2 = L2 * sin(Te2) + x1$$
$$Te12 = Te1 - Te2$$
$$VTe12 = VTe1 - VTe2$$
$$D = -L1 * L2 * (m1 + m2 * sin(Te12)\hat{}2)$$
$$D1 = L2 * (m2 * cos(Te12) * (L1 * VTe1\hat{}2 * sin(Te12) - g * sin(Te2)) + \\ + g * m * sin(Te1) + m2 * L2 * VTe2\hat{}2 * sin(Te12))$$
$$D2 = -L1 * (g * m * (sin(Te1) * cos(Te12) - sin(Te2)) + \\ + sin(Te12) * (m2 * L2 * cos(Te12) * VTe2\hat{}2 + m * L1 * VTe1\hat{}2))$$

$g = 9.8$ $m1 = 1$ $m2 = 1$ $m = m1 + m2$ $L1 = 1$ $L2 = 1$ $Te10 = 1.4$ $Te20 = -1.4$ $VTe10 = 0$ $VTe20 = 0.2$	Auxiliary variables
$t = 0$ $Te1 = Te10$ $Te2 = Te20$ $VTe1 = VTe10$ $VTe2 = VTe20$	$t' = 1$ $Te1' = VTe1$ $Te2' = VTe2$ $VTe1' = D1/D$ $VTe2' = D2/D$

EXAMPLE 3. *This one and further examples in this chapter are the n-body problem. Here are ODEs for the planar three body problem (Fig. 4):*

$$
\begin{array}{l}
i15 = -1.5 \\
m1 = 1 \\
m2 = 1 \\
m3 = 1 \\
x1c = 1 \\
y1c = 0 \\
x2c = cos(120) \\
y2c = sin(120) \\
x3c = cos(240) \\
y3c = sin(240) \\
vx1c = 0 \\
vy1c = 1 \\
vx2c = cos(210) \\
vy2c = sin(210) \\
vx3c = cos(330) \\
vy3c = sin(330) \\
k = 0.2
\end{array}
$$

$$
\begin{array}{l}
dx12 = x1 - x2 \\
dy12 = y1 - y2 \\
dx23 = x2 - x3 \\
dy23 = y2 - y3 \\
dx31 = x3 - x1 \\
dy31 = y3 - y1 \\
r12 = (dx12\hat{}2 + dy12\hat{}2)\hat{}i15 \\
r23 = (dx23\hat{}2 + dy23\hat{}2)\hat{}i15 \\
r31 = (dx31\hat{}2 + dy31\hat{}2)\hat{}i15
\end{array}
$$

$$
\begin{array}{l}
t = 0 \\
x1 = x1c \\
y1 = y1c \\
x2 = x2c \\
y2 = y2c \\
x3 = x3c \\
y3 = y3c \\
vx1 = k * vx1c \\
vy1 = k * vy1c \\
vx2 = k * vx2c \\
vy2 = k * vy2c \\
vx3 = k * vx3c \\
vy3 = k * vy3c
\end{array}
$$

$$
\begin{array}{l}
t' = 1 \\
x1' = vx1 \\
y1' = vy1 \\
x2' = vx2 \\
y2' = vy2 \\
x3' = vx3 \\
y3' = vy3 \\
vx1' = m3 * dx31 * r31 - m2 * dx12 * r12 \\
vy1' = m3 * dy31 * r31 - m2 * dy12 * r12 \\
vx2' = m1 * dx12 * r12 - m3 * dx23 * r23 \\
vy2' = m1 * dy12 * r12 - m3 * dy23 * r23 \\
vx3' = m2 * dx23 * r23 - m1 * dx31 * r31 \\
vy3' = m2 * dy23 * r23 - m1 * dy31 * r31
\end{array}
$$

With the Z coordinate and for a greater number n of variables the system gets much more cumbersome, yet the program *generates the system automatically* for the n-body problem.

The program also visualizes variability of the radius of convergence along the trajectory (the ticks in the progress bar in the lower part of the Fig. 4):

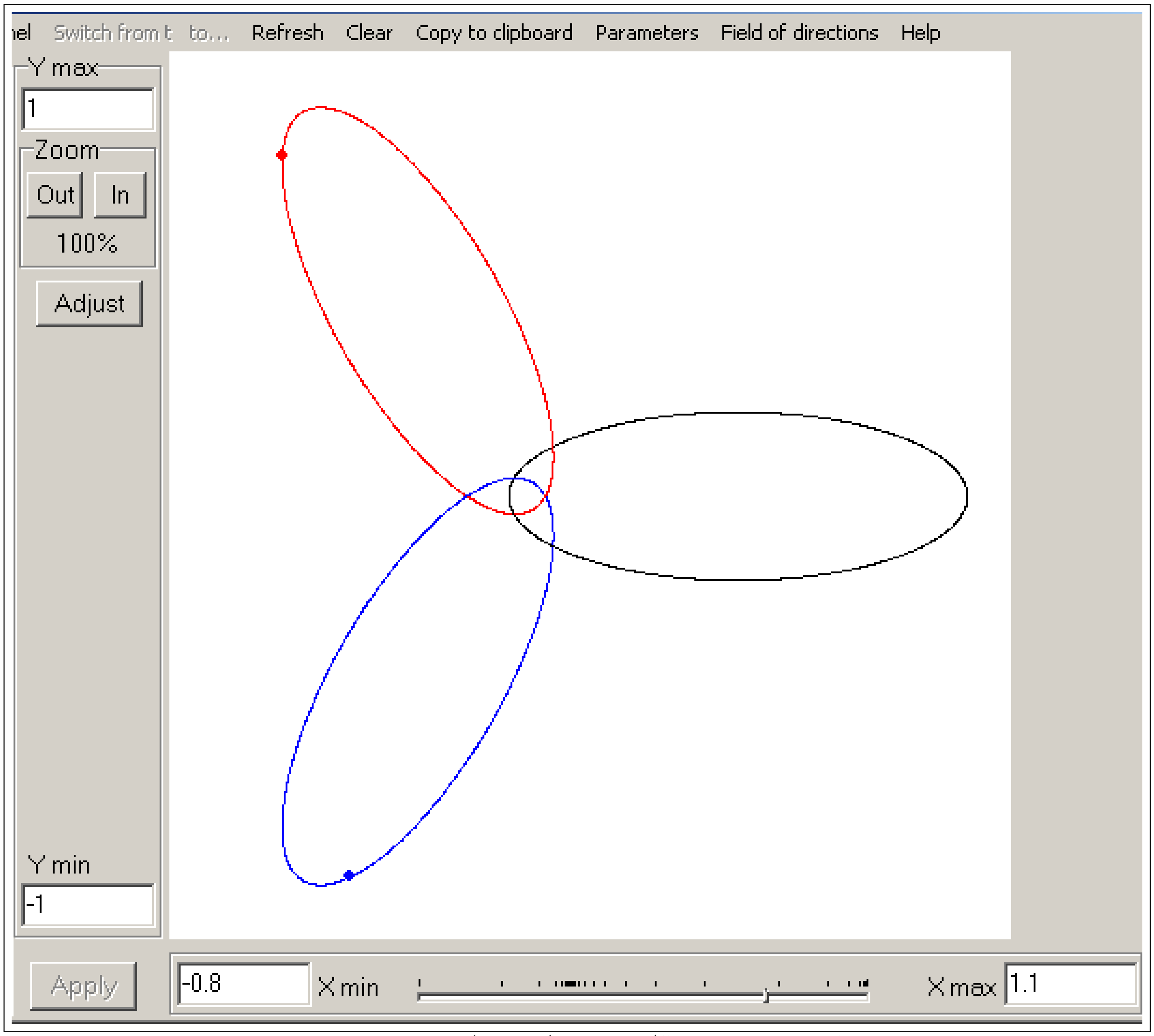

Fig. 4. The three body Lagrange case. (Demo/3 Bodies/Symmetircal or file *3Bodies2D.ode*)

The direct observation of the dramatic acceleration when the bodies approach the center of the masses is a perfect illustration when teaching Kepler's laws. The program is pre-loaded with a variety of commonly taught classical problems such as:

- Pendulums (planar in files *Pendulum2D.ode*, *DoublePendulum.scr*, and non-planar in files *PendulumFlower.scr*, *PendulumApple.scr*);
- Spirals (*CornuSpiral.scr*, *AlgSpiral.ode*, *IntSpiral.ode*);
- Bessel functions (in folder *Samples\SpecPoints*);
- Knot curves in 3D (*KnotChain3D.scr*, *TrefoilKnot3D.scr*);

- Great variety of $n-$body problems under different conditions, including the illustration of the Lagrange points (under the Demo menu and in the folder *Samples*).

Also, teachers can add samples of their own interest.

Among mathematical tools, the Taylor Center perhaps is unique in employing stereo vision for displaying non-planar curves. It is always a challenge to draw non-planar trajectories in the conventional axonometric projection. That is why the Taylor Center uses the Red/Blue anaglyph stereo as a cheap, yet efficient system of stereo vision. The curves literally pop up from the screen into the 3D space in front of the viewer, who can turn them and explore them with a 3D cursor controlled with the mouse wheel (the respective 3D coordinates being continuously displayed).

Dynamic playing of trajectories is desirable for almost every ODE problem in mathematics and physics, especially in the celestial mechanics. There are numerous pre-loaded script files (in the sub-folder *Samples*) defining common mechanical problems such as pendulums to sophisticated examples in celestial mechanics illustrating the 5 Lagrange (libration) points (*Demo/5 Lagrange points* or file *LagrangePoints.scr*, to be covered with more details in a future article).

In the Taylor Center, we can see the immediate effect of parameters controlling the behavior of the solution. In particular, it is instructive to illustrate instability, for example in the Lagrange solutions of the $n-$body problem.

A solution of the $n-$body problem is called the Lagrange case if the n masses are equal, and in the initial moment:

- *The bodies are positioned at the apexes of a regular polygon;*
- *Their initial velocities are equal in absolute value;*
- *Their vectors are inclined at the same non-zero angle to the respective radii.*

The initial polygonal formation (defined by the properties 1-3) is preserved during the motion, in which all the bodies move alone the trajectories of the same conical type with the center being the center of the polygon (Fig 3).

The instability of the Lagrange case motion (and of the Lagrange points as well) may be observed in various ways: In failure to numerically integrate it for big enough number of periods (especially for oblong ellipses), or in sensitivity of the solution to slight changes in the initial values. Compare Fig. 4 showing the accurate Lagrange setting, with the disturbed case in a plane (Fig. 5), where all possible pairs of the three bodies couple randomly in turn (you would appreciate to watch it as a real time motion):

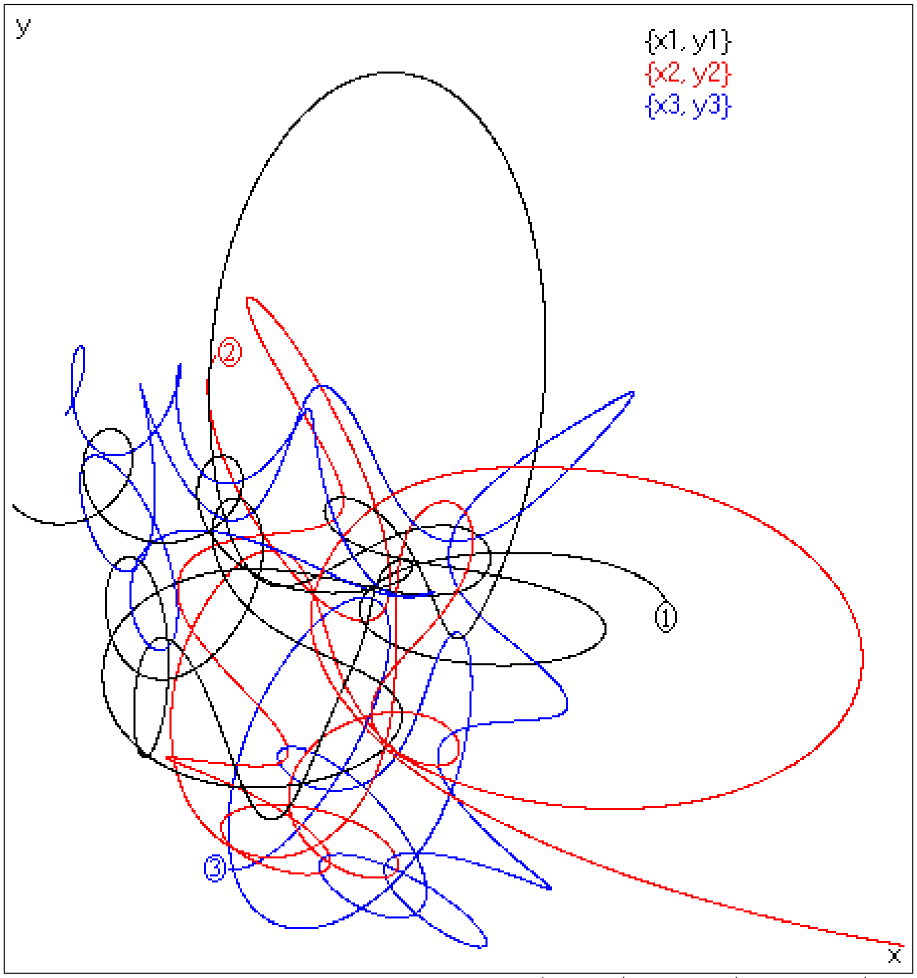

Fig. 5. Disturbed Lagrange setting in a plane. (Demo/3 Bodies/Disturbed/2D or file *3Bod9995.scr*)

Finally, see what happens when the initial setting was disturbed in the direction perpendicular to the plane pushing the trajectories into 3D space:

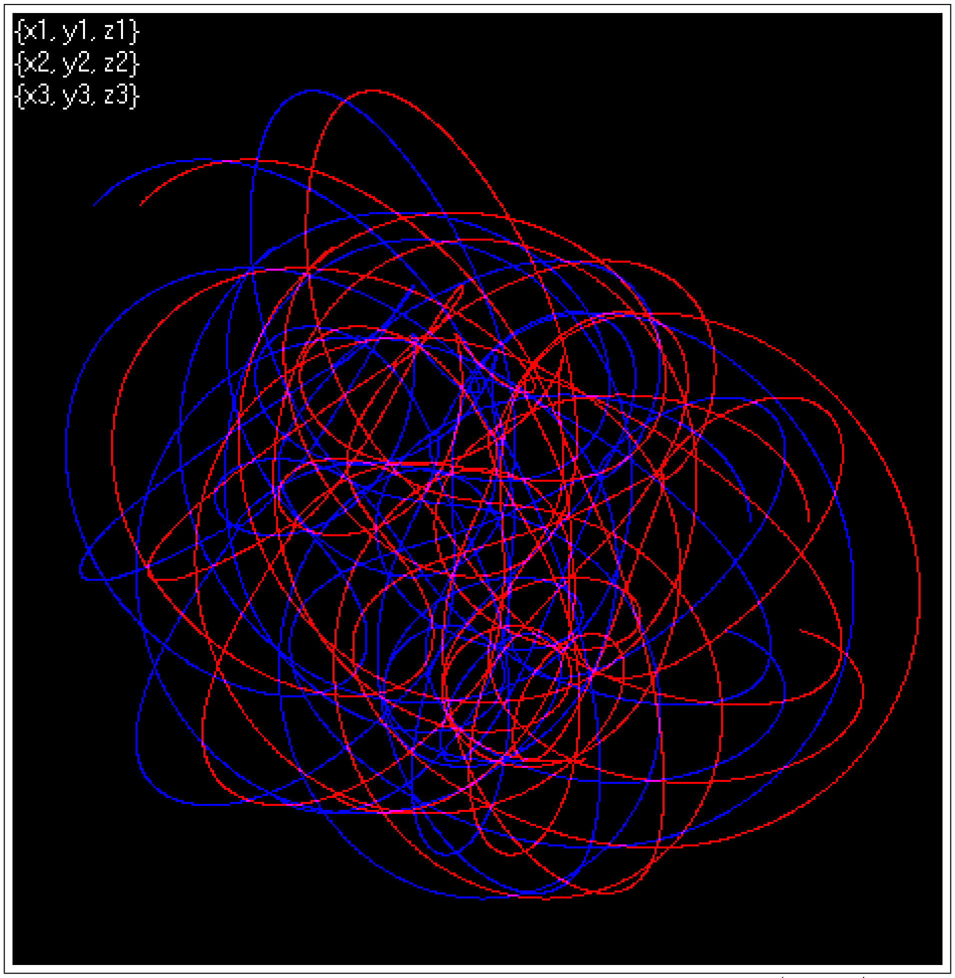

Fig. 6. The three body disturbed into a non-planar motion (Demo/3 bodies/Disturbed/3D or file *3Body3D.scr*)

You can show students the Euler formation (in line) of 3 bodies (files *3EqBodEuler.scr* or *3NonEqBodEuler.scr*) and then demonstrate instability of their motion. Or you can generate the Lagrange setting (circular or elliptic) for the n-body problem (n may be up to 99, but at a PC of an average power try numbers not exceeding 20). Here you may explain to the students that the circular Lagrange motion also exemplifies the simplest case of the *Choreography*.

A solution of the $n-$body problem is called a Choreography solution if all the n bodies move along the same periodic trajectory.

For a long time the circular Lagrange motion was the only known case of Choreography. It was not until 2000 when a non-circular case of choreography was discovered [10]: the amazing 8−shape motion of 3 bodies (Demo/Three Bodies/Choreography or file *Simo.scr*). Many others have been found since then.

Now ask the students a provocative question if they think the Lagrange case of $n-$body motion may be *non-planar*: Say if 4 equal mass bodies are placed into the apexes of the regular tetrahedron (or if the n bodies are positioned at the apexes of the other known regular polyhedra called Platonic bodies). Ask them to suggest the directions for the initial velocities and to try them in the Taylor Center: for a tetrahedron, a cube...

(The correct answer is that a non-planar Lagrange motion is impossible - except the trivial radial collision case, because in 3D space it is impossible to turn a solid non-planar pencil of rays in such a way, that all the angular increments were equal - see Appendix 2).

Finally you may ask the students what are their expectations about the possibility for n equal mass bodies each to move along some cyclic *near planar* orbit so that all the orbits are reciprocally perpendicular planes in 3D space? Then show them the remarkable 4 body orbits inscribed into a cube discovered just recently (by Moore & Nauenberg):

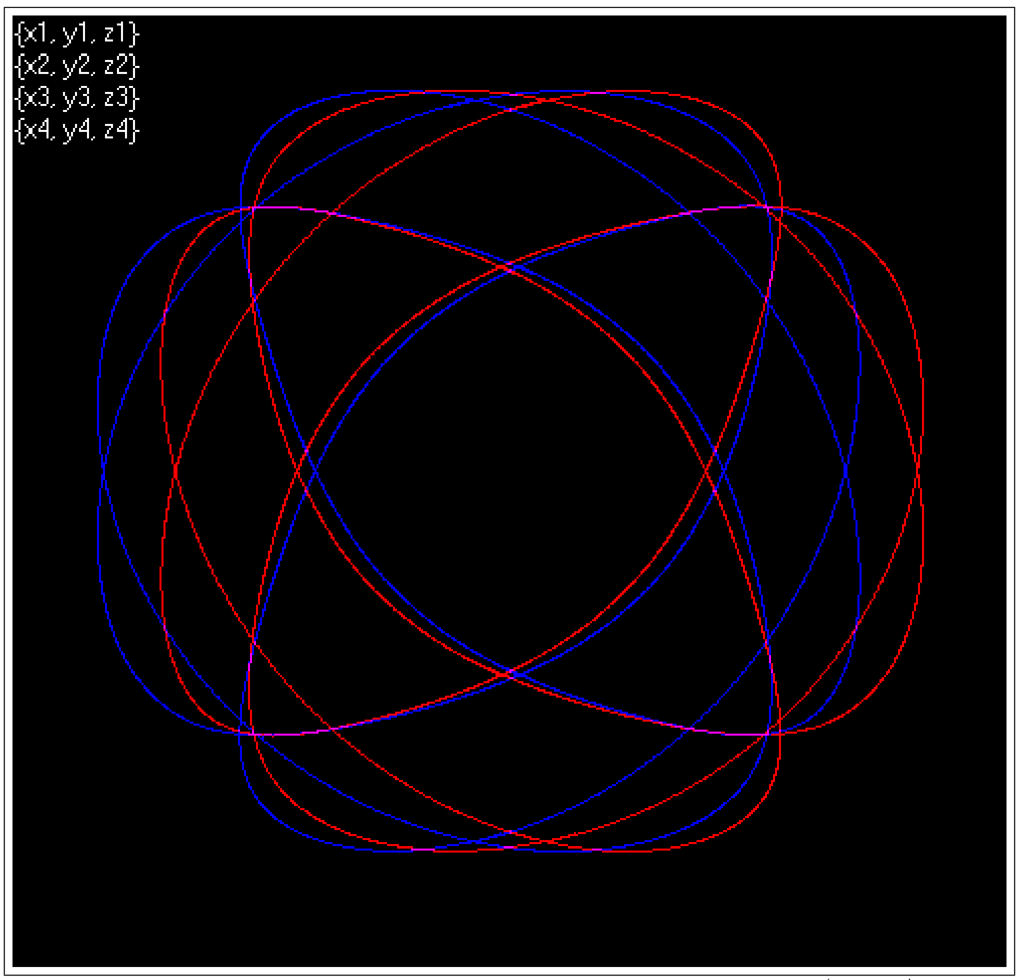

Fig. 7. The 4 body problem, the trajectories inscribed into a cube (Demo/4 bodies/Cube or file *4BodiesCubic.scr*)

In the following sections, we will consider ideas where the Taylor Center provides an illustration or a helpful hint beyond mere graphing the solutions.

4. ODE as the most straightforward tool for generating the Taylor expansion of the solution

In this chapter we are going to deal with concepts such as:

- Numeric series, Taylor series and its convergence radius;
- Points of singularity of a function as the boundaries of its Taylor series' convergence radius;
- Numeric integration of ODEs, the step of integration, its accuracy, and sources of integration errors.

Typically in numeric methods for integration of ODEs the input is a vector of initial values and the routine computing the right hand sides of ODEs. The output is a table of the values of the solution at a grid with a step small enough to satisfy the accuracy requirements.

Any Taylor solver differs from conventional integrators in that the input – an IVP – should be provided not simply as a numeric vector and a subroutine computing the right hand sides, but rather as the arithmetic expressions as such representing the right hand sides in order to enable automatic differentiation.

Correspondingly, the output and interaction of a Taylor solver with other applications has its particularity too. The result is not just tabulated values of the solution, but rather its expansion into the Taylor series (an analytical element), or a sequence of such elements.

The possibility to expand the solution into the Taylor series presumes that the solutions and the right-hand sides of the ODEs are holomorphic. So the behavior of the solution as a real valued function is determined by its properties as a complex holomorphic function (while the derivatives in all subsequent *real valued* ODEs in fact stand for *complex differentiation*)[5]. The Taylor expansion at every point is characterized by its finite (or infinite) radius of convergence equal to the distance to the nearest point of singularity of the solution (usually unknown). Therefore the Taylor Center operates with the so called *heuristic convergence radius* r_e (discussed below) always displayed during the process of integration, while the expansions themselves may be viewed at the Debugging page.

Observing the expansion of the solution may be instructive. The Debugging page of the Taylor Center allows to see the expansion either in numeric form, or as bar diagrams (if the check box Show Taylor profile is checked).

For example, it would be useful to show the students how the expansions differ for the elliptic vs. the circular case of the Lagrange motion. In the elliptic motion example, stop at the slowest and fastest locations of the trajectories to observe how the expansions of the solution dramatically differ, and so does the r_e. The applicable integration step h must always make the fraction $k = \dfrac{h}{r_e} < 1$, (by default $k = \frac{1}{2}$).

[5]In the definition of a derivative of a real valued function at a point, the argument approaches the point along the real axis.

In the definition of a derivative of a complex function at a point, the argument approaches the point along any path in the complex plane.

Existence of a complex derivative is a much stronger condition than existence of the derivative on the real axis only. However the elementary functions we deal with have complex derivatives everywhere (except at a few isolated points of singularity).

The Taylor center can deal only with finite partial sums

$$S_n = \sum_{k=0}^{n} a_k (t - t_0)^k$$

of the Taylor series, whose exact convergence radius (given by the Cauchy–Hadamard formula)

$$R = \frac{1}{\sup |a_k|^{\frac{1}{k}}}$$

usually is unknown. To obtain the *heuristic convergence radius*, the program uses the Cauchy–Hadamard formula [9] based on the available n terms of the Taylor expansion (by default $n = 30$). The comparison Table 1 contains the heuristic vs. exact values of convergence radii for various types of singularities, demonstrating that the heuristic values reasonably fit the exact radii. (Indeed the examples of the solutions were chosen such a way that their points of singularities be available allowing to easily compute the exact convergence radius).

Function	Heuristic r_e		Exact R
	$n = 30$	$n = 100$	
$\frac{1}{1-t}$	0.951	0.984	1
$\frac{1}{(1-t)^2}$	0.803	0.885	1
$\frac{1}{(1-t)^3}$	0.692	0.848	1
$\frac{1}{1-t^2}$	0.971	0.992	1
$\frac{1}{1-t^3}$	0.966	0.991	1
$e^{\frac{1}{1-t}}$	0.696	0.798	1
$\sqrt{1-t}$	1.244	1.110	1
$\ln(1-t)$	1.156	1.058	1
$\tan t$	1.52	1.558	$\frac{\pi}{2} \approx 1.57$
$\frac{t}{e^t - 1}$	5.93	6.133	$2\pi \approx 6.28$

Table 1. Comparison of the heuristic and exact radii in cases of a finite convergence radius

You can ask the students now what to expect for solutions which happen to be entire functions, i.e. those which have an infinite convergence radius. Will the program work out the heuristic radius equal to the machine infinity? Does it mean that an arbitrarily large step of integration may be practically applied?

In fact, the program does work out nearly "infinite" heuristic radius for polynomial solutions, or for certain non-polynomial holomorphic functions. For example, for the system[6]

$$\begin{aligned} x' &= -y^7, \qquad x|_{t=0} = 1 \\ y' &= x^5, \qquad y|_{t=0} = 0 \end{aligned}$$

[6]Courtesy of Harley Flanders

(file *y7x5_in_t.ode*) the Taylor Center computes $r_e = 2.18 \times 10^{1192}$. (To see it, you will have to temporarily change the default radius limit from the value 10 to say 10^{2000}).

Now you can demonstrate the student an effect of a violent bell-shape growth of the Taylor coefficients (or of the Taylor terms at an attempt to apply a big enough step). In order to do it, enter the trivial ODE $t' = 1$ and the function $x = e^{-100t}$ as an auxiliary variable. Compile it and immediately look into the Debugging page to see the bell-shape growth of the Taylor coefficients particular to functions having an infinite convergence radius.

$x = e^{-100t}$ on $[0; +\infty)$ is a typical example of such a function. For $k = 0,\ 1,\ 2,\ 3,\ 4, ...$ its Taylor coefficients $a_k = 1,\ -100,\ 5000, -16667,\ 4.16667 \times 10^6$ violently grow in absolute value reaching the maximum for $k = ...114,\ 115,\ 116, ...$ $a_k = 3.9315 \times 10^{41},\ -3.41869 \times 10^{41},\ 2.94715 \times 10^{41}$.

Beginning from this number and further on, the coefficients decrease in absolute value. For example, for $k = ...268,\ 269,\ 270, ... a_k = 1.09019,\ -0.405277,\ 0.150103, ...$and for $k = ...398,\ 399,\ 400, ... a_k = 2.49241 \times 10^{-68},\ -6.24663 \times 10^{-69},\ 1.561665 \times 10^{-69}$ they finally subside.

The same bell shape pattern may be observed not only for the coefficients a_k proper, but also for the terms $a_k h^k$ in the Taylor expansions $\sum a_k h^k$ of entire functions.

Remark 1. *The Taylor expansion for every (non-polynomial) entire function* $x(t_0 + h) = \sum_{k=0}^{\infty} a_k h^k$ *converges for an arbitrary* h, *with* $a_k h^k \to 0$ *as a consequence. Yet for any given number* k, *there exists such a large step* h, *that the term* $|a_k h^k|$ *will exceed any arbitrarily large value.*

(This is obvious for any term for which $a_k \neq 0$, and there must be infinitely many of them in non-polynomial expansions).

Indeed, the integration step h is a finite part of the convergence radius R (whether it is finite or infinite). Moreover, R is usually unknown, so only the available Taylor coefficients allow to determine the applicable integration step h in order to meet the given error tolerance criteria. The Taylor coefficients allow us to determine the step via the algorithm elaborating the heuristic convergence radius r_e. Table 2 displays values of r_e obtained for various entire functions.

Function	Heuristic r_e		Exact R
	$n = 30$	$n = 100$	
e^{-t}	5.506	17.4	∞
e^{-10t}	0.505	1.746	∞
e^{-100t}	0.059	0.171	∞
e^{-1000t}	0.0058	0.0174	∞
$e^{-10000t}$	0.00055	0.00170	∞
$\sin t$	8.46	32.15	∞
$\sin 10t$	0.922	3.223	∞
$\sin 100t$	0.0917	0.321	∞
$\sin 1000t$	0.0093	0.0314	∞
$\sin 10000t$	0.00092	0.00321	∞
$\frac{\sin t}{t}$	11.753	34.29	∞

Table 2. Comparison of the heuristic radii in cases of an infinite convergence radius

Observe: not only are the radii obtained by the program *finite* (rather than being the machine infinity). They tend to get smaller and smaller for those entire functions, whose beginning terms in the expansion behave violently showing the bell shape pattern. Although computed by the Cauchy formula, the heuristic r_e has nothing to do with the infinity of the actual convergence radius. Indeed, if the order of the method in the program were specified much bigger then the numbers at which the Taylor coefficients subside to disappearance, the computed heuristic radius r_e would approach the machine infinity. Otherwise, what the program outputs as r_e is in fact just a numeric characteristic of the available Taylor coefficients helpful for elaboration of the integration step to satisfy the specified accuracy.

Although theoretically the series' for entire functions converge for any *arbitrarily large* step, practically the number of terms required for achieving high accuracy may be enormous. Also because of the fixed length of the mantissa, the violent growth of the terms of the series causes the loss of accuracy and the so called *catastrophic subtractive error* (explained further).

Fortunately, the algorithm in the Taylor Center works out such a computationally viable heuristic radius for entire functions, that the step splitting in a loop and recalculations (to reach the required accuracy) happen rarely.

5. Is the highest accuracy in the Taylor method always achievable?

In this chapter we are raising the question of accuracy of numeric methods in general, and of the numeric ODEs integration in particular. It would be helpful here to remind the students about the concepts of rounding errors in computation, and about the absolute and relative error tolerances. The chapter will be focused on one particular type of error emerging while computing differences of close numbers, called catastrophic *cancellation* or *subtraction* error.

The distinct feature of the Taylor Method is its potential to achieve the highest accuracy at a given fix length float point representation in a particular computer: the "all-correct-digits" accuracy for the entire integration pass. This potential derives from (but is not guaranteed by) the following two facts.

(1) During *one finite step* integration the "all-correct-digits" accuracy is achievable because of an arbitrary high order of approximation in the Taylor method. For the PC the native highest float point format is a 63 bit mantissa of the 10 byte type *extended*. However, the 64th and all subsequent (virtual) digits are assumed zeros being the source of the *rounding error*. Therefore even after the very first integration step, the "all-correct-digits" result ends up slightly not on the original trajectory. The 2nd and all subsequent steps will inevitably cause the computed trajectories to slide away from the exact trajectories defined by the previous steps. (Whether this sliding process goes more and more away from the original trajectories depends on the property of stability of the given ODEs.)
(2) During *multi-step* Taylor integration process the finite number of steps is minimized because the step size is large. The fewer number of integration steps – the fewer incidents of sliding from the original trajectory due to the rounding error. Ideally, to avoid the sliding at all, we would need to reach the final point in one step.

To specify the "all-correct-digits" accuracy in the Taylor Center, the user has to set the values of the relative error tolerance (for the variables of interest) to something less than 2^{-64} or 10^{-22}.

Beside the inevitable rounding error and possibly intrinsic instability of the ODEs, there is one more effect which may prevent achievement of the "all-correct-digits" accuracy: it is *the catastrophic subtraction* (also called *cancellation*) error. This effect is particular not only for the Taylor method. It may occur in any computations with float point binary numbers having the form $m2^n,\ 2^{-1} \le |m| < 1$.

The mantissa m (in the native machine representation proper to the processor) is usually of a fixed length of 64 bits. (For emulated operations it may be 128 binary digits or something bigger, yet still fixed). The binary exponent n, however, is allowed to be between -4951 and $+4932$. To accurately represent a sum of two numbers having such extreme values of the exponents, the mantissa ought to be something nearly 10000 binary digits.

Because of the limited length mantissa, in the Intel generic float point machine arithmetic

$$1 + 10^{-22} = 1$$

and

$$0.1234567890123456789 - 0.1234567890123456788 = 0$$

Therefore, summation of Taylor expansions having violently growing terms may cause a loss of accuracy, just as a difference of two very close values.

To clarify the concept of catastrophic subtraction error and its fundamental distinction from the rounding error, consider the following two seemingly similar expressions for some differentiable function $f(x)$ when $h \to 0$:

Catastrophic subtraction error	Rounding error
$\lim \dfrac{f(x_0+h) - f(x_0)}{h}$	$\lim \dfrac{f(x_0+h) + f(x_0)}{2}$

The first one inevitably becomes machine zero for small enough h. It therefore never approaches the derivative $f'(x_0)$ if $f'(x_0) \neq 0$, and may differ from it dramatically. The second one always approaches $f(x_0)$ and may differ from it only in the 64th binary digit.

In ODEs the catastrophic subtraction error emerges when the integration pass approaches a point of singularity of the ODEs or some other special points. Such examples are provided in the Chapter 5 "Tricks and traps of Automatic Differentiation" in the User Manual.

6. Regular solutions of singular ODEs.

This chapter provides a ground for a discussion about points of singularities in ODEs and their solutions, and the pre-loaded examples (see the User Manual) are instructive for such a discussion.

First, advise the students about the distinction between points of singularity of the *solution* vs. points of singularities of the *ODEs* as such in their phase space. For example, the holomorphic function $x = \dfrac{1}{1-t}$, or $y = \tan t$ have singularities respectively at point $t = 1$ and point $t = \dfrac{\pi}{2}$. However, each of them satisfies a polynomial ODE ($x' = -x^2$ and $y = y^2 + 1$), whose every finite point of the phase space is regular indeed.

And vice versa, the right hand sides of ODEs may happen to be singular at particular points of the phase space. For example the ODE $x' = \dfrac{ax}{t}$ is singular when $t = 0$. Yet its solution $x = t^a$ is regular for any natural (non-negative integer) parameter a. This solution also happens to satisfy a regular ODE $x' = at^{a-1}$.

However, there exist regular solutions (in fact entire functions) which at certain points can satisfy no explicit polynomial ODE, nor any rational ODE with the non-zero denominator [7]. For example, such functions are $x = \dfrac{e^t - 1}{t}$, $x(0) = 1$, or $y = \dfrac{\sin t}{t}$, $y(0) = 1$, or $z = \cos\sqrt{t}$. All the above mentioned functions are holomorphic at all finite points. The specialty of the point $t = 0$ for them is in that the explicit Taylor method (i.e. the explicit formulas for evaluation of the derivatives implied by the Taylor method) is not applicable at this special point. (The elementariness of these functions is possibly violated at this point [7]). Therefore some other – implicit ODEs and implicit formulas – must be used at such points, generating the respective Taylor expansions. (For many classical functions these expansions in the special point are known).

The feature of the recent version of the Taylor Center is that it can integrate some ODEs even at the points of singularity of these ODEs – providing that the Taylor expansions in the special points are known from other sources (the above mentioned samples are pre-loaded and their description provided in the User Manual).

The following chapter may serve as a good illustration to the statement of Borrelli and Coleman [2]:

"*Using a numerical solver to produce an approximate solution of an initial value problem is not a mindless operation; It is not merely inserting an IVP into a package solver and out pops a decent approximate solution*".

7. Weird examples of real valued solutions vs. their complex properties.

Usually we expect that even simple looking ODEs (polynomial or rational) may happen to have a solution that is not "simple" at all. The following sample however exemplifies the opposite situation.

Consider the initial value problem:

$$x' = -\sqrt{x}, \qquad x|_{t=0} = 1.$$

In the neighborhood of $t = 0$, its solution is a polynomial $x = \frac{1}{4}(t-2)^2$. Indeed, the solution itself (as a polynomial) exists and may be continued analytically into all points of a complex plain, but the right hand side $-\sqrt{x}$ of the ODE cannot. Here the right hand side is deliberately chosen to be the negative branch of the 2-branched function $\sqrt{x}$. Therefore, this ODE may be satisfied only by the *decreasing* horn of the parabola $x = \frac{1}{4}(t-2)^2$ - the example considered in the User Manual to illustrate various strange effects which may be encountered during a naïve attempt of integration of such an ODE. (Fig. 8).

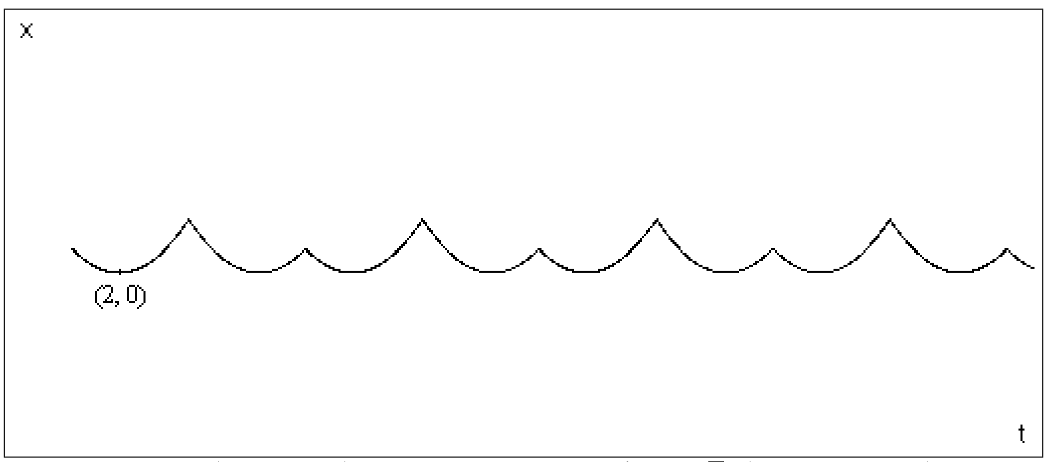

Fig. 8. A naïve (and wrong) attempt to integrate $x' = -\sqrt{x}$ (file *strange.ode*). This piecewise curve (instead of a parabola) is an artefact of the program.

The other remarkable example[7] is the function $x = \cos\sqrt{t}$, also pre-loaded and integrable in the Taylor Center: both for negative and positive t. Indeed, this version of the Taylor Center cannot deal with complex variables directly. Observe: in spite of that $\sqrt{t}$ becomes imaginary for $t < 0$, the cosine of purely imaginary values is real (and bigger than 1 because $\cos it = \cosh t$).

It is worth noting a fundamental fact of automatic differentiation [7], that ODEs whose right hand sides contain non-rational elementary functions (transcendental or algebraic) may be equivalently transformed into larger systems of ODEs whose right hand sides are rational only. The function $\cos\sqrt{t}$ is elementary (except at the point $t = 0$). Hence the problem may be treated as though it has real valued variables as soon as we find a rational ODE satisfied by this elementary function.

[7] Courtesy of George Bergman

There exists a general way for elimination of non-rational functions in ODEs [7]. In this particular case, differentiate x two times

$$x' = -\frac{\sin\sqrt{t}}{2\sqrt{t}};$$

$$x'' = -\frac{(\cos\sqrt{t})\dfrac{2\sqrt{t}}{2\sqrt{t}} - (\sin\sqrt{t})\dfrac{1}{\sqrt{t}}}{4t} = -\frac{x+2x'}{4t},$$

obtaining the required rational ODE:

$$x'' = -\frac{x+2x'}{4t}, \qquad x|_{t=0} = 1, \qquad x'|_{t=0} = -\frac{1}{2}.$$

This ODE still has $t = 0$ as a point of singularity indeed (because this is the *unremovable* or "*regular*" singularity [7] of the function $x(t)$). For it the Taylor expansion at $t = 0$ is easily available and pre-loaded into the Taylor Center, so that the program can integrate this ODE and graph the solution in both directions.

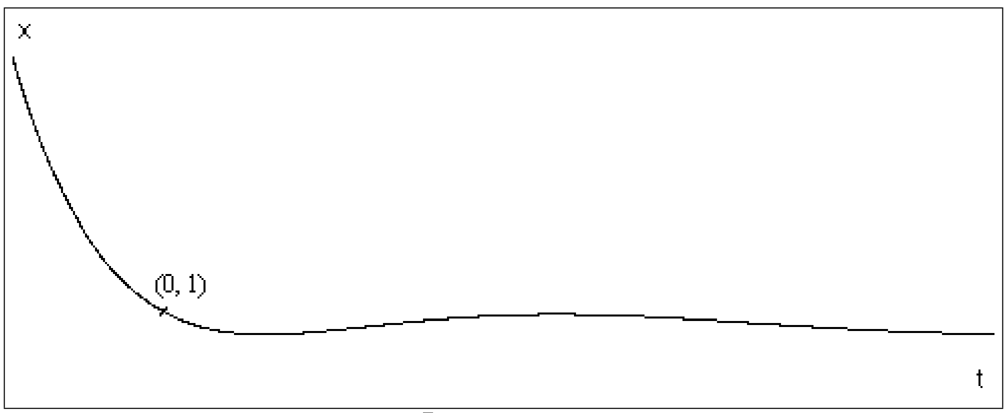

Fig. 9. Function $x = \cos\sqrt{t}$ (file *SpecPoints\cos(sqrt(t))-2.ode*)

8. Conclusions

The Taylor Center may assist in teaching elementary and advanced ODEs. Moreover, it helps also in a few other mathematical disciplines such as complex analysis, general and celestial mechanics, numerical methods, and indeed Automatic Differentiation (in the frame of the Unifying View [7]).

In the simplest and straightforward way, the Taylor Center helps to teach due to its sophisticated dynamic graphics. The teachers therefore can immediately illustrate examples of ODEs and examine the effects of their parameters. From the very beginning the article offered several such examples occurring in the basic courses. Indeed, teachers will be able to enter their own examples of interests.

However possible applications of the Taylor Center are not limited only by the basic ODEs. It helps even more to illustrate various ideas in the advanced courses, as it was shown in the article. Additionally, it is indispensable for numeric experiments in research and advanced student projects because of its potential to achieve the all-correct-digits accuracy in the processes of integration, to obtain the roots of the solutions, to explore their convergence radii and expansions, and indeed to view the real time dynamics.

9. Appendix 1

The full list of features of the Taylor Center

With the current version of the Taylor Center you can:

- Specify and study any Initial Value Problem presented as a system of explicit first order *elementary* ODEs (the standard format) with numeric and symbolic constants and parameters;
- Perform numerical integration of IVPs with an arbitrary high accuracy along a path without singularities, while the step of integration remains finite and does not approach zero (presuming the order of approximation or the number of terms may increase to infinity, and the length of mantissa is unlimited);
- Apply an arbitrary high order of approximation (by default 30), and get the solution in the form of the set of analytical elements - Taylor expansions covering the required domain;
- Study Taylor expansions and the radius of convergence for the solution at all points of interest up to any high order (the terms in the series must not exceed the maximum value of about 10^{4932} implied by the Intel processor generic implementation of the real type *extended* as10-bytes with 63-bit mantissa);
- Perform integration either "blindly" (observing only the numerical changes), or graphically visualized. Perform integration for a given number of steps, or until an independent variable reaches the terminal value, or until a (former) *dependent* variable (now a new independent) reaches a terminal value (as explained in the next item);
- Switch integration between several states of ODEs defining the same trajectory, but with respect to different independent variables. For example, it is possible to switch the integration in respect to t to that by x, or by y to reach the terminal value of a former dependent variable (x, or y). In particular, if the initial value is nonzero and the terminal value is set to zero, the root (the zero) of the solution may be obtained directly without iterations.
- Integrate piecewise-analytical ODEs;
- Specify different methods to control the accuracy and the step size;
- Specify accuracy for individual components either as an absolute or relative error tolerance, or both;
- Graph curves (trajectories) in color for any pair of variables of the solution (up to 99) on one screen - either as plane projections, or as 3D stereo images (for triplets of variables) to be viewed through anaglyphic (Red/Blue) glasses. The 3D cursor with audio feedback (controlled by a conventional mouse) enables "tactile" exploration of the curves virtually "hanging in thin air";
- Play dynamically the near-real time motion along the computed trajectories either as 2D or 3D stereo animation of moving bullets;
- Graph the field of directions - actually the field of curvy segments, whose length is proportional to the radius of convergence.

- Explore examples such as the problem of Three and Four Bodies supplied with the package. Symbolic constants and expressions allow parameterization of the equations and initial values to try different initial configurations of special interest.
- Automatically generate ODEs for the classical Newtonian $n-$body problem for n up to 99 and then integrate and explore the motion. For $n = 99$, there are 298 ODEs, 19404 auxiliary equations, compiled into over 132000 variables and over 130000 AD processor's instructions: a "heavy duty" integration!
- Integrate a few special instances of singular ODEs having regular solutions near the points of the "*regular singularities*" [7].

In particular, the Demo version of this software comes with numerous instructive ODEs including the Choreography for the Three Body motion - a figure eight-shaped orbit, discovered in 2000 by Chenciner and Montgomery [10]. Users can "feed" the ODEs of their interest into the Taylor Center, integrate them, draw the curves, and play the motion in the real-time mode all in the same program. Another example describes the four body non-planar trajectories inscribed in a cube - a recent discovery by Cris Moore and Michael Nauenberg [11].

The Taylor Center is a 32-bit software which runs under both 32- and 64-bit Windows (up to Windows-7). The executable module is only 1 Mb. As a 32-bit application, the program can use no more than 4 Gb of available memory for variables and their expansions - the limit far exceeding any practical needs - see the memory requirements below. (Now when the new 64-bit Delphi compiler became available, the project is recompiled into a 64-bit application doing away with this 4 Gb limitation).

The memory consumption depends on the number of variables *VarNum* (a function of the number of ODEs and their complexity) and on the specified *Order* of approximation. If the expansions are not stored, the program takes $2 \times VarNum \times Order \times 10$ bytes of memory. If the expansions in P points are stored, it additionally requires $P \times VarNum \times Order \times 10$ bytes.

A benchmark for the 10 body planar problem comprised of 41 ODEs, $45 + 90 = 135$ auxiliary equations, parsed into 811 AD instructions, takes 38 s for 10000 steps of integration (or 3.8 ms per step) at 2.4 GHz Pentium.

Generally for each system of ODEs there exists such a small value of the accuracy tolerance, that at this high accuracy the Taylor methods beats any fixed order method due to the unlimited order of approximation in the Taylor method (this is known since Moore in 1960s).

10. Appendix 2

Impossibility of the non-planar Lagrange motion

Consider the earlier given definition of the Lagrange case for the n-body problem hypothetically applied to one of the five regular polyhedra in 3D. Let call it a *non-planar Lagrange case.*

LEMMA 1. *If a non-planar Lagrange case with the masses at the apexes of a regular polyhedron is possible, the pencil of rays from the center to the apexes in this regular polyhedron must be rotatable in such a way that the angular increments are equal for all the rays.*

Proof. Absolute values of the initial velocities must be equal and inclined at the same angle to the radii at all the apexes. Therefore, they must cause equal angular increments. □

The issue of possibility of a non-planar Lagrange motion therefore relies on a purely geometric question: whether a solid non-planar pencil of rays is rotatable preserving all its angular increments (no regularity of the pencil is now assumed). A *planar* solid pencil of rays (Fig. 10) *is* definitely rotatable this way in its plane.

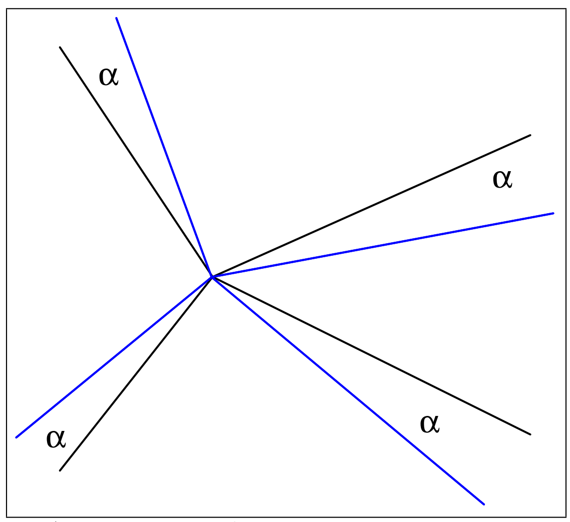

Fig. 10. A solid pencil of rays in a plane turned at angle α

Now consider an arbitrary non-planar pencil of rays rotating in 3D around the point of apex. According to Euler's Theorem, the motion of a rigid body about a fixed point is equivalent to the rotation of the body about an instantaneous axis of rotation.

Let this instantaneous axis be OQ (Fig. 11).

Lemma 2. *During rotation around an axis of a pencil of rays, a ray with a bigger angle to the axis has a bigger rotational angular increment.*

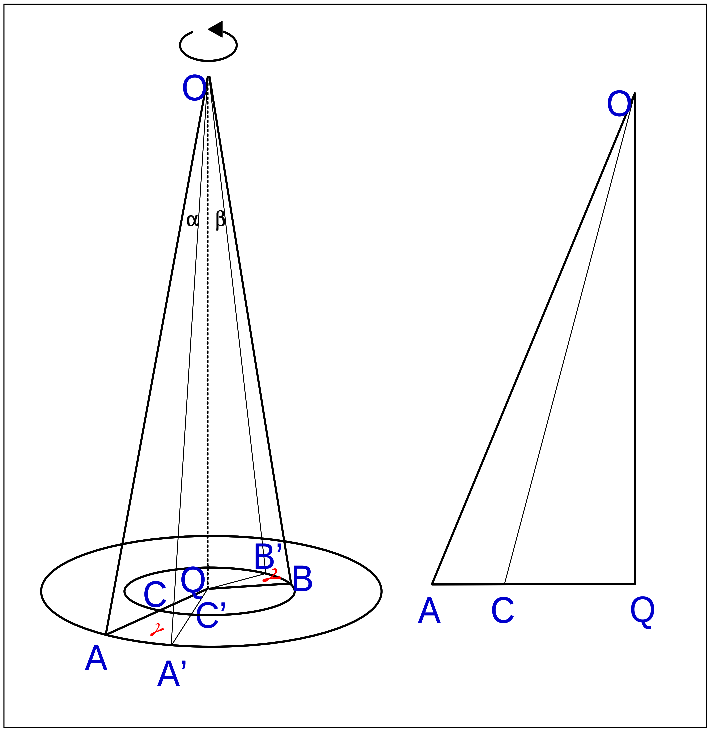

Fig. 11. Rotation of a solid bunch of rays in 3D

Proof. Let the ray OA be at angle α to the axis OQ, the OB - at angle β to the axis, and $\alpha > \beta$. Let the pencil of rays turn around the axis at angle γ so that $\angle AQA' = \angle BQB' = \gamma$, while $CC' = BB'$. Observe that

$$\frac{CO}{CQ} > \frac{AO}{AQ}$$

because $\angle OCQ > \angle OAQ$. Therefore

$$\frac{CO}{AO} > \frac{CQ}{AQ} = \frac{CC'}{AA'}$$

(due to similarity of $\triangle CQC'$ and $\triangle AQA'$), and

$$\frac{CC'}{CO} < \frac{AA'}{AO}$$

meaning that $\angle BOB' < \angle AOA'$. □

Conclusion 1. *A rotation of a non-planar pencil of rays preserving all the angular increments in the 3D space is possible if and only if the rays belong to the surface of a direct circular cone.*

Proof. Follows from the Lemma. □

The Conclusion may be also proved in analytical geometry. Denote the rays as vectors $\mathbf{a}_k$, which rotate around an unknown axis $\mathbf{x}$. In order that axis $\mathbf{x}$

be inclined to each of the vectors $\mathbf{a}_k$ at the same angle, all the cosines expressed through the scalar product must be equal to the same unknown value α:

$$\frac{(\mathbf{a}_k, \mathbf{x})}{|\mathbf{a}_k| \cdot |\mathbf{x}|} = \alpha. \tag{10.1}$$

If $\alpha \neq 0$, this non-linear system expresses the fact that all vectors $\mathbf{a}_k$ belong to a direct circular cone. Otherwise if $\alpha = 0$, (10.1) means that the axis $\mathbf{x}$ must be perpendicular to all vectors $\mathbf{a}_k$, which is possible only if $\mathbf{x}$ belongs to a space of dimension 4 or higher.

Indeed, in no of the Platonian regular polyhedra the pencil of rays from the center to the apexes of the polyhedra belongs to a direct circular conic surface. Therefore, there exists no way to orient the vectors of the initial velocity at the apexes of the regular polyhedra so that the bodies preserve the initial formation during the motion - unless all these vectors are collinear with the respective radii. If this is the case, the motion takes place along the radii, and it either ends up with a collision, or the bodies escape into infinity.

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