Physics for Computer Science Students

Lecture 2: Modeling of physical processes

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1 Modeling

During the lecture some fundamental facts from the modeling theory are given. The connection of models with the real world is shown and next, some examples from physics are discussed.

Physical models are mainly formulated in the form of the systems of differential equations, so at the end of the lecture some simple methods of numerical solving of differential equations are presented. These methods can be used for the computer simulations in which the physical laws are adopted.

Citations:

Cum Deum calculat, fit mundus (G.W. Leibniz)

Computo ergo sum (variation from De'Cart)

Everything should be made as simple as possible but not simpler (A. Einstein)

Definitions:

Modeling is: research of the model properties in itself

Simulation **is:** experimenting with the model with the goal to predict the dynamic behaviors of the original

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Is the reality able to be modeled?

The question has an philosophical character. The answer given by Laplace says that the model of the system has to be a certain simplification for one be able to say something about the fundamental features of the studying object. The lack of knowledge about the reality should be a reason to more intensive research.

Laplace demon

Laplace strongly believed in the causal determinism, which is expressed in the following quote from the introduction to the Essai:

"We may regard the present state of the universe as the effect of its past and the cause of its future. An intellect which at a certain moment would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes."

Pierre Simon Laplace, Essai philosophique sur les probabilities, Paris, 1814

It should be noted that the existence of this hypothetical intellect depends on a number of assumptions:

1. It is possible to know all the information about the past and present states of the universe (contra some interpretations of both Quantum Mechanics and Relativity).

2. It is possible to know all the natural laws governing the universe.

3. These natural laws are fully deterministic, computable and do not underdetermine the physical outcomes.

4. That an "intellect" could be capable of computing the future states of the universe faster than they actually occur.

5. That such an intellect could exist without being inside the universe.

6. That such knowledge would not change or alter the universe in such a way that the state of the universe would change.

Laplace's demon met its end with early 19th century developments of the concepts of irreversibility, entropy, and the second law of thermodynamics. In other words, Laplace's demon was based on the premise of reversibility and classical mechanics; thermodynamics, i.e. real processes, however, are, under current theory, thought to be irreversible.

1.1 Model and its definitions

Representation of something, either as a physical object which is usually smaller than the real object, or as a simple description of the object which might be used in calculations.

Cambridge International Dictionary of English (1995)

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By the mathematical model the system of equations describing qualitatively the phenomena included into the physical model is understand.

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Mathematical model: the operator H_t transforming the given input signal $X(t)$ (input data) into the output signal $Y(t)$ (output data) of a given object, i.e.:

$$Y(t) = H_t\, X(t)$$

Cezary Szczepaniak, Podstawy modelowania systemu, Wydawnictwo Naukowe PWN (1999)

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Mathematical model: the set of mathematical relations describing the physical phenomena, being *the subjects of the physical laws, in the unambiguous, consistent and stable ways.*

Andrzej Krawczyk, Podstawy elektromagnetyzmu matematycznego, (2001)

###

- **The model is unambiguous ,** if for the one input data the only one answer is generated.
- **The model is consistent,** if all its elements are of the same nature.
- **The model is stable,** if it is not sensitive to the small disturbaces of the input data or steering parameters, and if these disturbaces cause on the output the changes of the same order.

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Modelling is the central element of the scientific reasning.

A. Rosenbluth i N. Wiener

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Dealing with the modelling, one has to take into account many factors, like:

- the level of the simplification,
- the needs of the experiment,
- the validity,
- the tractability,
- the credibility,
- the aim.

In the first step one has to define the elementary components of the model (e.g. elements of the electrical circuits). Every component is described by the descriptive variables, classified as

- input variables,
- state variables,

- output variables.

1.2 Model and reality

The set of the all descriptive variables allows to plan the experiment. For the same real system many different experiments can be carried out. E.g. in the one experiment with the electrical circuit voltages and currents in the all elements of the circuit can be studied. In the other experiment one can measure the temperatures of these elements and the temperature distribution in the circuit. It is clear that different experiments need different models. Every experiment leads to a certain simplified model as it is shown in Fig. 1.

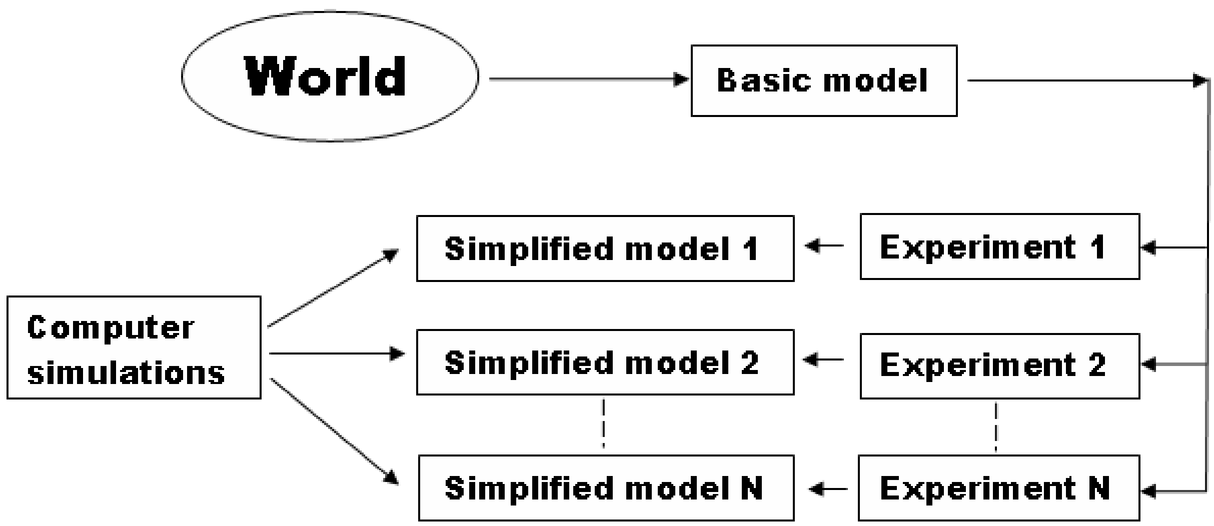

Figure 1: World and its models

Basic model describes the real world exactly. Such models in general do not exist.

The formulated job and the technological restrictions (e.g. the eficiency of the computer used for simulations) in the natural way limit the number of the possible simplified models. If there are more then one simplification fulfilling the criteria, one has to apply other choice rules, e.g. modelling costs.

Model validation is one of the main problems of the modelling and the computer simulations. Let us consider the real dynamical system and its model. Let S be the modelling operation (tranfer fro the real system to the model). Let $x(t)$ describes the system state at the instant t, $y(t)$ - output data, and f - transition function, mapping the state $x(t)$ and the input data in the time interval $[t,\ t+h]$ into the new state $x(t+h)$. The ame symbols with the subscript S desribe the model quantities. The given model is choosed properly if the diagram in Fig. 2

comutes.

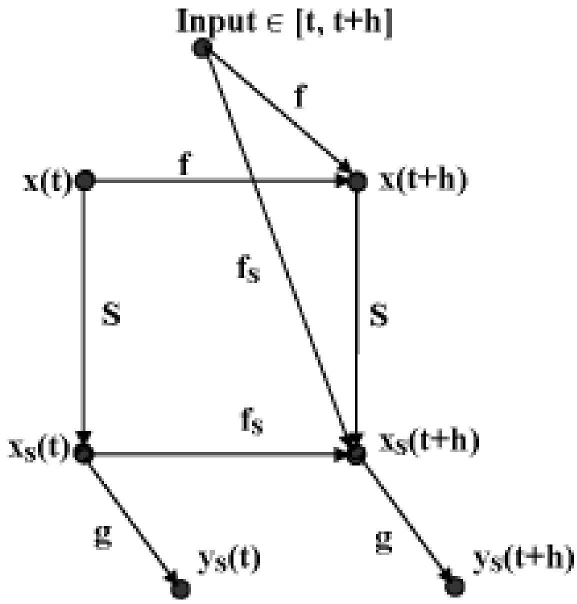

Figure 2: Comutation

The given above definition of validation of the model is difficult in application in the real situations. The more useful approach is the input-output validity reperesenting by the diagram in Fig. 3.

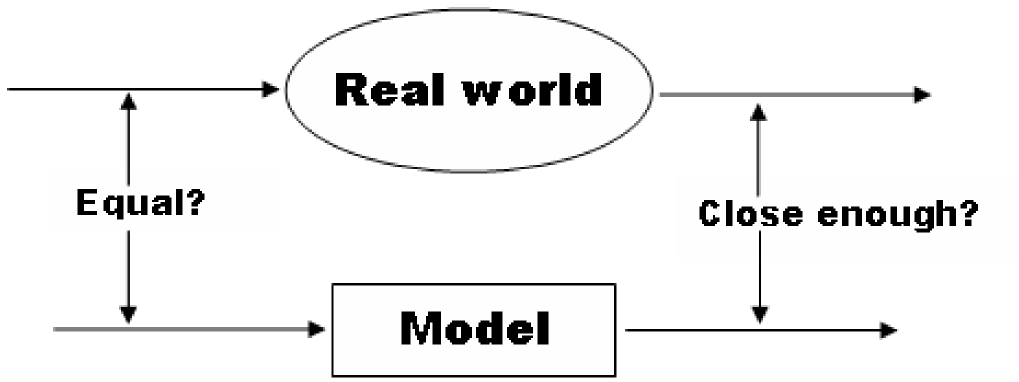

Figure 3: Validity of a model

Let us note that the every approximation of the real system continuous in time by the model with the discrete time is not valid.

Example 1. In the real process disturbances can appear in time intervals smaller than the time step of the time discretization, so they are not detected by the discrete model.

Erroneous models relatively often result from the wrong assumptions. One has to take care constructing simplified models because they can produce incorrect physical outputs.

Model tractability

It is well known, that some problems having beautiful mathematical description can not be solved with the help of available methods. The same concerns models being assigned to the computer simulation. They are either too time consuming or too costly.

The model or the simulation task is untractable, if the complexity of calculations increase exponentially as the number of the descriptive variables grows up. Calculation complexity can be defined as the minimal cost that assures that the answer for the question (simulation task) will be obtained below the assumed error level.

Example 2. *The most often citied example of such a problem that can not be solved is the (travelling) salesman problem. Another problem: computer simulation of the come back to Earth the space shuttle (problem from the dynamics of fluids).*

Josef F. Traub, Henryk Woźniakowski, Breaking intractability, Scientific American, January 1994

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Model credibility

The model is crdible, if the user believes that it is correct and useful. It means, that the model can be correct but not credible. Of course, credible model can be not correct.

The best way to construct the credible models is to join the prospective user into the of the model process construction.

2 Examples from physics

2.1 Lagrange formalism

Lagrange formalism is one of the most powerful technics of describing the physical phenomena. It relies on writing down the model in the form of one function, called Lagrangean. It is easy to show, that from Lagrangean the equations of motion can be derived. If the Lagrangean is invariant with respect to a certain group of transformations (in the classical mechanics it is the Galilean group of translations and rotations in the Cartesian space), then the Noether theorem can be used and the all conservation laws,such as energy conservation law, momentum conservation law, moment of momentum conservation law, ...

In order to find the equations of motion, i.e. the so called Euler-Lagrange equations, one has to find the extremum of the Lagrange functional. To make it more clear some remarks about the variational calculus will be made. We mention about that in order to show that in physics there are quite well developed and beautiful methods of construction and analysis of the models of the physical systems. Lagrange formalism is also very important from the point of view of the computer simulations, becuse it gives the possibilty to study the behaviour of the system either by solving the system od Euler-Lagrange equations or by finding the exteremum of the Lagrange fuctional, using e.g. the Ritz method.

Variation of a function

The variation $\delta y(x)$ of the function $y(x)$ is called the difference between the given function $y(x)$ and a "near" to it the function $y_1(x)$:

$$\delta y(x) = y_1(x) - y(x). \tag{1}$$

The first variation of the function

$$\delta F(y,\ y',\ x) = \frac{\partial F}{\partial y}\delta y + \frac{\partial F}{\partial y'}\delta y', \tag{2}$$

where

$$\delta y' = \frac{d\delta y}{\mathrm{dx}}. \tag{3}$$

The first variation of the functional

$$\delta I[\gamma] = \int_a^b \delta F(y,\ y',\ x)\,\mathrm{dx}. \qquad (4)$$

The Hamilton's principle

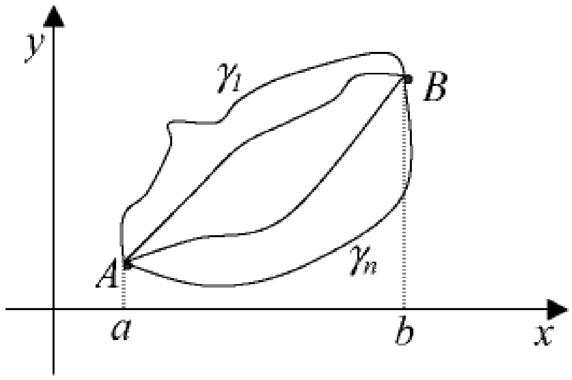

Figure 4: Reference curves of the motion

The Hamilton's principle says that out of the all possible trajectories γ_i of the transition of the system from the point A to the point B only this one is realized, which minimize the Lagrange functional. The condition the fuctional arrives its mininimum is the vanishing of the first variation of the functional (see Eqn (5)).

Euler-Lagrange equation

$$\delta I = 0 = \int_a^b \left\{ \frac{\partial F}{\partial y} - \frac{d}{\mathrm{dx}} \frac{\partial F}{\partial y'} \right\} \delta y\,\mathrm{dx}. \qquad (5)$$

Eqn (5) has to be fulfiled for an arbitrary variation of the variable y, so the wxpression under the integral has to vanish, and these considerations give us the E-L equations.

Second variation

$$\delta^2 I = \frac{1}{2}\int_a^b \left\{ \frac{\partial^2 F}{\partial y^2}(\delta y)^2 + 2\frac{\partial^2 F}{\partial y\,\partial y'}\delta y\,\delta y' + \frac{\partial^2 F}{\partial y'^2}(\delta y')^2 \right\} \mathrm{dx}. \qquad (6)$$

when $\delta^2 I < 0$ - maximum; when $\delta^2 I > 0$ - minimum. Second variation gives us the condition for the extremes.

Noether theorem

If the equations of motion are the Euler-Lagrange equations for a certain functional I and if this functional is invariant for a certain group of of transformations, then there exists a certain number of the conservation laws. The number of the resulting conservation laws is exactly the same as the number of the parameters of the symmetry transformation group of the functional I.

Emma Noether, 1916

Some examples

Invariance with the respect to

- time translations gives energy conservation law: $E_k + V$ = const;
- space translations gives momentum conservation law: $\boldsymbol{p}$ = const;
- rotations gives moment of momentrum conservation law: $\boldsymbol{r}\times\boldsymbol{p}$ = const.

2.2 Plane simple pendulum

The simple (mathemathical) pendulum is the mechanical system consisting of the material point (geometrical point with the assigned mass m) located in the uniform gravitational field (force field) and with constrains allowing the motion of this material point around a certain another geometrical point.

If the constrains put on the motion of the pendulum or the specific initial conditions cause that the pendulum during its motion stays always in the same vertical plane, then the pendulum is called the plane pendulum.

Equation of the pendulum

$$m\,\ddot{s} = F_z\,\frac{d\,y}{d\,s}, \tag{7}$$

where s - length of the arc, (generalized coordinate); $F_y = -m\,g$ - y-component of the gravitational force (see Fig. 5).

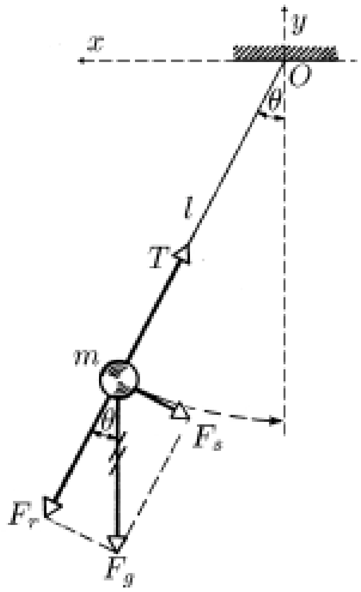

Figure 5: The simple pendulum

The motion is harmonic , if

$$\ddot{s} + \omega^2\,s = 0, \tag{8}$$

it is that

$$\frac{d\,y}{d\,s} = \frac{\omega^2}{g}\;s, \tag{9}$$

and the integral of that equation equals

$$y = \frac{1}{2}\frac{\omega^2}{g}s^2. \tag{10}$$

Parametrization

Let us introduce the new generalized coordinate φ using the equation: $r = 4R\sin(\theta/2)$. It follows that

$$y = R(1 - \cos\theta). \tag{11}$$

where

$$R = \frac{1}{4}\ \frac{g}{\omega^2},$$

$$\left(\frac{d\,x}{d\,s}\right)^2 + \left(\frac{d\,y}{d\,s}\right)^2 = 1,$$

that is

$$\frac{d\,x}{d\,s} = \sqrt{1 - \frac{\omega^4}{g^2}\ s^2} = \cos\frac{\theta}{2},$$

and

$$x = R(\varphi + \sin\theta). \tag{12}$$

Equations (11) i (12) are the paramertic equation of a *cycloid*

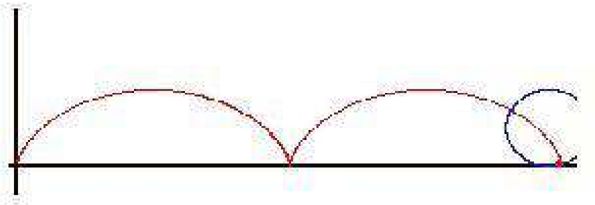

Figure 6: Cycloid

We are looking for the solution of Eqn (8) in the form

$$s = A\cos\omega t + B\sin\omega t, \quad \text{or} \quad s = C\sin(\omega t + \delta), \tag{13}$$

with the initial conditions

$v_0 = \dot{s}\,|_{t=0}$, and $s_0 = s|_{t=0}$. In this case

$$s = s_0\cos\omega t + \frac{v_0}{\omega}\sin\omega t, \tag{14}$$

or

$$s = \sqrt{s_0^2 + \left(\frac{v_0}{\omega}\right)^2}\,\sin\left[\omega t + \mathrm{arctg}\left(\frac{s_0\omega}{v_0}\right)\right]. \tag{15}$$

The *motion is isochronic*, if the period of vibrations does not depend on the amplitude

$$T = \frac{2\pi}{\omega} = 4\pi\sqrt{\frac{R}{g}}. \tag{16}$$

The cycloid is a *brachistochron* - the time of sliping down is minimal.

Let us consider the circular motion.

$$y = R(1 - \cos\theta). \tag{17}$$

Equation of motion takes the form

$$R\ddot{\theta} = -g\sin\theta. \tag{18}$$

If θ is small, then $\sin\theta \approx \theta$, and

$$\ddot{\theta} + \omega^2\theta = 0, \quad \omega = \sqrt{\frac{g}{R}}. \tag{19}$$

For small inclinations, vibrations of the circular pendulum are isochronic.

For big inclinations solutions of the Eqn. (18) are given by the elliptic integrals of the first kind.

Elliptic intgral of the first kind

$$F(k, \psi) = \int_0^{\psi} \frac{d\varphi}{\sqrt{1 - k^2\sin^2\varphi}}. \tag{20}$$

The integrals of such typen can be solved numerically only, and the results are given in the mathematical tables.

It was shown what are the real equations describing the motion of a simple pendulum and where the simplifying assumptions are made. For computer models usually the simplified models are satisfactory. Nowadays the very powerfull computers are available, so the more complicated models can be considered as well.

3 Numercal solving of differential equations

3.1 Euler method

Let us consider the differential equation

$$\frac{d\,y}{d\,x} = f(x,\,y), \qquad y(x_0) = y_0. \tag{21}$$

There are many numerical recipes how to solve such equations, and we demonstrate the simplest which can be easy implemented. Our goal is to show during the laboratory exercises how to obtain the spectacular visualizations making use of the physical laws. the more important role will be given to the efficiency of the solutions then to the numerical accuracy. The more information about the numerical methods of solving the differential equation van be find elsewhere.

Euler method (method of tangents)

Let us consider the one dimensional case. The domain of the solution $y(x)$ of the differential equation (21) is divided into segements of the length h. The formula below (22) is the simple consequence of the definition of the derivative, as the limit of the difference quotient (here the limit is omitted)

$$y_{n+1} = y_n + h\,f(x_n,\,y_n), \quad n \geqq 1. \tag{22}$$

this method is very simple and is well-suited to our needs. Unfortunately it is weak convergent. There exits the modification of the Euler method with better convergence. It is defined by the formula (23)

$$y_{n+1} = y_n + \frac{1}{2}h\,(\,f(x_n,\,y_n) + f(x_n + h,\,y_n + h\,f(x_n + y_n)), \tag{23}$$

Error of the method is of the order $O(h^2)$.

Midpoint method

The midoint method was constructed as the generalization of the Euler method: the expansion into the Taylor series takes into account the one term more. The iterative formula obtains the following form:

$$y_{n+1} = y_n + h\, f(x_n + \frac{h}{2},\, y_n + \frac{h}{2}\, f(x_n,\, y_n)), \qquad n \geqq 1. \tag{24}$$

Error of the method is of the order $O(h^2)$. The midpoint method is often considered as the one of the Runge-Kutta methods.

3.2 Runge-Kutta methods

The Runge-Kutta method of solving the differential equations is very well adapted for the computer applications. It is a case especially if one needs to learn about the quality of the phenomenon studied and the precision of the calculations is not very important. The basis of the RK method is Eqn. (25).

$$y_{n+1} = y_n + \sum_{i=1}^{s} w_i K_i, \tag{25}$$

where $K_1 = h\ f(x_n,\ y_n)$, and

$$K_i = h\, f(x_n + a_i\, h,\ y_n + \sum_{j=1}^{i-1} b_{\mathrm{ij}}\, K_j, \qquad i > 1,$$

$w_i,\ a_i,\ b_{\mathrm{ij}}$ - constants, and s - order of the Runge-Kutta method.

When selecting the integration step h the stability and the precision of the solution should be taken into account, and one one has to notice that

- Runge-Kutta methods are not stable and h should be chosen in a way to assure the reasonable stability;
- the precision of the obtained result depends on the methodological error and the round errors. Usually the round errors are not very important and the methodological error is the main component of the total error.

3.2.1 Second order methods s = 2

For $s = 2$ one has the following relations between the constants:

$$w_1 + w_2 = 1, \quad \alpha_2 w_2 = \frac{1}{2}, \quad b_{21} = \alpha_2. \tag{26}$$

Three interesting methods of the second order Runge-Kutta method can be obtained for $\alpha_2 = \frac{1}{2},\ \frac{2}{3},\ 1$. Eqn (25) takes the form

$$y_{n+1} - y_n = h\, f(x_n + \frac{1}{2}h,\ y_n + \frac{1}{2}h\, f_n), \tag{27}$$

$$y_{n+1} - y_n = \frac{1}{4}h\,(f(x_n,\ y_n) + 3f(x_n + \frac{2}{3}h,\ y_n + \frac{2}{3}h\, f_n)), \tag{28}$$

$$y_{n+1} - y_n = \frac{1}{2}h\,(f(x_n,\ y_n) + f(x_n + h,\ y_n + h\, f_n)). \tag{29}$$

The error of the method is of the order $O(h^2)$.

3.2.2 Third order methods $s = 3$

Here the following equations have to be fulfiled:

$$w_1 + w_2 + w_3 = 1, \quad \alpha_2 w_2 + \alpha_3 w_3 = \frac{1}{2}, \tag{30}$$

$$\alpha_2^2 w_2 + \alpha_3^2 w_3 = \frac{1}{3}, \quad \alpha_2 b_{32} w_3 = \frac{1}{6}, \tag{31}$$

$$\alpha_2 = b_{21}, \quad \alpha_3 = b_{31} + b_{32}, \tag{32}$$

with the two-parametric family of solutions

$$\begin{aligned} w_1 &= 1 + \frac{2 - 3(\alpha_2 + \alpha_3)}{6\alpha_2\alpha_3}, \quad w_2 = \frac{3\alpha_3 - 2}{6\alpha_2(\alpha_3 - \alpha_2)}, \\ w_3 &= \frac{2 - 3\alpha_2}{6\alpha_3(\alpha_3 - \alpha_2)}, \quad (\alpha_2 \neq \alpha_3, \ \alpha_2, \ \alpha_3 \neq 0). \end{aligned} \tag{33}$$

$$\begin{aligned} b_{21} &= \alpha_2, \quad b_{31} = \frac{3\alpha_2\alpha_3(1 - \alpha_2) - \alpha_3^2}{\alpha_2(2 - 3\alpha_2)}, \\ b_{32} &= \frac{\alpha_3(\alpha_3 - \alpha_2)}{\alpha_2(2 - 3\alpha_2)}. \end{aligned} \tag{34}$$

The two next methods are interesting:

the first method:

$$\begin{aligned} y_{n+1} - y_n &= \frac{2}{9}k_1 + \frac{1}{3}k_2 + \frac{4}{9}k_3, \\ k_1 &= h\,f(x_n, \, y_n), \\ k_2 &= h\,f(x_n + \frac{1}{2}h, \, y_n + \frac{1}{2}k_1), \\ k_3 &= h\,f(x_n + \frac{3}{4}h, \, y_n + \frac{3}{4}k_2). \end{aligned} \tag{35}$$

the second method:

$$
\begin{aligned}
y_{n+1} - y_n &= \tfrac{1}{6}(k_1 + 4k_2 + k_3), \\
k_1 &= h\, f(x_n,\, y_n), \\
k_2 &= h\, f(x_n + \tfrac{1}{2}h,\, y_n + \tfrac{1}{2}k_1), \\
k_3 &= h\, f(x_n + h,\, y_n - k_1 + 2k_2).
\end{aligned} \tag{36}
$$

The error of the method is of the order $O(h^3)$.

3.2.3 Fourth order methods $s = 4$

Here the following equations have to be fulfiled:

$$
\begin{aligned}
w_1 &= \frac{1}{2} + \frac{1-2(\alpha_2+\alpha_3)}{12\alpha_2\alpha_3}, \quad w_2 = \frac{2\alpha_3 - 1}{12\alpha_2(\alpha_3-\alpha_2)(1-\alpha_2)}, \\
w_3 &= \frac{1-2\alpha_2}{12\alpha_2(\alpha_3-\alpha_2)(1-\alpha_3)}, \; w_4 = \frac{1}{2} + \frac{2(\alpha_2+\alpha_3)-3}{12(1-\alpha_2)(1-\alpha_3)} \;, \\
b_{32} &= \frac{\alpha_3(\alpha_3-\alpha_2)}{2\alpha_2(1-\alpha_2)}, \quad \alpha_4 = 1, \\
b_{42} &= \frac{(1-\alpha_2)(\alpha_2+\alpha_3-1-(2\alpha_3-1)^2}{2\alpha_2(\alpha_3-\alpha_2)(6\alpha_2\alpha_3-4(\alpha_2+\alpha_3)+3)}, \\
b_{43} &= \frac{(1-2\alpha_2)(1-\alpha_2)(1-\alpha_3)}{\alpha_3(\alpha_3-\alpha_2)(6\alpha_2\alpha_3-4(\alpha_2+\alpha_3)+3)}.
\end{aligned} \tag{37}
$$

The most often used Runge-Kutta of the fourth order one has $\alpha_2 = \alpha_3 = \frac{1}{2}$.The corresponding equations take the forms:

$$
\begin{aligned}
y_{n+1} - y_n &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4), \\
k_1 &= h\, f(x_n,\, y_n), \\
k_2 &= h\, f(x_n + \frac{1}{2}h,\, y_n + \frac{1}{2}k_1), \\
k_3 &= h\, f(x_n + \frac{1}{2}h,\, y_n + \frac{1}{2}k_2), \\
k_4 &= h\, f(x_n + h,\, y_n + k_3).
\end{aligned} \tag{38}
$$

The best estimation of the error is recived for $\alpha_2 = 0.4$, $\alpha_3 = \frac{8}{7} - \frac{3}{16}\sqrt{5}$. The error of the method is of the order $O(h^4)$.

In all these methods the integration step h can be selected separately for the every iteration. In such a case instead of h the h_n should be written.

The End of the Lecture 2

4 Problems to think about

1. Answer the questions:

i. Is the Laplace postulate possible to complete, now or in any time? If yes/no, then explain why?

ii. Which one of the given definions of the model you like at most?

iii. What conditions have the model to fulfil to be aceptable?

iv. How the Noether theorem can be summarized?

v. What kind of the motion can be called the harmonic motion?

vi. Enumerate the differences between the Euler and the Runge-Kutta methods. Do you know other methods of solving the differential equations?

2. Construct the model of the arbitrarily selected physical phenomenon.