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Analysis of the correlation properties of direct and inverse composite Walsh functions

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Abstract: The article discusses the correlation properties of pseudo-random sequences (PRS) used in the formation of noise-like signals in code division coupled communication systems. The direct and inverse composite Walsh functions are considered. Comparative analysis of the correlation properties of the PRS is carried out in the Matlab medium. It is shown that the correlation properties of certain ensembles of composite Walsh functions are independent of the time shift. The possibility of using these signals in the development of systems with channels code separation in order to reduce the level of interference of multiple access is justified. Directions for further research have been determined.

Keywords: PSEUDO-RANDOM SEQUENCES, NOISE-LIKE SIGNALS, AUTOCORRELATION FUNCTION, CROSS CORRELATION FUNCTION, DIRECT COMPOSITE WALSH FUNCTION, INVERSE COMPOSITE WALSH FUNCTION

1. Introduction

Information transmission systems (ITS) are currently one of the most developing areas in radio communication engineering. The flows of information and the speed of its transmission are increasing, the requirements for the accuracy and reliability of the transmitted information are increasing, the requirements for electromagnetic compatibility with other devices and the use of the frequency resource are becoming more stringent. Among a large number of various ITSs, communication systems using noise-like signals (NLS) are of the greatest interest [1-5].

The use of broadband methods makes it possible to obtain such results in the field of communication systems that cannot be obtained using conventional signals, namely: the energy, structural and informational secrecy of the ITS. In addition, systems with NLS are capable of providing code addressing of a large number of subscribers and their code division when operating in a common frequency band, and have much better electromagnetic compatibility compared to narrowband radio communication systems.

Pseudo-random sequences (PRS) are widely used to generate noise-like signals (NLS) in communication systems with direct-sequence spread spectrum (DSSS) or frequency hopping spread spectrum (FHSS). Examples of such systems are DS-CDMA, GPS / Navstar, Glonass, and IEEE 802.11b wireless networks.

2. Preconditions and means for resolving the problem

2.1. Theoretical Data

As noted above, PRS is widely used in various systems and devices of data transmission systems. When using noise-like signals for data transmission, correlation methods of processing the received signals are used. In this case, the degree and quality of using the PRS largely depends on the correlation characteristics of the sequences used. In general, the following requirements are imposed on pseudo-random sequences used to spread the spectrum of signals [1,2,5]:

a large volume of an ensemble of sequences formed using a single algorithm;

- "good" auto- and cross-correlation properties of the sequences included in the ensemble;

- balanced structure;

- the maximum period for a given length of the shift register that forms the sequence;

- unpredictability of the structure of a sequence by its undistorted segment of limited length.

The simplest method of receiving NLS is correlation. The main subject of comparison is the autocorrelation function (ACF) of the sequence. ACF is a measure of the similarity of a signal and its time-shifted copy. When the signal coincides with its copy, we get the maximum (main) ACF overshoot, thanks to which the detection equipment can detect and extract a useful signal from the noise. The characteristic and comparison of broadband signals is based on the value of the maximum lateral ejection (lobe) of the ACF. Sometimes it is provided as a percentage of the value of the main emission.

The autocorrelation function of discrete signals is calculated by the formula:

$$R_u(n) = \sum_{j=-\infty}^{\infty} u_j u_{j-n}, \quad (1)$$

where n is an integer, positive, negative, or zero.

The cross-correlation function (CCF) between two discrete signals is calculated using a similar formula:

$$R_{uv}(n) = \sum_{j=-\infty}^{\infty} u_j v_{j-n}, \quad (2)$$

In order to improve the correlation characteristics of the PSP, various methods are proposed. In [6-9], various modifications of Barker codes are considered - composite Barker codes, Barker-Volynskaya codes. However, the use of such modifications of Barker codes does not allow obtaining large PSP ensembles, which is a necessary condition for their use in multichannel code division multiplexing systems. In addition, to reduce the level of multiple access interference, the applied PRSs should be orthogonal, since in this case the CCF between any other PRSs will be equal to zero. Codes with such properties include Haar, Rademacher, Walsh codes. However, a feature of orthogonal codes is that the orthogonality of these codes is performed only at the "point", i.e. in the absence of time shifts. In real conditions, such conditions are not met, orthogonality is violated, which in turn leads to an increase in the level of multiple access interference and the appearance of errors in the processing of input data. Therefore, various methods are used to eliminate these disadvantages [10-12].

Let us consider the application of the so-called composite Walsh codes from this point of view. The method for obtaining such codes is as follows - this code is formed by multiplying two standard sequences. The first of them (for example, the Walsh function) is called a generator, and the second (for example, M is a sequence) is called elementary. Each character in the generating sequence is replaced by a direct or inverse elementary sequence, depending on what value the character has (+1 or -1) in the generating sequence. As a result of multiplying the first sequence by the second, sequences with a large number of digits are obtained. We call such a sequence the direct composite Walsh function. If M - a sequence is taken as the first, and the Walsh function is taken as an elementary one, then such a sequence will be called the inverse composite Walsh function.

As an M - sequence, we take a primitive, irreducible polynomial of the 3rd order - $h(x) = x^3 + x + 1$, with the help of which we can obtain several PRSs depending on the initial state of the shift register. The most important feature of M - sequences is that their periodic autocorrelation function is optimal in the class of possible autocorrelation functions of binary sequences of length $L = 2^n - 1$. It is the good autocorrelation properties of M - sequences and the simplicity of their formation that have led to their widespread use in communication systems [1,2,6,12].

As the Walsh function, we choose the 4th order Walsh function, which can take the following values: $\{(+1, +1, +1, +1), (+1, +1, -1, -1), (+1, -1, -1, +1), (+1, -1, 1, -1)\}$. Given the values of the PRS generated by the shift register corresponding to the polynomial $h(x) = x^3 + x + 1$, the following direct composite Walsh functions can be obtained:

$(1, -1, 1, -1) \cdot (1, -1, -1, 1, 1, 1, -1) = 1, -1, -1, 1, 1, 1, -1, -1, 1, 1, -1, -1$
 $1, -1, 1, 1, -1, -1, 1, 1, 1, -1, -1, 1, 1, -1, -1, 1$;

$(1, -1, -1, 1) \cdot (1, -1, -1, 1, 1, 1, -1) = 1, -1, -1, 1, 1, 1, -1, -1, 1, 1, -1, -1$
 $1, -1, 1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1$.

And also, the inverse composite Walsh functions:

$(1, -1, -1, 1, 1, 1, -1) \cdot (1, -1, 1, -1) = 1, -1, 1, -1, -1, 1, -1, 1, -1, 1, -1, 1$
 $1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, 1, -1, 1, -1$;

$(1, -1, -1, 1, 1, 1, -1) \cdot (1, -1, -1, 1) = 1, -1, -1, 1, -1, 1, 1, -1, -1, 1, 1, -1, 1, 1, -1, -1$
 $1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, -1, 1, 1$.

2.2. Experimental Data

The analysis of the correlation characteristics of direct composite Walsh functions, which are presented above, performed in the Matlab environment, gave the following results (Fig. 1, ..., Fig. 4).

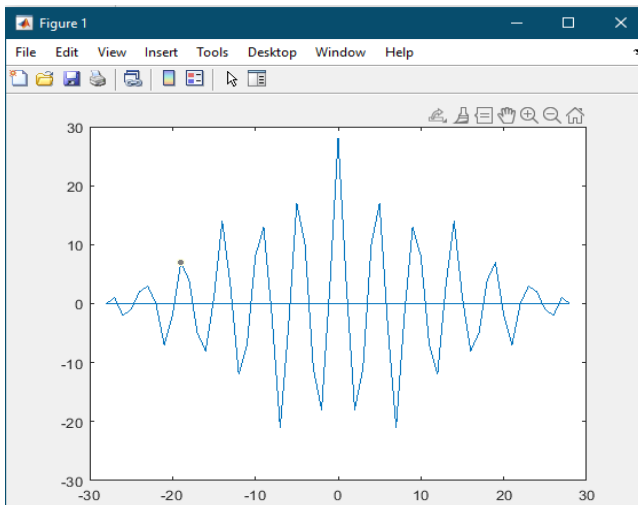


Fig. 1 ACF of direct composite Walsh functions and *M*-sequences:
 $(1, -1, 1, -1) \cdot (1, -1, -1, 1, 1, 1, -1)$

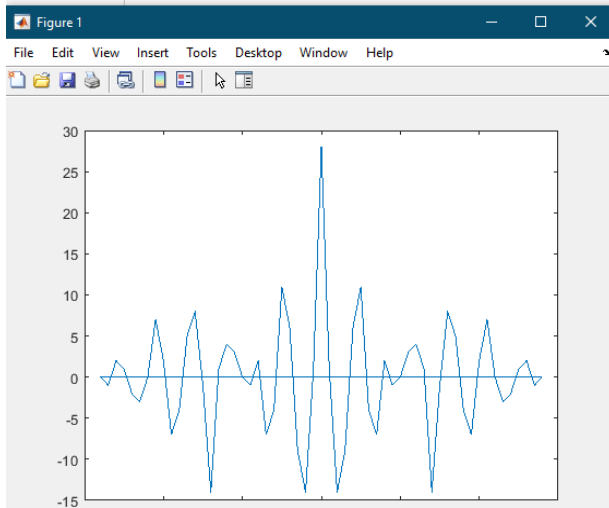


Fig. 2 ACF of direct composite Walsh functions and *M*-sequences:
 $(1, -1, -1, 1) \cdot (1, -1, -1, 1, 1, 1, -1)$

In the Fig. 3 the cross-correlation characteristic of direct composite Walsh functions is given.

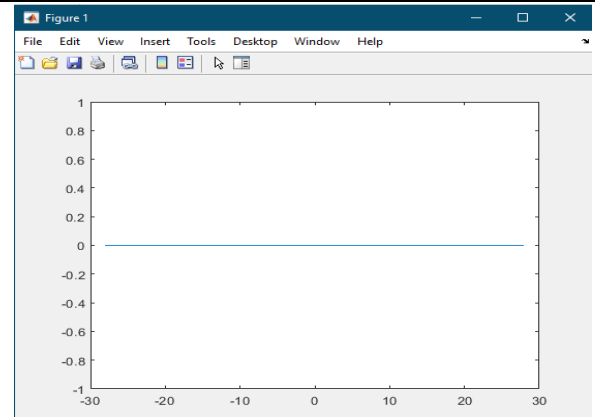


Fig. 3 CCF of direct composite Walsh functions.

From Fig. 1, ..., Fig. 3 it follows that direct composite Walsh functions based on *M*-sequences have poor ACFs - there is no pronounced central lobe of the characteristic and large levels of side lobes, but very good cross correlation characteristics. Thus, direct composite Walsh functions cannot provide reliable synchronization on reception, correct decoding of input data, but provide a minimum level of multiple access interference, since the CCF is zero at any time offsets.

Fig. 4, ..., Fig. 6 shows the correlation characteristics of the inverse composite Walsh functions.

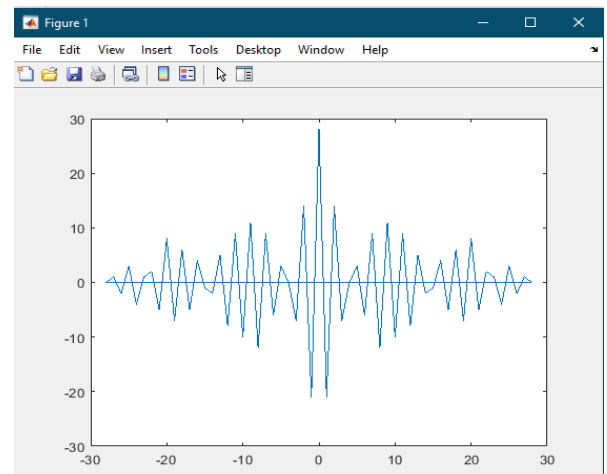


Fig. 4 ACF of inverse composite Walsh functions and *M*-sequences:
 $(1, -1, -1, 1, 1, 1, -1) \cdot (1, -1, 1, -1)$

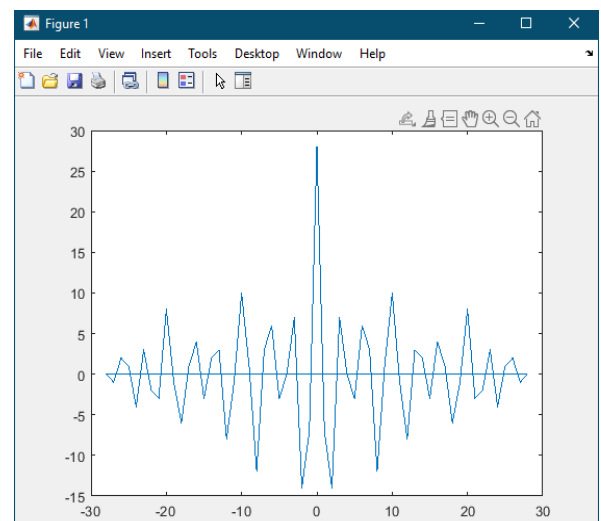


Fig. 5 ACF of inverse composite Walsh functions and *M*-sequences:
 $(1, -1, -1, 1, 1, 1, -1) \cdot (1, -1, -1, 1)$

Fig. 6. the cross-correlation characteristic of the inverse composite Walsh functions is given.

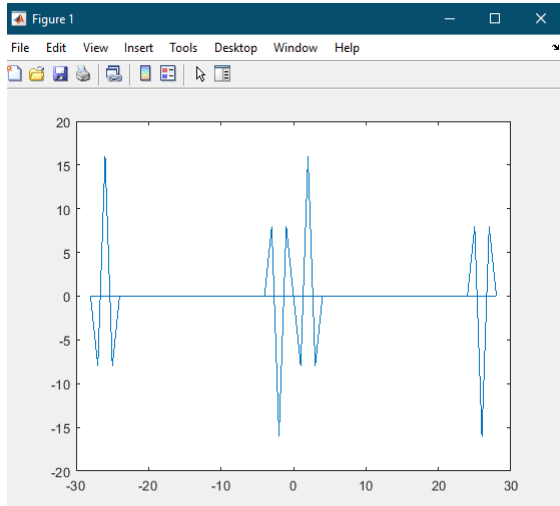


Fig. 6 CCF of inverse composite Walsh functions.

From Fig. 4, ..., Fig. 6 it follows that the inverse composite Walsh functions have better ACFs compared to the direct ones - there is a pronounced central lobe of the characteristic and lower levels of side lobes, but not very good CCF.

Thus, inverse composite Walsh functions can provide reliable timing on reception, correct decoding of input data, but slightly increase the level of multiple access interference at small time offsets, and significantly less at large time offsets.

Consider the case when the de Bruijn sequences are used as a standard sequence - $(1, -1, 1, 1, 1, -1, -1, -1)$ and $(1, 1, 1, -1, 1, -1, -1, -1)$. In this case, the following direct composite Walsh functions can be obtained:

$$\begin{aligned} (1, -1, 1, -1) \cdot (1, -1, 1, 1, 1, -1, -1, -1) &= 1, -1, 1, 1, 1, -1, -1, -1, 1, -1, -1, \\ &1, 1, 1, 1, -1, 1, 1, 1, -1, -1, -1, 1, -1, -1, 1, 1, 1; \\ (1, -1, -1, 1) \cdot (1, 1, 1, -1, 1, -1, -1, -1) &= 1, 1, 1, -1, 1, -1, -1, -1, -1, -1, \\ &1, -1, 1, 1, 1, 1, -1, -1, 1, 1, 1, 1, -1, -1, -1, -1, \end{aligned}$$

as well as the inverse composite Walsh functions:

$$\begin{aligned} (1, -1, 1, 1, 1, -1, -1, -1) \cdot (1, -1, 1, -1) &= 1, -1, 1, -1, -1, 1, 1, -1, \\ &1, -1, 1, -1, 1, -1, 1, -1, -1, -1, 1, -1, 1, -1, 1, -1, 1; \\ (1, 1, 1, -1, 1, -1, -1, -1) \cdot (1, -1, -1, 1) &= 1, -1, -1, 1, 1, -1, -1, -1, \\ &1, 1, -1, 1, 1, -1, -1, -1, 1, -1, 1, 1, -1, -1, 1, -1. \end{aligned}$$

The analysis of the correlation characteristics of the composite Walsh functions, which are presented above, carried out in the Matlab environment, gave the following results (Fig. 7, ..., Fig. 9).

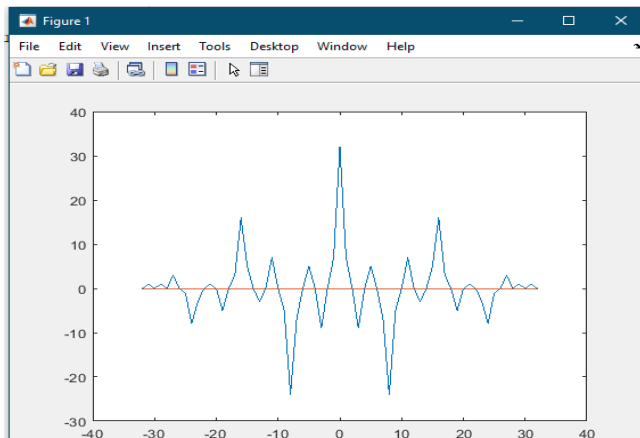


Fig. 7 ACF of direct composite Walsh functions and de Bruijn sequences: $(1, -1, 1, -1) \cdot (1, -1, 1, 1, 1, -1, -1, -1)$

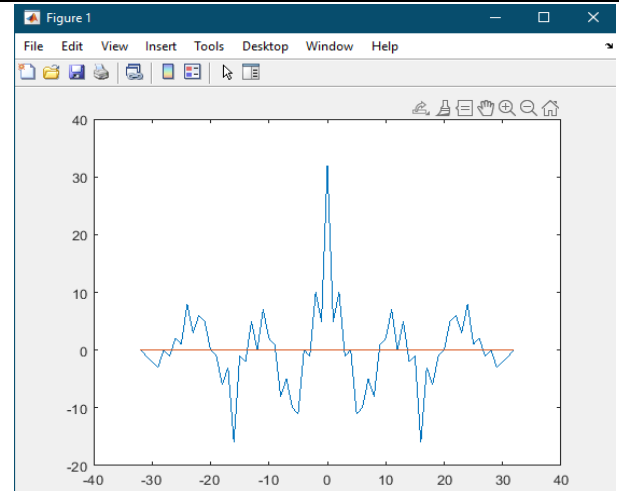


Fig. 8 ACF of direct composite Walsh functions and de Bruijn sequences: $(1, -1, -1, 1) \cdot (1, 1, 1, -1, 1, -1, -1, -1)$

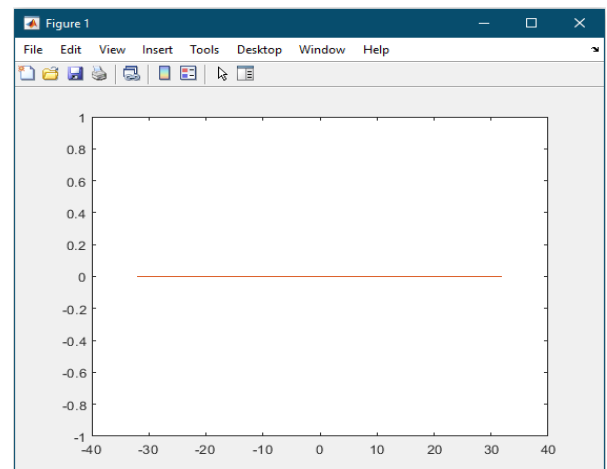


Fig. 9 CCF of direct composite Walsh functions.

From Fig. 7, ..., Fig. 9 it follows that direct composite Walsh functions based on de Bruijn sequences have relatively good ACFs - there are pronounced central lobes of characteristics, the suppression coefficient - the ratio of the amplitude of the central lobe to the maximum side lobe is equal to two, and very good CCF. Thus, direct composite Walsh functions based on de Bruijn sequences can provide reliable synchronization on reception, correct decoding of input data, and provide a minimum level of multiple access interference, since the cross-correlation function is zero at any time offsets.

Fig. 10, ..., Fig. 12 show the correlation functions of the inverse composite Walsh functions.

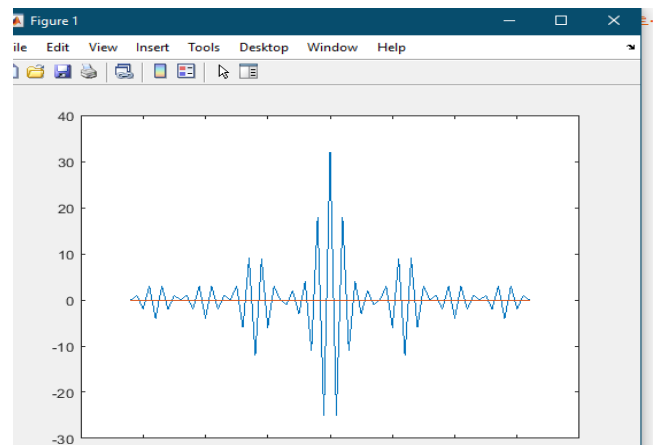


Fig. 10 ACF of inverse composite Walsh functions and de Bruijn sequences:
 $(1, -1, 1, 1, 1, -1, -1, -1) \cdot (1, -1, 1, -1)$

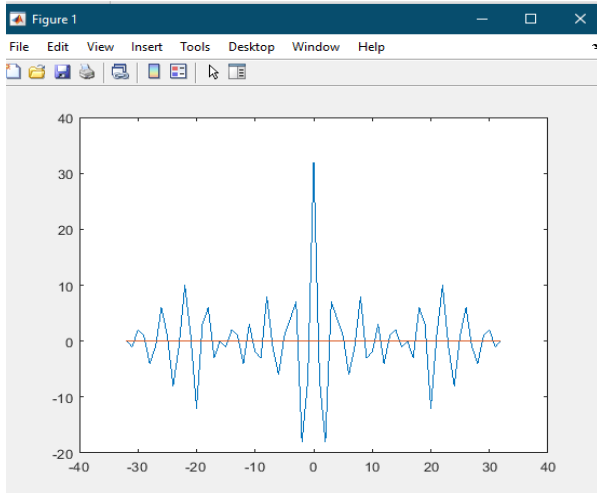


Fig. 11 ACF of inverse composite Walsh functions and de Bruijn sequences:
 $(1, -1, 1, 1, 1, -1, -1, -1) \cdot (1, -1, 1, -1)$

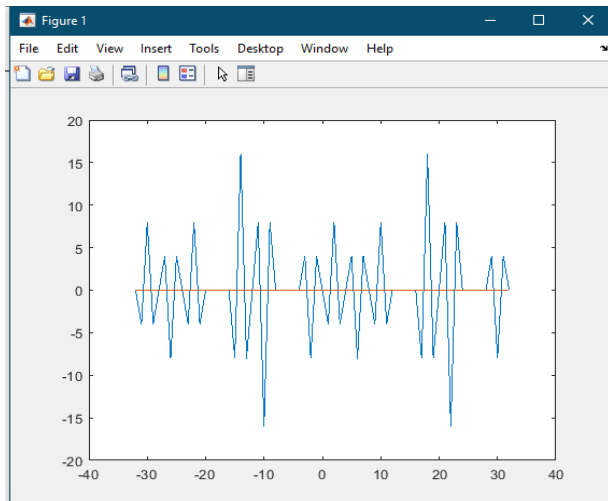


Fig. 12 CCF of inverse composite Walsh functions.

From Fig. 10, ..., Fig. 12 follows that the inverse composite Walsh functions based on de Bruijn sequences have approximately the same autocorrelation functions as the direct ones - there are pronounced central lobes of characteristics, the suppression coefficient is the ratio of the amplitude of the central lobe to the maximum side lobe is two, but poor cross-correlation characteristics. Thus, inverse composite Walsh functions based on de Bruijn sequences can provide reliable synchronization on reception, correct decoding of input data, but have a large level of multiple access interference.

Consider the case when the following arbitrary sequences are used as a standard sequence:

$$(1, 1, 1, -1, -1, -1, 1) \text{ and } (-1, -1, -1, 1, 1, 1, -1).$$

In this case, the following direct composite Walsh functions can be obtained:

$$\begin{aligned} (1, -1, 1, -1) \cdot (1, 1, 1, -1, -1, -1, 1) &= 1, 1, 1, -1, -1, -1, 1, -1, -1, \\ &-1, 1, 1, 1, -1, 1, 1, -1, -1, 1, 1, 1, -1, 1, -1, 1; \\ (1, -1, -1, 1) \cdot (-1, -1, -1, 1, 1, 1, -1) &= -1, -1, -1, 1, 1, 1, -1, 1, 1, 1, 1, \\ &1, -1, -1, 1, 1, 1, -1, -1, -1, -1, 1, 1, 1, 1, -1, 1, \end{aligned}$$

as well as the inverse composite Walsh functions:

$$\begin{aligned} (1, 1, 1, -1, -1, -1, 1) \cdot (1, -1, 1, -1) &= 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, \\ &-1, 1, 1, 1, -1, -1, 1, -1, 1, -1, 1, 1, -1, 1, -1, 1; \end{aligned}$$

$$\begin{aligned} (-1, -1, -1, 1, 1, 1, -1) \cdot (1, -1, -1, 1) &= -1, 1, 1, -1, -1, 1, 1, -1, 1, 1, \\ &-1, -1, 1, 1, -1, -1, 1, 1, -1, 1, 1, -1, 1, -1, 1, 1. \end{aligned}$$

The analysis of the correlation characteristics of the composite Walsh functions, which are presented above, carried out in the Matlab environment, gave the following results (Fig. 1.13, ..., Fig. 1.15).

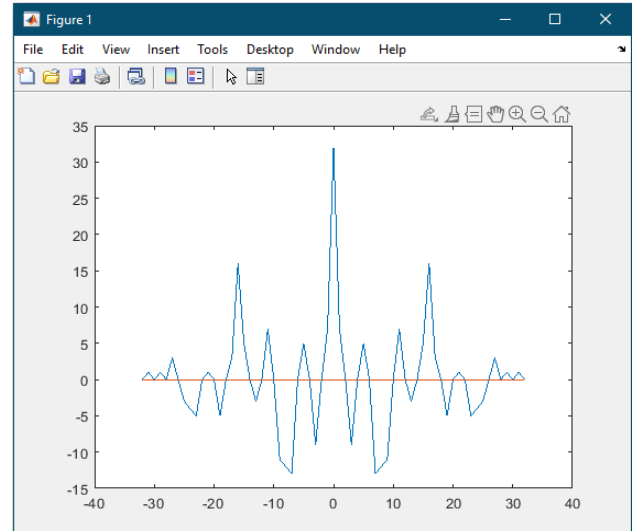


Fig. 13 ACF of direct composite Walsh functions and arbitrary sequences:
 $(1, -1, 1, -1) \cdot (1, 1, 1, -1, -1, -1, 1, -1, 1, 1)$

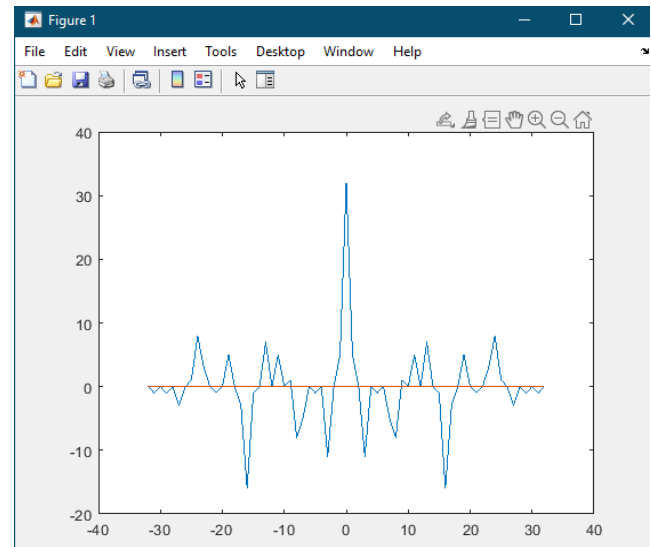


Fig. 14 ACF of direct composite Walsh functions and arbitrary sequences:
 $(1, -1, -1, 1) \cdot (-1, -1, -1, 1, 1, 1, -1, 1)$

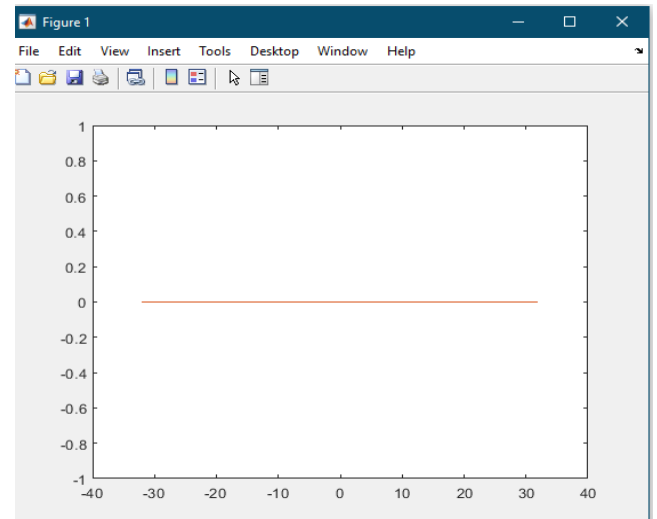


Fig. 15 CCF of direct composite Walsh functions and arbitrary sequences.

Fig. 16, ..., Fig. 18 show the correlation characteristics of the inverse composite Walsh functions and arbitrary sequences.

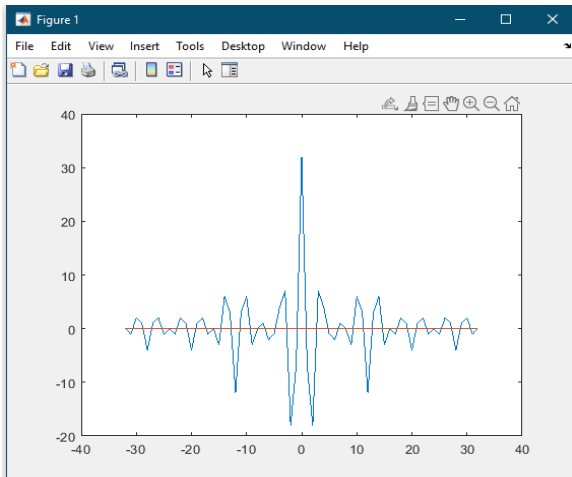


Fig. 16 ACF of inverse composite Walsh functions and arbitrary sequences: $(-1, -1, -1, 1, 1, -1, 1)$ $(1, -1, -1, 1)$.

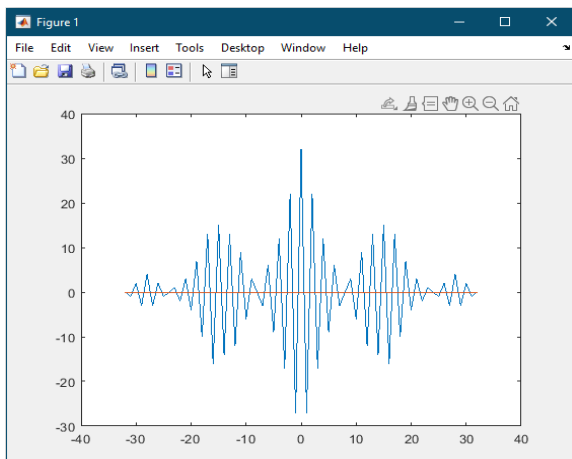


Fig. 17 ACF of inverse composite Walsh functions and arbitrary sequences: $(1, 1, 1, -1, -1, -1, 1)$ $(1, -1, 1, -1)$.

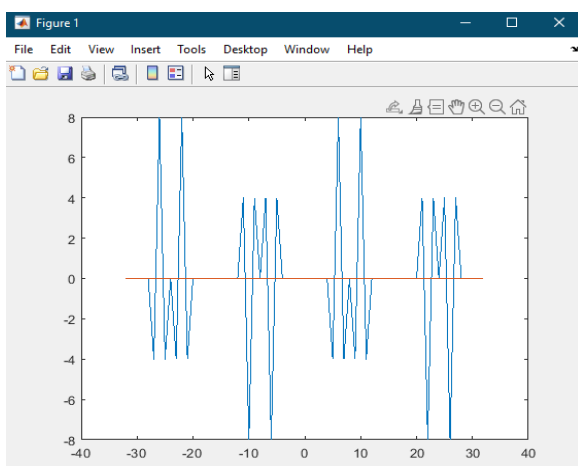


Fig. 18 CCF of inverse composite Walsh functions and arbitrary sequences.

From Fig. 13, ..., Fig. 15 it follows that direct composite Walsh functions based on arbitrary sequences have relatively good autocorrelation functions – there are pronounced central lobes of characteristics, the suppression coefficient-the ratio of the amplitude of the central lobe to the maximum lateral is equal to two, and very good cross-correlation characteristics. Thus, direct composite Walsh functions based on arbitrary sequences can provide reliable synchronization at reception, correct decoding of input data, and

provide a minimum level of multiple access interference, since the cross-correlation function is zero at any time shifts.

From Fig. 16, ..., Fig. 18 follows that inverse composite Walsh functions based on arbitrary sequences have worse auto - and cross-correlation functions than direct ones. Thus, inverse composite Walsh functions based on arbitrary sequences cannot provide reliable synchronization at reception, correct decoding of input data, have a high level of multiple access interference, and cannot be used in data transmission systems.

3. Conclusion

The analysis of the correlation characteristics of the composite Walsh functions allows to draw the following conclusions:

- Direct composite Walsh functions have slightly better correlation characteristics than inverse composite Walsh functions.
- Direct composite Walsh functions are time-shift invariant, i.e., the cross-correlation of such functions is independent of the time shift and is orthogonal.
- The type of correlation characteristics of composite Walsh functions largely depends on the type of generators and elementary sequences that are conjugated with the corresponding Walsh functions.
- Pseudo-random sequences of composite Walsh functions are well balanced.

The area of application of PSP, which are based on various approaches, is huge and varied. By selecting the appropriate properties of the generators or elementary sequences, a satisfactory result can be achieved in most cases of operation of broadband systems. Generation of PSP ensembles of arbitrary length with given correlation properties is an urgent practical problem.

Consequently, further careful study of the properties of derivatives and elementary sequences is required for the formation of various composite functions for solving the corresponding applied problems.

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Mathematical software tools applicable to remote learning and scientific research in case of isolation

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Abstract: This paper is devoted to some up-to-date computational tools, which are on-line available and appropriate to remote learning as well as to scientific research implementation relevant to mathematics and their applications.

The following aspects are concerned and discussed: some of the opportunities and benefits afforded by the software tools which are taken into consideration; necessary requirements which have to be met in order to use these tools; some disadvantages and drawbacks which may arise.

Comparison of fees and prices for different mathematical software tools is done.

For purpose of illustration realistic examples are also given.

Keywords: MATHEMATICAL SOFTWARE, COMPUTER ALGEBRA SYSTEMS, FREE SOFTWARE, CLOUD COMPUTING

1. Introduction

Nowadays, the mathematical software tools used in research and engineering play a crucial role in the development of technology, education and science. For example, the treatment of complex numerical analysis with the aid of mathematical software is currently used in all branches of physical, medical and social sciences. For that matter, by means of Computer aided design (CAD) software the level of scientific research and in particular of engineering science can be significantly improved. Computer solutions to large algebraic systems are implemented by users in form of algorithms using instruction codes and special syntaxes [3].

Strategic use of technology makes stronger mathematics teaching and learning [1]. But, the global pandemic has posed significant obstacles to education and scientific researches. So that, it is absolutely indispensable to change the approach when using on-line the modern computer software. The purpose here is to present some peculiarities in the use of mathematical software, computer algebra systems in particular and especially free software resources for remote learning and scientific research.

2. Mathematical Software

In the last two years, in the conditions of the new reality, scientists, teachers and students in Bulgaria are facing a serious problem. With the increasing isolation and as a consequence -- working from home (permanently or for different periods of time), most often they do not have appropriate software tools in their home office. This naturally makes it necessary for them to make a reasonable decision and a wise choice of suitable mathematical software with which they can conduct their work remotely.

This is the place, according to the problem taxonomy of the National Institute of Standards and Technology (USA), to recall what does mathematical software mean:

Definition 1. *Mathematical software* is software used to model, analyze and/or calculate numeric, symbolic and geometric data.

According to this definition, even computer (software) calculators are mathematical software of the simplest kind, through which one is able to perform simple mathematical operations and data input is usually done by hand.

At the other side are the so-called computer algebra systems, which are the subject of this work (see, e.g. [2]):

Definition 2. *Computer Algebra System (CAS)*, also called *Symbolic Algebra System (SAS)*, is a package which includes mathematical algorithms and special functions for performing symbolic manipulations on algebraic objects, a language for their

implementation and an environment in which the language to be used.

This means that, using CAS, one may manipulate mathematical expressions in a way as if he do it manually.

Computer algebra systems can be conditionally divided into two types:

- specialized, which are devoted to a specific part of mathematics;
- general-purpose, which are useful to a user who works in any scientific field in which it is necessary to perform manipulation of mathematical expressions.

Usually symbolic manipulations in CAS include: expression simplification; substitutions of symbols or numeric values in expressions; modifications of the form of expressions (expanding products and powers, factorization, transforming trigonometric functions in exponential form, transforming logic expressions, etc.); differentiation (partial and total); symbolic integration for some functions (indefinite and definite), symbolic optimization (constrained and non-constrained); linear and some nonlinear equations solving over various domains; some differential and difference equations solving; some limits solving; integral transforms; series operations (expanding, sums, products); matrix operations; statistical computations and even theorems verification and proving.

Also, for the purposes of teaching and research in mathematics and its engineering and economic applications, CAS needs to include: arbitrary precision numeric operations; exact integer arithmetic; plotting graphs and parametric plots (2D and 3D) and animation of them; mathematical expressions in two-dimensional form editing; a programming language for purpose of implementation of own algorithms.

The choice of a particular mathematical software tool by a scientist/teacher/student is determined by at least the following several factors, given not necessarily in order of importance:

- Research area and problem statement;
- Goals and level of work of the user;
- Financial capacity and attitudes of the user;
- The user's long- and short-term developmental intentions and prospects;
- User's available hardware, operating platforms, etc.;
- Consistency with the team the user is working with.

3. Computer Algebra Systems

Nowadays, there is a wide variety of computer algebra systems. Among the commercial systems, Maple, Mathematica and Matlab seem to be the most popular and commonly used.

Maple (<https://www.maplesoft.com/>) is a symbolic and numeric computing environment as well as a multi-paradigm programming language, developed commercially by the Canadian software company Maplesoft. Several areas of technical computing are covered: symbolic operations, numerical analysis computations, data processing, data visualization, etc. A toolbox MapleSim adds functionality for multidomain physical modeling and code generation.

Maple is a general-purpose computer algebra systems, because of its capacity for symbolic computation and visualization. At the same time numeric computations to arbitrary precision are supported.

Users can enter mathematics using traditional mathematical notation. Custom user interfaces can also be made. There is also opportunity to convert expressions from traditional mathematical notation to markup suitable for LaTeX system.

Maple is compatible with: Linux, macOS, Windows. Maple 2021 system requirements are: 4 GB recommended RAM (disk space 10 GB).

MATLAB, which is an abbreviation of "matrix laboratory" (<https://www.mathworks.com/>), is a programming language and numeric computing environment developed by MathWorks. By means of MATLAB one is able to make matrix manipulations; to plot functions and data, to implement some algorithms; to transfer results and incorporate them into other packages.

Most functions accept arrays as input and operate element-wise on each element.

Although MATLAB is intended primarily as a system for numeric computations, an optional toolbox uses the MuPAD symbolic engine thus providing access to symbolic computing capabilities. Its additional package, Simulink, adds graphical multi-domain simulation and model-based design for dynamic and embedded systems, which in a number of cases makes MATLAB preferable in engineering investigations.

MATLAB is compatible with: Linux, macOS, Windows. MATLAB and Simulink requirements are: 3.4 GB of HDD space for MATLAB only, 5-8 GB for a typical installation; RAM 4GB minimum, 8 GB recommended.

Wolfram Mathematica, which is usually termed **Mathematica** (<https://www.wolfram.com/mathematica/>), is a software system with built-in libraries for several areas of technical computing that allow symbolic computation, manipulating matrices, plotting functions and various types of data, implementation of algorithms, creation of user interfaces, and interfacing with programs written in other programming languages. Features include instant dynamic interactivity, high-impact adaptive visualization, symbolic interface construction, load-on-demand curated data, image and audio-processing, neural networkings, 3D printing, and tools for connecting to DLL, SQL, Java, .NET, C++, Fortran, CUDA, OpenCL, and http-based systems. Together with Maple, it is one of the major general-purpose computer algebra systems. The programming language used in Mathematica is the Wolfram Language.

Mathematica is available for onsite machines running Windows, Mac OS X, Linux, or Unix. Home-use licenses are available for machines running Windows, Mac OS X, or Linux.

Mathematica 12 System Requirements are: 4 GB+ recommended RAM (disk space 19 GB).

Mathematica was conceived by Stephen Wolfram and is developed by Wolfram Research of Champaign, Illinois.

Some additional opportunities and computational resources provided by Wolfram Research will be considered into the next section.

Based on the data from the table below, a comparison can be made of the prices of the three computer algebra systems considered. Given the objectives of this paper, the table is limited to Student, Home/Personal and Education/Academic Plan.

Table 1. Annual fees (in EUR) of the most popular and major computer algebra systems [6-8]

	Student	Home/ Personal	Educatio n/ Academic
Maple	101 €	195 €	1274 €
MATLAB & Simulink	35/69 €	119 €	250 €
Mathematica	152 €	328 €	1428 €

Along with commercial ones, there are many free computer algebra systems, some of which are more than a successful alternative. It is in place here to give the Free Software definition written by Richard Stallman [5] and published by the Free Software Foundation [11]:

Definition 3. *Free software* is computer software distributed under terms that allow users to run the software for any purpose as well as copy, distribute, study, change and improve it and any adapted versions.

A program is free software if some necessary conditions are fulfilled. Namely, a program is free software if the program's users have the four essential freedoms (see [11]):

- The freedom to run the program as you wish, for any purpose (**Freedom 0**);
- The freedom to study how the program works, and change it so it does your computing as you wish (**Freedom 1**). Access to the source code is a precondition for this;
- The freedom to redistribute copies so you can help others (**Freedom 2**);
- The freedom to distribute copies of your modified versions to others (**Freedom 3**). By doing this you can give the whole community a chance to benefit from your changes. Access to the source code is a precondition for this.

While MATLAB is a very popular numerical computation software package, some other free alternatives are available, such as the open source GNU Octave.

GNU Octave (www.gnu.org/software/octave/) is an open-source and free mathematical modeling and simulation software and computation language that provides a command interface for solving linear and nonlinear equations numerically and for executing other numerical experiments using a language that is mostly compatible with MATLAB.

Moreover, it may also be used as a batch-oriented language. GNU Octave is primarily intended for numerical computations. As a part of the GNU Project, it is free software under the terms of the GNU General Public License.

The syntax of GNU Octave is math-oriented which makes it preferred by many mathematicians.

GNU Octave is compatible with Linux, macOS, BSD, Windows.

Other free alternatives to MATLAB include Scilab and FreeMat. In fact, GNU Octave is more compatible with MATLAB than Scilab is; as for FreeMat, it has not been updated since 2013.

Scilab (<https://www.scilab.org/>) is a free and open-source, sophisticated, cross-platform numerical computational package and a high-level, numerically-oriented programming language. Scilab is well-suited for engineers and offers a powerful platform for numerical computation. It can be used for signal processing, statistical analysis, image enhancement, fluid dynamics simulations, numerical optimization, modeling, simulation of explicit and implicit dynamical systems, etc. It also supports more than 2000 mathematical functions; can produce complex algorithms and if the corresponding toolbox is installed, symbolic manipulations are also available.

In Scilab, users can display their 2D and 3D data, to animated figures, charts, graphs. This platform comes along with source code, help menu and user guide in English.

Scilab is available free of cost under an open source license. Due to the open source nature of the software, some user contributions have been integrated into the main program.

Scilab is compatible with Windows, Linux, macOS.

SageMath (<https://www.sagemath.org/>), previously **Sage** – an abbreviation of "System for Algebra and Geometry Experimentation", is a computer algebra system with features covering many aspects of mathematics, including algebra, combinatorics, graph theory, numerical analysis, number theory, calculus and statistics.

SageMath is free software, distributed under the terms of the GNU General Public License version 3, which serves as a real open source alternative to Maple, Mathematica, and MATLAB. It is very useful for education, studying, and research as it covers various mathematical areas.

The interface of this program is a notebook in a browser or the command-line. With the help of a notebook, SageMath connects either locally to your own Sage installation or to a Sage server on the network. Notebooks can be examined locally or remotely, and the connection can be secured with HTTPS. Inside any notebook, one can draw graphics in a perfect way, typeset mathematical expressions, add/delete input, and share his work across the network.

SageMath is compatible with Windows, Linux, macOS.

4. Wolfram|Alpha and Wolfram Cloud

This section is devoted to resources powered by Wolfram Research, which can be used on-line and/or free. In case of isolation and remote learning and scientific work they are useful, powerful and effective tool for students, teachers, scientists in any scientific branch related to mathematics, structural mechanics, physics, chemistry, etc.

Wolfram|Alpha (www.wolfram.com) is an online computational knowledge engine or answer engine that answers factual queries directly by computing the answer from externally

sourced curated data, rather than providing a list of documents or web pages that might contain the answer, as a search engine might. Additional data is provided from both academic and commercial websites and some of the data is kept updated in real time. The data sets include astronomical, chemical, geopolitical, language, biomedical and weather data, in addition to mathematical data. Wolfram|Alpha is developed by WolframAlpha LLC, a subsidiary of Wolfram Research. The service was officially launched on May 18, 2009 with purpose to provide integrated storage, interface, computation, knowledge, linguistics and deployment capabilities.

In Wolfram|Alpha users submit queries and computation requests via a text field. Then Wolfram|Alpha computes answers and relevant visualizations from a knowledge base of curated, structured data that come from other sites and books.

In Wolfram|Alpha is built-in free form input (Fig. 1), which is most often preferred by the students and young scientists. Of course, it is also possible to use the syntax of Wolfram Language.

Example 1. If we want to compute $\int_a^b f(x)dx$ using

Wolfram|Alpha, we can enter

`Integrate[f(x),{x,a,b}]`

according to Wolfram Language (Fig. 2); on the other hand we can give a request in free form (Fig. 1):

integrate f(x) from a to b.

It is also possible to enter only *integrate* into the text box, and then fill in the attributes of the corresponding integral in the fields that appear (Fig. 3).

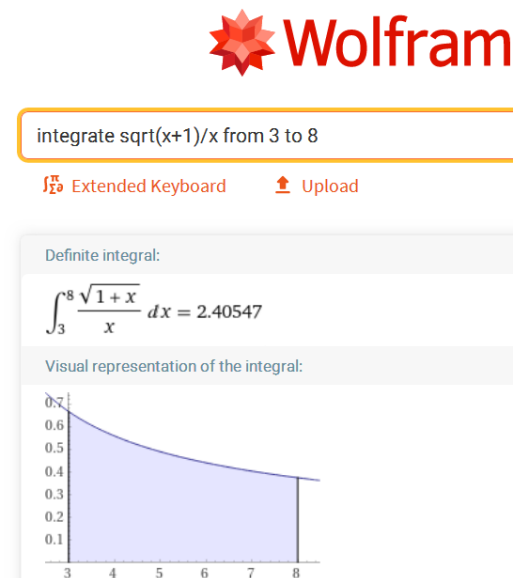


Fig. 1: $f(x) = \frac{\sqrt{x+1}}{x}$, $a=3, b=8$

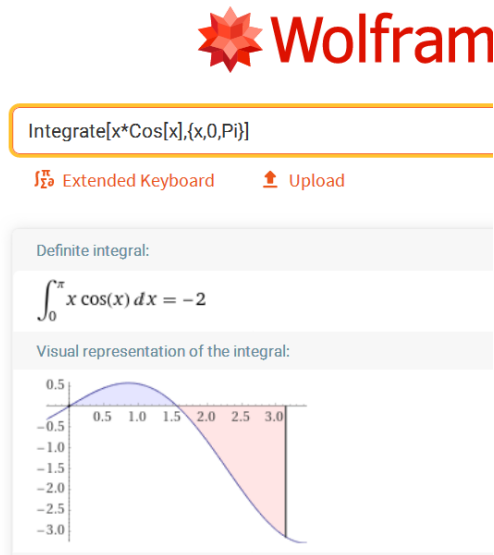


Fig. 2: $f(x) = x \cos x$, $a=0$, $b=\pi$

If we have to compute an indefinite integral, the fields corresponding to lower and upper integration limit have remain empty.

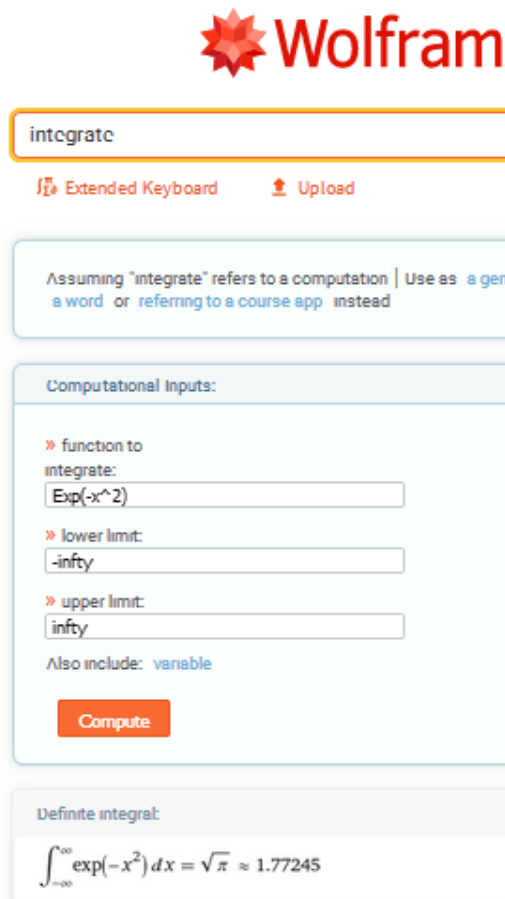


Fig 3: $f(x) = e^{-x^2}$, $a=-\infty$, $b=+\infty$

Although the use of a free form inputs has its reasons and brings some advantages, the authors believe that it is better to stick to Wolfram Language [4]. A user of Wolfram|Alpha, who has taken advantage of the free form of queries for some time, would find it difficult to switch and adapt to some of the computer algebra systems, which have strict syntactic rules and are usually case sensitive.

Wolfram|Alpha can be directly, on-line used successfully and completely free of charge, without any registration. This manner of work has been effectively applied by the authors in remote learning for immediate demonstration and illustration of theoretical facts, dependencies and statements (some plots; derivatives; functions and sequences properties; integrals; integral transforms, matrix manipulations; equations and systems solving; vector calculations; data fit; statistics as well as some strong mathematical definitions). The engine is also used by the authors and their students as a very useful auxiliary tool during practical exercises and when doing homework. Given this, sometimes the lack of step-by-step solutions capabilities is a very positive fact!

Using Wolfram|Alpha without registration brings a number of disadvantages: a sequence of actions cannot be set for execution and we have to enter a separate request at each stage of the work without being able to use previous results; the results are not saved as a working document and the user has to decide for himself how to do this; the options for many of the functions are restricted and so on.

On the other hand, we can easily copy inputs and results in math mode to clipboard; the Wolfram Language code of the corresponding request and result is also available. This fact is extremely useful for improving the user's Wolfram skills.

However, in order to get wider and more complete opportunities which Wolfram|Alpha provides, one can make a user registration for Wolfram|Alpha and choose some of the offered user plans. In 2012, Wolfram|Alpha Pro (<https://www.wolframalpha.com/pro/>) was released. Wolfram|Alpha Pro lets us to do much more than Wolfram|Alpha: to upload our own data and images for analysis, to get customized and interactive visuals for presentations, to download data, to get more computation time, to access optimized Web Apps.

The following user plans are available (see [9]):

Students: Basic - Personalized experience with customizable settings; does not include step-by-step solutions capabilities; it is free with sign-in; **Pro** - Enhanced features with step-by-step solutions, increased computation time and calculator Web Apps; 47 € annually; **Pro Premium** - Complete access to all features and priority customer support; 79 € annually;

Educators: Basic - Personalized experience with customizable settings; does not include step-by-step solutions capabilities; it is free with sign-in; **Pro** - Unlock additional classroom resources with step-by-step solutions, printable worksheets and extended computation time; 47 € annually; **Pro Premium**: Complete access to all features and priority customer support; 79 € annually.

Another opportunity is **Wolfram|Alpha Notebook Edition** (<https://www.wolfram.com/wolfram-alpha-notebook-edition/>), which combines the best of both Wolfram|Alpha and Wolfram Mathematica into a single, unified tool perfect for teaching and learning. Free-form input, like in Wolfram|Alpha, can be used to get instant answers to questions, create and customize graphs, and turn static examples into dynamic models. Inputs and results are saved as an interactive Wolfram Notebook. In a Wolfram Notebook the user can not only save, but also use previous results, and build up or work through a whole computation. Notes can be added and notebooks can be used as class or reference materials, or can be presented as dynamic slide shows.

Let us note that the question how does Wolfram|Alpha Notebook Edition work depends on the machine the software package is running on. The plans available can be seen from [10].

Wolfram Cloud (<https://www.wolfram.com/cloud/>) is a computational cloud-based platform for symbolic and numeric computations, analysis, programming and visualization. It is

accessible in a direct way in the web-browser of the user -- no installation and configuration required.

The platform contains the following features: libraries of mathematical functions; matrix and data manipulation tools; 2D and 3D data, function and geo-visualization and animation tools; solvers for systems of equations; finite element analysis with 2D and 3D adaptive mesh generation; database collection for mathematical, scientific, and socio-economic information and access to Wolfram|Alpha data and computations; tools for parallel programming and many others.

Wolfram Cloud technology powers a number of products including Wolfram Mathematica, Wolfram|Alpha, Wolfram|One, Wolfram Programming Lab, Wolfram Enterprise Private Cloud, instant Web Apps and others. Paid subscription plans for Wolfram|One, Mathematica Online, Wolfram|Alpha Notebook Edition and Wolfram Programming Lab are offered. It is also possible to use a Basic Plan subscription, for which only user registration is required.

With any paid subscription plan, all files stored in the Wolfram Cloud do not expire, while with a Cloud Basic plan, any file expires 60 days after its creation. One way to prevent this is to upgrade to a paid Wolfram Cloud subscription plan; another one is to convert the files to pdf format and save them to hard drive. It is not a good idea to copy notebook-files to the disk; to open the files you need an installed desktop version not earlier than Wolfram Mathematica 11. Cloud Basic plan includes 200 MB of file storage and when it is exceeded, the user will not be able to upload or create new files.

When files expire, they will still be visible in the account, but will not be accessible. Expired files will still count towards limits on cloud storage, so that they should be deleted from the account.

Users who upgrade to a paid Wolfram Cloud subscription from Cloud Basic will be able to recover any previously expired files, but not any deleted files.

There is a huge variety of different paid Wolfram Cloud subscription plans. For scientists conducting high-level research, we recommend, for example *Wolfram|One Personal* (Desktop and loud access, Upgrades; 2 GB file storage; 207 € annually) or *Standard Desktop +Cloud Wolfram Mathematica* (Desktop and Cloud Mathematica, Upgrades, Standard support, Personal-computer license; 15 GB file storage; 720 € annually).

For students it is best to use a Cloud Basic plan. In this case, they can easily switch from Wolfram|Alpha (unregistered user) to Wolfram Cloud.

Example 2. Given $X=\{0, 200, 400, 600, 800, 1000, 1200, 1400, 1600, 1800\}$ and $Y=\{373, 156.1, 113.6, 93.1, 81.5, 73.7, 67.2, 62.4, 58.3, 55\}$, find the least squared best fit.

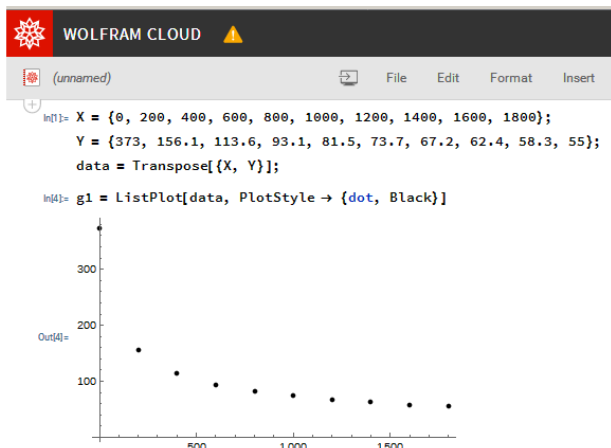


Fig 4: Wolfram Cloud Notebook (Basic Plan)

We will work by means of Wolfram Cloud, Basic Plan. We open a cloud notebook and our first step is to enter both X and Y and to pair them (see Fig. 4, input 1).

Plotting the data, we decide to search for logarithmic least squares best fit into the form $f(x) = a \ln(x+0.01)+b$.

The Wolfram implementation can be seen in Fig. 5 below. Nonlinear model function is used (Fig. 5, input 5); some indicators can be computed (Fig. 5, input 6) as well as the standard deviation (input 7). Finally, we can show the plot the logarithmic fit which we obtained together with the data (input 8).

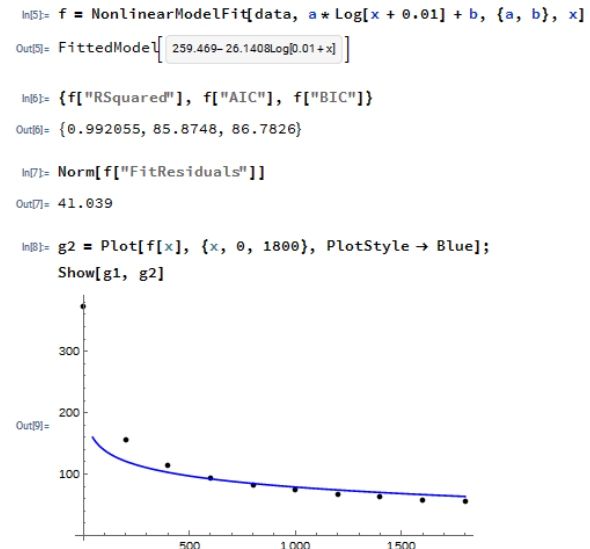


Fig 5: Wolfram implementation of least squares best fit

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Use of algorithms in semaphoric regulation. Tirana, Durrës case

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Abstract: In the design phase of transport systems, a significant step is also the traffic light regulation. In world practice, to evaluate the efficiency of the proposed theoretical methods, experiments on test transport systems and on real systems are carried out. The obtained results allow for the confrontation between different methods and the definition of those to be used in professional practice. For the semaphoric adjustment project, the algorithms proposed by the world literature were used in test networks with a non-large number of defining variables, so with as much semaphorized crossings in the project. This small number of variables makes it possible to find the optimal solution of the problem and evaluate how much the proposed approximation approaches this solution. While for the common topology project and traffic light regulation, algorithms were experimented in real transport systems. For this we chose two areas with about 60,000 inhabitants, respectively in Tirana and Durres. Since many of the half hypotheses used in the phase when acting on topology variables depend on one or several parameters, different values were used in order to reach their calibration. Next, the algorithms, with the calibrated parameters, will be used in another city. But this will be the subject of a future study.

KEYWORDS: TOPOLOGICAL PROJECT, STOCHASTIC LOAD FUNCTION, CONTROL PARAMETER, JOINT FLOWS.

1. Selection of Algorithms

Given that finding project solutions as close to reality is a difficult problem, the selected algorithms are of approximate type. This choice comes from the fact that solutions must be effectively implemented in practice and to be realized within a reasonable time. Even in the literature [1] no precise algorithm is proposed that manages to find the optimum of the semaphore adjustment problem by linking the equilibrium of users behavior.

In solving the common problem of topology and semaphore regulation, some algorithms are proposed below. The overall structure of all solutions is given in two stages. During the first phase it deals with the internal variables (semaphore network topology), while in the second it deals with the continuous variables (semaphore regulation), taking the topology defined. The proposed algorithms, starting from an initial configuration of the “ $y_{C,0}$ ”, setting, alternate two phases in each “ i ” approximation:

- Updating flows

Given the semaphore regulation vector “ $y_C^{(i-1)}$ ”, an equilibrium determination is performed from which the equilibrium flow vector

“ $f_{SUE}^{(i)}$ ” is obtained. The objective function “ $w(f_{SUE}^{(i)}, y_C^{(i-1)})$ ” can be precisely estimated from the production of the flux vector and the cost vector.

- Updating the setting variables

Calculate a displacement direction from the inverse gradient “ $\tilde{\nabla}_{y_C}$ ”, by the determinant variables “ y_C ” at the point “ $f_{SUE}^{(i)}, y_C^{(i-1)}$ ”. In defining the step “ $\mu^{(i)}$ ” a relatively small constant value is obtained.

The stopping condition can be determined by the approximate gradient

$$\|\tilde{\nabla}_{y_C}(f_{SUE}^{(i)}, y_C^{(i-1)})\| < \omega$$

or based on the difference of two adjustment vectors obtained in successive approximations

$$\|y_C^{(i)} - y_C^{(i-1)}\| < \omega$$

with constant positive “ ω ”. The flowchart of the proposed algorithm is given in Fig. 1.

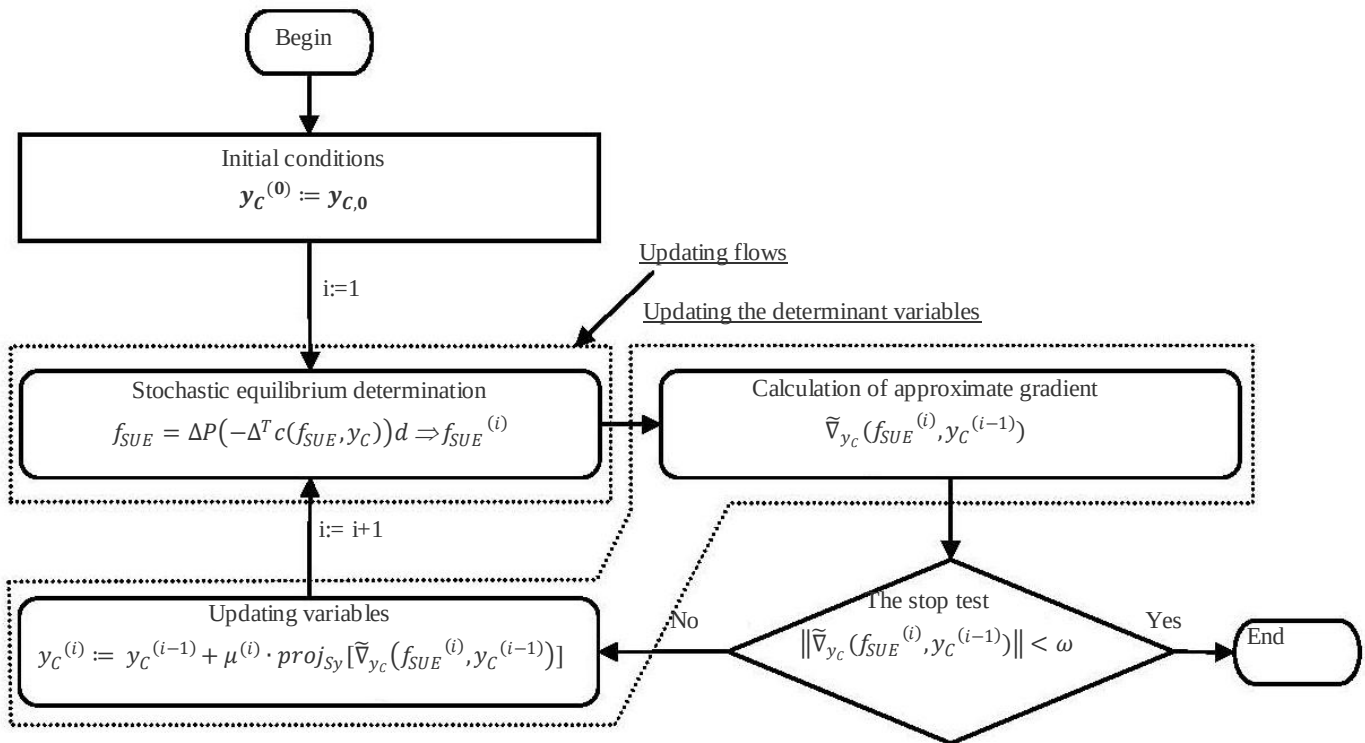


Fig.1 General structure of the design algorithm of the traffic light regulation

The new thing that this algorithm carries lies in calculating the search direction, so let's look at it in more detail. Relation to users behavior $y_C^* = \arg \min_{y_C} c(f_{SUE}, y_C)^T f^*$ can also be written based on the function of stochastic network load " f_{SNL} "

$$f_{SUE} = f_{SNL}(c(f_{SUE}, y_C), d) \quad (1)$$

The objective function, after substitution and without considering dependency on the demand vector " d ", can be written:

$$w(f_{SUE}, y_C) = c(f_{SUE}, y_C)^T f_{SNL}(c(f_{SUE}, y_C)) \quad (2)$$

After the replacement, (2) again depends on the vector " f_{SUE} ". The general element " i " of the gradient of (2), against the vector of the determinant variables, i.e. the derivative of the objective function against "time with green $y_{C,i}$ ", is given by the expression:

$$\frac{\partial w(f_{SUE}, y_C)}{\partial y_{C,i}} = \left[\frac{\partial c(f_{SUE}, y_C)}{\partial y_{C,i}} \right]^T \cdot f_{SNL}(c(f_{SUE}, y_C)) + c(f_{SUE}, y_C)^T \left[\frac{f_{SNL}(c(f_{SUE}, y_C))}{\partial y_{C,i}} \right]$$

which after deriving the compound function and replacing (1), has the form:

$$\frac{\partial w(f_{SUE}, y_C)}{\partial y_{C,i}} = \left[\frac{\partial c(f_{SUE}, y_C)}{\partial y_{C,i}} \right]^T f_{SUE} + c(f_{SUE}, y_C)^T \text{Jac}[f_{SNL}(c)] \left[\frac{\partial c(f_{SUE}, y_C)}{\partial y_{C,i}} \right]$$

The calculation of the " i " element of the gradient requires the calculation of:

- Jakopian of the stochastic grid load function by cost (this matrix is identical for each gradient term, so it is enough to calculate only once).
- Derivative vector of cost functions, against the variable $y_{C,i}$.

The Jacobian of the stochastic grid load function by cost can be calculated analytically. The general term of this Jacobian, i.e., the derivative of the stochastic grid load term belonging to a general branch ' l ', to the relative cost of a general branch ' l ' is given:

$$\frac{\partial f_{SNL,l}(c)}{\partial c_{l'}} = \frac{\partial}{\partial c_{l'}} \left(\sum_{rs \in RS} d_{rs} m_{l,rs} \right) = \sum_{rs \in RS} d_{rs} \sum_{k \in K_{rs}} \delta_{lk} \frac{\partial}{\partial c_{l'}} p_{rs,k} \quad (3)$$

The probability of choosing the route " $p_{rs,k}$ " can be given by a C-Logit choice model. In this case formula (3) turns out:

$$\frac{\partial f_{SNL,l}(c)}{\partial c_{l'}} = \sum_{od} d_{od} (-m_{rs,l \rightarrow l'} - m_{rs,l' \rightarrow l} + m_{l,rs} m_{l',rs})$$

in which the term $m_{rs,l \rightarrow l'}$ represents the probability that a user, going from the origin " r " to the destination " s ", traversed a route that has the " l " and " l' " branches.

Some of the most recommended algorithms in today's studies of semaphore regulation will be described below.

Hill Climbing Method (HC) is the simplest method used to design the topology of the semaphore network. It is a defined method and allows finding a local minimum value. In this method, for each approximation the best value of the single circle of that solution is found. The algorithm stops when it is no longer possible to improve this value, ie when a local minimum is reached.

This method is not controlled by any parameters. The flow diagram of this algorithm is given in Fig. 2.

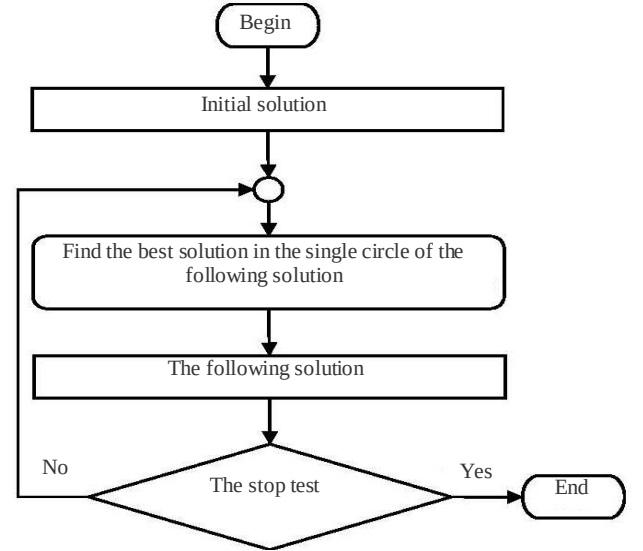


Fig.2 Hill Climbing (HC) flow chart

Simulated Annealing (SA) Method is a stochastic method, which, in contrast to (HC), does not require the whole circle of the following solution. It does not guarantee that the next choice will be better than the preceding one, enabling, especially in the initial phase, the shift towards solutions that aggravate the objective function.

In this method, each approximation is randomly selected (ie "with uniformly distributed probability") a solution belonging to the following solution circle. If this solution meets the Metropolis criterion, it becomes the next new solution. Temperature (as a parameter governing the selectivity of the Metropolis criterion), is cooled according to a geometric progression after a phase in which a predetermined number of approximations is executed. The method (SA) is controlled by three parameters:

- Initial temperature τ_0 - the value at which the temperature starts;
- Final temperature τ_f - the temperature value when the algorithm stops;
- Step length λ_p - number of solutions required at constant temperature, fixed in advance.

The flux diagram of the algorithm is given in Fig. 3.

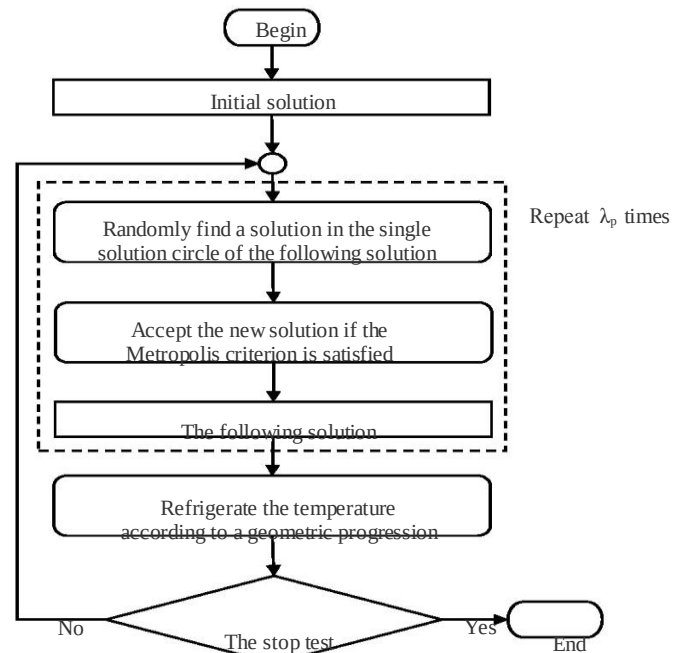


Fig.3 Simulated Annealing Method flow chart

Tabu Search Method (TS) is based on the caching of recent measures taken to avoid returning to search in previously explored areas.

In this method the best solution of the following solution circle is obtained from each approximation, which has no sequence located in the list tabu. This represents, for all sequences examined, the configuration that they had prior to this variation. So if a sequence was characterized by a configuration and it was processed, then any action that restores that configuration is forbidden.

The prohibitions imposed by the tabu list can only be violated if the solution considered satisfies the aspiration criterion, which provides that the considered solution has a value of objective function, better than the following optimal solution (ie, the best solution found until that moment).

The specificity used for (TS), especially the aspiration criterion, guarantees that this algorithm leads to finding a solution certainly not worse than the one dealing with (HC).

The Tabu Search is controlled by a single-dimension tabu list parameter denoted by the symbol λ_1 , which represents the number of approximations during which a given configuration is listed and considered prohibited. In some cases a stochastic variant of the algorithm is implemented, in which the tabu list dimension changes during the approximations from a value λ_{1min} to a value λ_{1max} .

In this stochastic variant, starting from a randomly selected value in the interval considered, for each approximation the tabu list dimension increases or decreases by one unit equilibrium.

The flow diagram of the algorithm is given in Fig. 4.

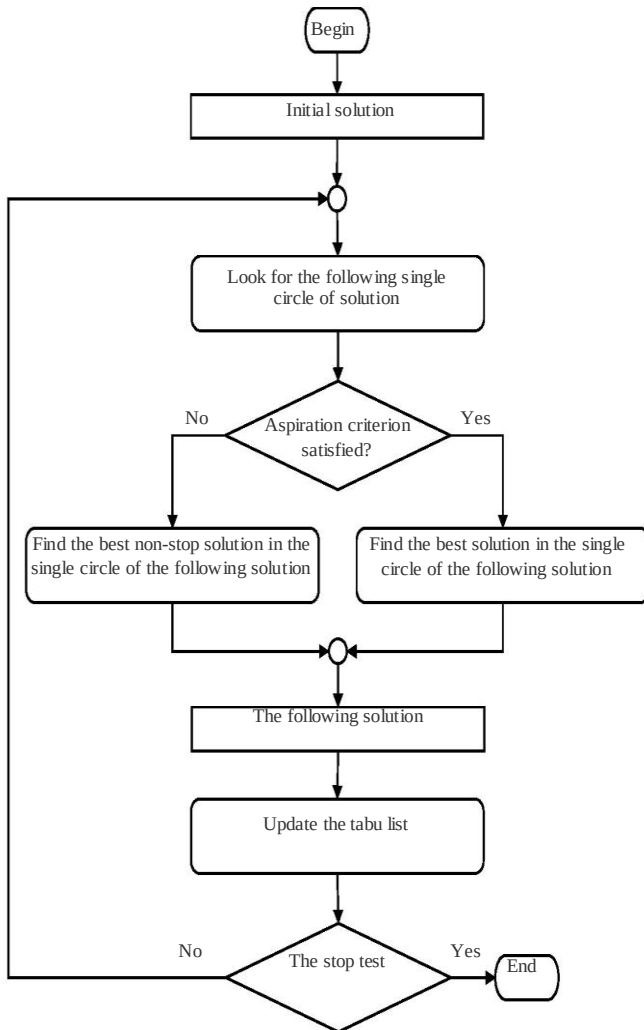


Fig. 4 Tabu Search Method flow chart

2. Applications of the combined intersections project

In designing successive semaphoric intersections, the need arises for information on the maneuvers performed in each of them. The most appropriate method for resolving these intersections is that of "joint flows" [2].

Let us consider two successive intersections as in Fig. 5, assuming each is regulated so that there are two phases: the first with green light traffic lights for vehicle streams coming from horizontal branches and the second with green lights from vertical branches.

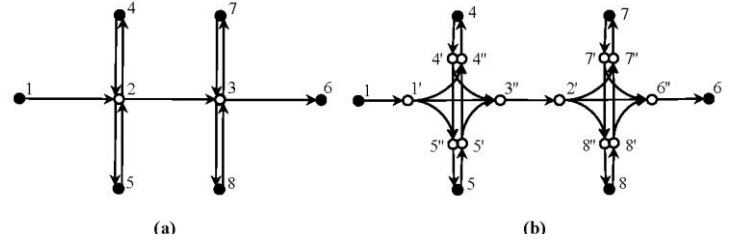


Fig. 5 Simple (a) and developed (b) representation of two consecutive intersections

The vehicles coming to junction "3" after passing through junction "2", have a phase change that depends on the phase at which they passed junction "2":

the flux " f_{11} " coming from node "1" crosses the junction "2" in the first phase, while the flux " f_{12} " coming from nodes "4" and "5" crosses the junction "2" at the second stage. In order to coordinate both traffic lights, the values of both flows must be known, which can be obtained from the representation of part (b) of the figure :

$$f_{11} = f_{1',3'}$$

$$f_{12} = f_{4',3'} + f_{5',3'}$$

In cases where intersections are also regulated with left turn phases (ie when there is more than one green phase for any of the entrances), more complete data is required. Therefore, without considering all combinations, consider the flow of vehicles passing from node "5" to node "7". If this flux is significant, then the phase allowing the left (2', 7'') crossing to coincide with the phase when the green is given the node "5" should be coordinated. When the flow is not large, then other combinations are given priority.

It is not possible to identify the vehicle flux from node "5" to "7" from the defined flows vector. Considering the matrix of joint flows, this flow is given by the term $f_{5',3' \rightarrow 2',7''}$.

In the case where the intersections are not consecutive but nevertheless close to each other, the branch flux vector does not provide enough information to project the phase coordination, nor when we have only one green phase for each input.

To concretize, add the branch (9,10) as in Fig. 6 and assume that part of the flow passing at junction "2" does not reach junction "3". Even in this case it is necessary to use the common flow matrix, as we used above.

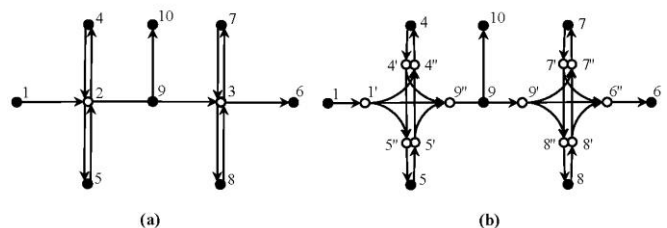


Fig. 6 Simple (a) and developed (b) representation of two intersections close to each other

Considering a general term of the matrix of joint flows, for example $f_{(1,2 \rightarrow (3,6))}$, it gives the flow passing branch (1,2) and then (3,6) but does not guarantee passage through branches (2,9) and (9,3). In this case the route could be (1-2-4... -7-3-6) and this complicates the calculation of the time needed to move from node "2" to node "3". Two cases can be observed:

- The portion of the flow that crosses a route other than the "direct" route (1-2-3-6) is insignificant. In this case we can continue to use the term $f_{(1,2 \rightarrow (3,6))}$ which appears quite close to the "direct" flux.
- The portion of the flow that crosses a route other than the "direct" route is not negligible. In this case the term $f_{(1,2 \rightarrow (3,6))}$ is no longer an acceptable approximation for "direct" flux.

The second hypothesis is more likely to increase the distance between semaphoric intersections (as the number of alternative routes may increase), while the benefits of coordination would be less significant. For this reason, we almost always consider the first case hypothesis. We note that in the case of successive intersections, by making the detailed presentation (b), an exact calculation can be made using the term $f_{(1',3' \rightarrow (2',6'))}$.

3. Conclusions

Given the complexity of the traffic light problem, especially in the case of successive intersections, we consider that the number of methods considered should increase. Since many of the half-hypotheses used in the phase when operating on topology variables depend on one or more parameters, the need arises to use different values to arrive at their calibration. To be as close to reality as possible, then the calibrated parameters will be used in another city and this will be the subject of a future study.

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On the question of the rational distribution of power between the hydrostatic and hydrodynamic branches of the complex steering mechanism for the tracked vehicle

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Abstract: The article presents a description of the mathematical model of the curvilinear movement of a tracked vehicle with a complex steering mechanism, which contains a control hydrostatic branch and an additional hydrodynamic branch for unloading the first. The adequacy of the presented mathematical model was verified by calculating the characteristics of the turn in place of the Leopard-2 tank. The resulting tool can become the basis for parametric optimization of similar steering mechanisms for tracked vehicles.

KEYWORDS: HYDROSTATIC STEERING MECHANISM OF A TRACKED VEHICLE, FILLABLE HYDRODYNAMIC COUPLINGS, MATHEMATICAL MODEL.

1. Introduction

Modern military tracked vehicles (TV), as a rule, have two-line hydrostatic steering mechanism (TLHSM), which make it possible to obtain a stepless change in the turning radius and provide the ability to turn the vehicle on the spot. The turn of the track vehicle on the spot mode is the most difficult for a two-line steering mechanism. This is due to the fact that in this mode, all engine power goes through the steering mechanism, and the main gearbox is simply locked. For heavy military TV, the weight has long exceeded 50 tons, and the power of the main engine has long exceeded 1000 hp. These vehicles have a width limitation due to the need to transport them by rail, which means that their length increases with increasing weight. This significantly increases the resistance to both turning and turning on the spot these vehicles. This means that the hydrostatic unit, which provides turning of the vehicle, with the classical approach to design, should significantly increase in size and weight. Back in the second half of the last century, an effective technical solution was found, which makes it possible to significantly relieve the hydrostatic unit (HSU) of the steering mechanism due to the fillable hydrodynamic couplings (HDU) [1, 2]. However, the design process for such steering mechanisms has always involved a large amount of complex engineering calculations. The problem of the optimal solution is associated with finding the ratio of the HSU and HDU parameters, which simultaneously provides the minimum volume and weight of the control system and good controllability of the vehicle.

2. Materials research.

2.1 Formulation of the Problem

In this paper, the authors set themselves the task of developing a mathematical model and software product that would allow to adequately simulate the process of turning a TV on horizontal terrain and at the same time be able to control all kinematic and power parameters in the transmission, including the pressure in HSU. The model should take into account slipping and skid of the tracked mover and be able to set different intensities and the law of rotation of the control wheel.

2.2 The Description of the Mathematical Model of the TV and the Calculation Assumptions

Assumptions and Simplifications that was Accepted.

- The movement of the TV is considered on horizontal terrain.
- The coordinate system associated with the TV has a beginning in the center of mass of the TV and axes: OX – forward, OY – to the left, OZ – up.
- The entrance to the turn and the movement in the turn are considered in the selected gear without switching in the gearbox.
- The engine is considered running on an external characteristic with full fuel supply.
- The ductility and resilience of shafts and other transmission elements is not taken into account due to the consideration of only low-frequency transients in the system without taking into account torsional vibrations.

– When the clutch in the base transmission are turned on, a linear increase in the friction torque is assumed from zero to the maximum value in 0.5 s.

– A turn is always viewed in one direction (to the left) and, accordingly, not the right and left, but the running and lagging sides are considered.

Initial data for modeling

TV parameters used for simulation:

- weight or mass of the TV;
 - track width of the TV;
 - length of the bearing surface of the TV;
 - drive wheel radius;
 - the height of the mass center;
 - maximum cross-sectional area of the TV;
 - the moment of inertia of the TV during rotation about a vertical axis passing through the center of mass;
 - the external characteristic of the engine (the dependence of the value of free torque on the frequency of rotation of the crankshaft at full fuel supply);
 - moment of inertia of the engine with a flywheel;
 - kinematic transmission scheme indicating the number of teeth on all gears;
 - the diameter and dependence of the torque on the turbine wheel on the frequency of its rotation during engine operation in maximum power mode;
 - the diameter and dependence of the torque on the HDU on the frequency of rotation of its turbine wheel at various levels of filling with the working fluid;
- Terrain parameters used for modeling:
- The coefficient of resistance to movement of the machine f ;
 - The coefficient of friction of track with the road φ ;
 - The coefficient of resistance to turning $\mu_{\max}$.

№	Type of terrain (road)	f	φ	$\mu_{\max}$
1.	Dry soddy loamy soil (humidity <8%)	0,08	0,9	0,9
2.	Dry loamy dirt road	0,065	0,8	0,8
3.	Loam plowing	0,1	0,7	0,7
4.	Wet road on loam	0,125	0,6	0,35
5.	Deep loose snow	0,25	0,3	0,3
6.	Asphalt	0,045	0,8	0,8

Structure of the Mathematical Model.

The mathematical model for studying the turn entry and the curved motion of the TV is based on the integration of differential equations describing the perturbed movement of the system and containing 6 generalized velocities (coordinates) [3, 4]:

- the longitudinal velocity of the TV, taking into account the skid (slipping) – v_X ;
- lateral sliding speed (drift) of the TV – v_Y ;
- the angular speed of rotation of the body of the TV relative to the vertical axis passing through the center of mass – ω_Z ;

- angular speed of rotation of the crankshaft of the engine and the associated pump of the hydrostatic steering control (HSU) and pump wheels of the HDU – ω_E ;
- angular speed of the turbine wheel of the torque converter, gearbox and epicycles of the summing planetary gear sets (steering epicyclic – SE) – ω_T ;
- angular speed of rotation of the HSU hydraulic motor and the associated turbine wheels of the HDU and solar gears of the SE – ω_{HSU} .

For each of the generalized velocities, a differential equation is compiled, which are grouped into a system:

$$\begin{cases} \frac{dv_X}{dt} = \frac{P_{D1} + P_{D2} - P_{F1} - P_{F2}}{G_M / g}; \\ \frac{dv_Y}{dt} = \frac{P_Y - P_{\phi 1} - P_{\phi 2}}{G_M / g}; \\ \frac{d\omega_Z}{dt} = \frac{0,5B(P_{D2} - P_{D1}) - M_{RR}}{I_Z}; \\ \frac{d\omega_E}{dt} = \frac{M_E - M_{ER}}{I_E + I_{ETR}}; \\ \frac{d\omega_T}{dt} = \frac{M_T - M_{TR}}{I_{TTR}}; \\ \frac{d\omega_{HSU}}{dt} = \frac{M_{HSU} + M_{HDU} - M_{HSUR}}{I_{HSUR}}. \end{cases}$$

Here the variables are:

P_{D1} and P_{D2} – traction (braking) forces on the lagging and running sides taking into account the sign, calculated by the slip or skid coefficients;

P_{F1} and P_{F2} – the forces of resistance to movement on the lagging and running sides taking into account the redistribution of normal reactions between the sides due to centrifugal force P_Y ;

P_Y – centrifugal force arising from the curvilinear movement of the TV;

$P_{\phi 1}$ and $P_{\phi 2}$ – cohesion (friction) force of the caterpillar mover with the soil in the transverse direction (the value $P_Y - P_{\phi 1} - P_{\phi 2}$ can be positive or equal to zero – the friction force cannot be driving);

M_{RR} – the moment of resistance to turning, depending on the geometric characteristics of the machine, its weight, turning radius and the characteristics of the soil (road);

M_E – engine torque;

M_{ER} – carried over to the crankshaft of the engine moment of resistance of the pump wheels of the torque converter and HDU, as well as the pump HSU;

M_T – torque on the turbine wheel of the torque converter;

M_{TR} – carried over to the turbine wheel moment of resistance to movement of the TV;

M_{HSU} – torque on the shaft of the HSU hydraulic motor;

M_{HDU} – torque on the HDU turbine wheel;

M_{HSUR} – the drag moment, transmitted from the sun gears of the SE, carried over to the shaft of the HSU hydraulic motor.

Constants:

G_M – weight (gravity) of the TV;

B – track width of the TV;

I_Z – the moment of inertia of the TV during rotation (turning) about a vertical axis passing through the center of mass;

I_E – moment of inertia of the engine with a flywheel;

I_{ETR} – carried over to the engine crankshaft moment of inertia of the pump wheels of the torque converter and HDU, as well as the HSU pump;

I_{TTR} – carried over to the turbine wheel of the torque converter the moment of inertia of the rotating parts of the transmission from the SE epicycles to the turbine wheel of the torque converter and part of the moment of inertia of the rotating parts of the transmission from the drive wheels to the SE carriers (levers);

I_{HSUR} – carried over to the shaft of the HSU hydraulic motor, the moment of inertia of the rotating transmission parts from the SE sun gears and from the turbine wheels of the HDU to the HSU hydraulic motor shaft.

Model of curved motion of a tracked vehicle on the terrain.

Input parameters of the “The turning” module.

“The turning” module as input parameters at each integration step uses the current values of the following generalized speeds:

– the longitudinal velocity of the TV, taking into account the skid (slipping) – v_X ;

– the angular velocity of rotation of the body of the TV relative to the vertical axis passing through the center of mass – ω_Z ;

– angular speed of the turbine wheel of the torque converter, gearbox and epicycles of the SE – ω_T ;

– angular speed of rotation of the HSU hydraulic motor and the associated turbine wheels of the HDU and solar gears of the SE – ω_{HSU} ;

as well as the gear number and all the constants characterizing the TV and the condition of the road (ground) on which the traffic is carried out.

The algorithm of work “The turning” module.

Given the linear v_X and angular ω_Z speeds of movement of the machine body, the actual longitudinal speeds of movement of the chassis of the lagging and running sides relative to the supporting surface are calculated:

$$V_1 = v_X - \omega_Z \frac{B}{2} \quad \text{and} \quad V_2 = v_X + \omega_Z \frac{B}{2}.$$

Further, the turning radii are determined for $\omega_Z \neq 0$ – central and along the sides:

$$R_C = \frac{v_X}{\omega_Z}, \quad R_1 = \frac{v_X}{\omega_Z} - \frac{B}{2} \quad \text{and} \quad R_2 = \frac{v_X}{\omega_Z} + \frac{B}{2}.$$

Knowing the radius of turning of the machine, we can determine the actual coefficient of resistance to turning μ on a given road (terrain) and the centrifugal force P_Y that occurs when turning:

$$\mu = \frac{\mu_{\max}}{0,85 + 0,15 \cdot R_2 / B},$$

where $\mu_{\max}$ – maximum turning resistance coefficient corresponding to turning around a stopped side.

$$P_Y = \frac{G_M v_X^2}{R_C}.$$

Knowing the centrifugal force P_Y and the actual coefficient of resistance to turning μ , we determine the absolute χ and relative χ_0 displacement of the pole of turning:

$$\chi = \frac{P_Y}{\mu G_M} \quad \text{and} \quad \chi_0 = \frac{2\chi}{L}.$$

If we get $\chi_0 > 1$, then we equating $\chi_0 = 1$ and recalculate the actual coefficient of resistance to turning μ :

$$\mu = \frac{P_Y}{G_M}.$$

Having finally decided on the coefficient of resistance to rotation μ , we find the moment of resistance to rotation:

$$M_{RR} = 0,25 \mu G_M L (1 + \chi_0^2).$$

Taking into account: the rotation speeds of the turbine wheel of the torque converter ω_T and the shaft of the HSU hydraulic motor

ω_{HSU} , current gear number and all gear ratios, we find the driving speeds of the driving wheels on the lagging and running sides: ω_{DW1} and ω_{DW2} .

Accordingly, the linear speeds of rewinding of tracks on the sides will be:

$$V_{T1} = \omega_{DW1} R_{DW} \quad \text{and} \quad V_{T2} = \omega_{DW2} R_{DW},$$

where R_{DW} – drive wheel radius.

Knowing the speed of rewinding the tracks, we find the efficiency of the caterpillar mover separately on the sides (η_{cat1} and η_{cat2}) and the slip coefficients (skid) σ_1 and σ_2 :

$$\eta_{cat1} = 0,95 - 0,018 \cdot V_{T1}; \quad \eta_{cat2} = 0,95 - 0,018 \cdot V_{T2};$$

$$\sigma_1 = \frac{V_{T1} - V_1}{V_{T1}} \quad \text{and} \quad \sigma_2 = \frac{V_{T2} - V_2}{V_{T2}}.$$

Knowing the centrifugal force P_Y , we determine the longitudinal component of the centrifugal force P_X and the actual normal reactions under the sides N_1 and N_2 , taking into account the redistribution of weight due to the force P_Y :

$$P_X = \frac{P_Y \chi}{R_C}; \quad N_1 = \frac{G_M}{2} - \frac{P_Y h_C}{B} \quad \text{and} \quad N_2 = \frac{G_M}{2} + \frac{P_Y h_C}{B}.$$

Here h_C – the height of the mass center. In the process of calculating the values N_1 and N_2 , it is necessary to control that the conditions $N_1 \geq 0$ and $N_2 \leq G_M$, that are responsible for the absence of the tipping of the machine are fulfilled.

Knowing the actual normal reactions under the sides N_1 and N_2 , we determine the maximum adhesion forces $P_{\phi 1}$, $P_{\phi 2}$ and the total resistance to movement under the sides P_{F1} , P_{F2} :

$$P_{\phi 1} = N_1 \varphi; \quad P_{\phi 2} = N_2 \varphi;$$

$$P_{F1} = N_1 f + \frac{0,65 F_{\max} v_X^2 + P_X}{2} \quad \text{and}$$

$$P_{F2} = N_2 f + \frac{0,65 F_{\max} v_X^2 + P_X}{2}.$$

Here φ and f – accordingly, the coefficients of adhesion of the mover to the road (terrain) and resistance to movement; $F_{\max}$ – maximum cross-sectional area of the TV.

Knowing the slipping (skid) coefficients σ_1 and σ_2 , we can determine the traction (braking) forces on the lagging P_{D1} and running P_{D2} sides taking into account the sign:

$$P_{D1} = \frac{\sigma_1}{0,3} R_{\phi 1}, \quad \text{if } \sigma_1 > 0,3, \quad \text{than} \quad P_{D1} = R_{\phi 1}, \quad \text{if } \sigma_1 < -0,3, \quad \text{than}$$

$$P_{D1} = -R_{\phi 1};$$

$$P_{D2} = \frac{\sigma_2}{0,3} R_{\phi 2}, \quad \text{if } \sigma_2 > 0,3, \quad \text{than} \quad P_{D2} = R_{\phi 2}, \quad \text{if } \sigma_2 < -0,3, \quad \text{than}$$

$$P_{D2} = -R_{\phi 2}.$$

Knowing the traction (braking) forces on the lagging P_{D1} and running P_{D2} sides, the direction of the power flows and all the gear ratios, we determine the load moments on the turbine wheel of the torque converter M_{TR} and the HSU hydraulic motor M_{HSUR} .

Output parameters of "The turning" module.

P_{D1} and P_{D2} – traction (braking) forces on the lagging and running sides taking into account the sign;

P_{F1} and P_{F2} – forces of resistance to movement on lagging and running sides;

P_Y – centrifugal force arising from the curvilinear movement of the machine;

$P_{\phi 1}$ and $P_{\phi 2}$ – adhesion forces of the caterpillar mover with the soil in the transverse direction;

M_{RR} – turning resistance torque;

M_{TR} – carried over to the turbine wheel torque resistance to movement of the TV;

M_{HSUR} – the drag moment carried over to the shaft of the HSU hydraulic motor transmitted from the sun gears of the SE.

The remaining modules of the model.

The «Engine» module.

The «Engine» module uses the speed of rotation of the crankshaft ω_E as an input parameter. The output parameter of the module is the engine torque M_E , calculated for the full fuel supply mode.

The «Torque Converter» module.

The «Torque Converter» module uses the crankshaft ω_E and turbine wheel ω_T speed of rotation as input parameters. The output parameters of the module are the torques on the turbine wheel of the torque converter M_T and on the pump wheel of the torque converter (part of the torque M_{ER}).

The «HSU» module.

The «HSU» module uses the speed of rotation of the shafts of the HSU hydraulic motor ω_{HSU} and the engine crankshaft ω_E , the HSU control parameter in fractions of unity (relative steering angle) as input parameters. The output parameters of the module are the torques on the HSU hydraulic motor M_{HSU} and on the HSU pump (part of the torque M_{ER}), as well as the pressure difference Δp .

The «HDU» module.

The «HDU» module uses the speed of rotation of the HSU hydraulic motor ω_{HSU} and the crankshaft of the engine ω_E as input parameters, as well as the pressure difference Δp in the HSU. The output parameters of the module are the torques on the HDU turbine wheel M_{HDU} and on the HDU pump wheel (the part of the torque M_{ER}).

Central integration unit.

The central integration unit is a classic solver module for integrating a system of differential equations using the Runge-Kutta method with constant or variable pitch. In this module, the right-hand sides of differential equations are formed that describe the behavior of a dynamic system taking into account changes in its structure during operation. As the initial data in the described module are entered:

- counting time;
- integration step in fractions of a second and the desired accuracy;
- a list of print options in the file of calculation results;
- gearbox operating mode (gear number);
- type of terrain (road) along which the VC is moving;
- initial conditions for each of the differential equations;
- cyclogram rotation of the helm.

From the central block in the required sequence, all previously described blocks are called up for the correct formation of the right-hand sides of the differential equations. Then, taking into account the accepted initial conditions, the differential equations are integrated and the counting results are written to disk. Processing of calculation results and construction of the necessary graphs is performed in the MS Excel program.

2.3. Calculations results

Parameters used for simulation:

- vehicle weight $G_M = 55$ t;
- vehicle track width $B = 2,785$ m;
- length of the supporting surface of the tracks $L = 4,73$ m;
- radius of the driving wheel $R_{DW} = 0,32125$ m;
- the height of the center of mass $h_C = 1,15$ m;
- maximum cross-sectional area of the vehicle $F_{\max} = 5$ m²;
- moment of inertia of the vehicle when rotating about the vertical axis passing through the center of mass $I_Z = 196200$ kgm²;
- moment of inertia of the engine with a flywheel $I_E = 78,48$ kgm²;

- a kinematic diagram of the transmission with an indication of the number of teeth on all elements (Fig. 1) [2];

- the external characteristic of the engine, the dependence of the torque on the turbine wheel of the torque converter on the frequency of its rotation when the engine is operating at maximum power, the dependence of the torque on the turbine of HDU on its rotation frequency at different levels of filling with the working fluid, characteristics of HSU are taken from [1, 6].

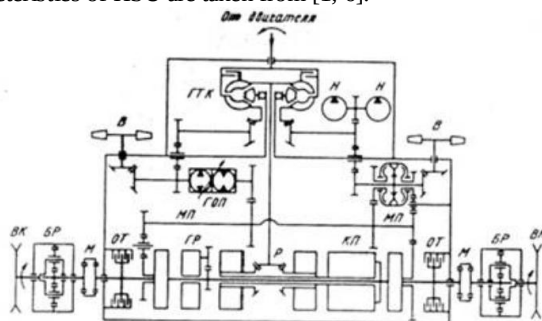


Figure 1 – Kinematic diagram of the transmission

When turning the vehicle on a horizontal asphalt surface, in the case of turning the steering wheel to the maximum position in 1 s, a 90° degree turn is completed in 3,6 s, 180° - in 6 s and 360° - in 10,7 s. At the same time, all transient processes in the engine and transmission completely calmed down in the first 2.5 seconds. Below (fig. 2-5) are the graphs of the main transient processes characterizing the distribution of power flows in the transmission when the vehicle turns in place.

In fig. 3-5, number 1 designates the parameter at the input to the device, and 2 - at the output from the device.

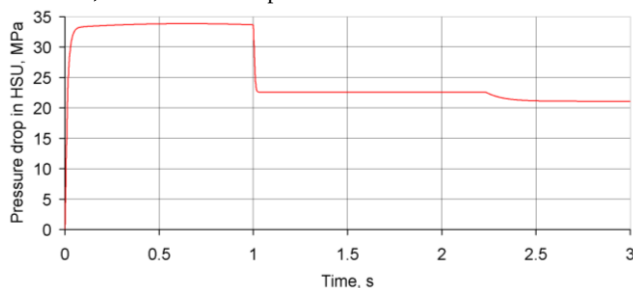


Figure 2 – Pressure drop in HSU

3. CONCLUSIONS

In accordance with the goals and objectives set for the results of the work done, the following conclusions can be drawn:

1) The calculated turn in place time of the Leopard-2 tank on a horizontal asphalt site using rubber asphalt pads when turning the steering wheel from the neutral position to the maximum in 1 second with an accuracy of 3% corresponds to those stated in the tactical and technical characteristics of this vehicle [1, 6]. This testifies to the adequacy of the developed mathematical model for this mode of motion.

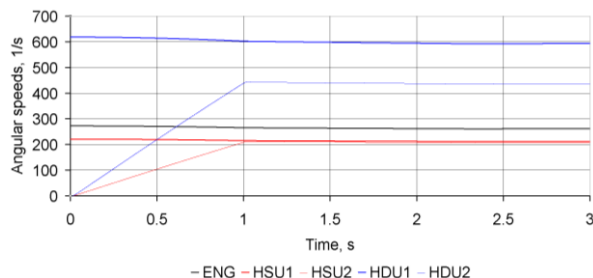


Figure 3 – Angular speeds in main units of transmission

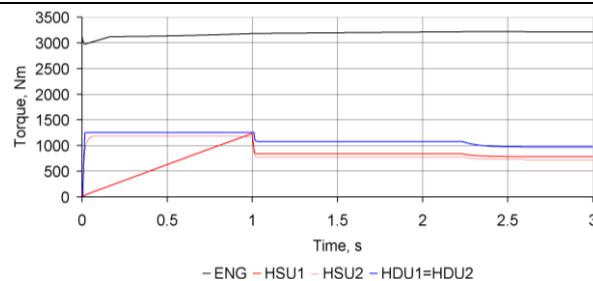


Figure 4 – Torque in main units of transmission

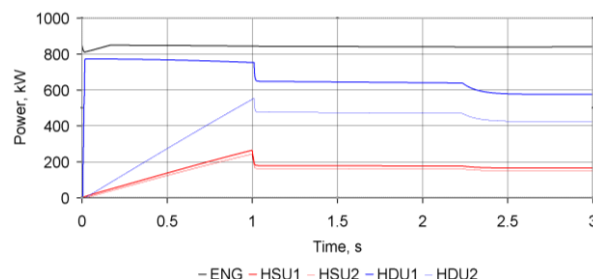


Figure 5 – Power in main units of transmission

2) The developed mathematical model and the software product that implements it make it possible to efficiently numerically study any planetary transmissions of tracked vehicles with TLHSM and hydrodynamic unloading in order to optimize their parameters at the design stage.

3) When designing TLHSM with hydrodynamic unloading for tracked vehicles, the power ratio of HDU and HSU should be approximately 3 to 1. This allows, on the one hand, to significantly relieve the HSU and, on the other hand, without disturbing the stability of the control system, to use the HSU as a link directly controlling the turning process.

4. LITERATURE

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Engine model for control concepts and e-fuel identification for recreational vehicles and hand-held tools

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Abstract: Mean value models are essential for developing control engineering methods, e.g., speed control concepts, failure monitoring features. This work briefly summarizes the main parts of such a second-order mean value model, suitable for control engineering purposes. The nonlinear model is linearized around one operating point, and a linear state controller is designed, both for single-input and multiple-input, without and with an integral component to eliminate steady-state deviations. Limitations of the proposed linear control concepts, potential advantages of nonlinear flatness-based control concepts, and possible extensions of the model for fuel identification are discussed in the outlook.

Keywords: MEAN VALUE MODELS, LINEAR STATE CONTROL CONCEPTS, PARAMETER ESTIMATION

1. Introduction

The European Union (EU) has agreed to reduce greenhouse gas emissions by 55 percent by 2030 compared to 1990 levels. To achieve this ambitious reduction, it is inevitable to drastically reduce CO₂ emissions from transport. In addition to the further development of novel drive concepts, e.g., electromobility or hydrogen-powered vehicles, it is required to reduce the emission of pollutants from conventional combustion engines. Lower Emissions can be achieved on the one hand by developing more intelligent engine management and control concepts, and on the other hand by using synthetic, means CO₂ neutral, fuels. However, one must adapt the engine control systems to the different fuel types to operate in the optimum range, e.g., low emissions. For such intelligent control concepts of modern combustion engines, mathematical models with reduced complexity but considering essential system dynamics with sufficient accuracy are crucial. Mainly when used in the low-cost segment or less computationally powerful ECUs, the models and algorithms used must be resource-efficient. Standard computational fluid dynamics (CFD) simulation models or characteristic curve fields are unsuitable for this purpose. For just such requirements, so-called mean value models have been developed, representing the essential system behavior as a function of time. The term mean value model was probably introduced by [1] and applied to internal combustion engines by [2]. A detailed overview of mean value engine models is given in [3, 4]. Such mean value models form the basis for developing linear and nonlinear control concepts, which serve as a fundamental tool for more in-depth analysis, e.g., for identifying the fuel characteristic. In [5–7], for example, the ethanol content of the fuel is estimated.

Section 2 briefly summarizes the main subsystems of a mean value model of a spark-ignition engine with port injection described in detail, e.g., [8]. Based on the linearized resulting nonlinear model, a linear state controller is designed in Section 3 for both the single-input and the multiple-input cases, which is then extended to include an integral component to suppress steady-state errors. Simulation results in Section 4 show the effectiveness of such control schemes. Finally, Section 5 gives a short outlook on nonlinear flatness-based control concepts.

2. Mean Value Model

Both highly complex CFD motor models and frequently used characteristic maps are not suitable for control engineering tasks. For the development or implementation of state-of-the-art control engineering methods, abstracted dynamic models reduced to the essentials are necessary. Usually, these mathematical models consist of a set of differential equations. So-called mean value models average over one engine cycle. For this reason, the independent parameter is also time and not the crankshaft angle, as is usually the case. Typically, mean value models have lumped parameter models, specified by nonlinear differential equations, often even ordinary differential equations. Such models are suitable for ECU implementation and offer online (real-time) monitoring

functionalities, e.g., online parameter estimation, or provide adaptive control features.

The mean value model presented here is a physics-based control-oriented model. It models the input-output behavior with a reasonable precision but with low computational complexity, suitable for ECUs. We assume a four stroke port injection engine, consisting of two dynamical systems, namely air path and mechanical system with the subsystems:

- Airpath (intake manifold pressure)
 - Air mass flow throttle valve
 - Air mass flow cylinder
 - Intake manifold
- Mechanical system (engine speed)
 - Torque generation
 - Engine speed

One finds an abstracted overview diagram in Fig. 1.

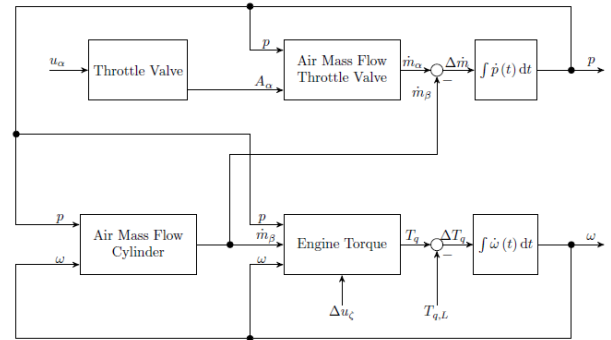


Fig. 1 Schematic diagram of a mean value engine model.

The essential subsystems with their fundamental mathematical relationships are presented and finally combined to form the complete engine model. For a better overview, the essential model parameters are listed in Tab.

As shown in Fig. 2, the incoming airflow $\dot{m}_\alpha$ depends on the opening area or the opening angle of the throttle. It applies

$$(1) \quad \dot{m}_\alpha \approx A_\alpha \frac{p_a}{\sqrt{2R_\beta T_a}}$$

where A_α is the opening area of the valve, p_a ambient pressure, T_a ambient temperature, and R_β is the specific gas constant of fresh air. The cylinder is modeled as a volumetric pump, resulting in an approximated speed-dependent engine mass flow $\dot{m}$. One can use a pressure- and speed-dependent efficiency parameter $\lambda_l(p, \omega)$ to describe the deviation of the behavior from an ideal volumetric pump. One obtains

$$(2) \quad \dot{m} = \dot{m}_\beta + \dot{m}_\varphi \approx \frac{p}{R_\beta T_\beta} \lambda_l(p, \omega) \frac{V_d}{N} \frac{\omega}{2\pi}$$

where $\dot{m}_\beta$ is the air mass flow into the cylinder, $\dot{m}_\varphi$ is the fuel mass flow into the cylinder, and R_β denotes the specific gas constant of fresh air with the corresponding air temperature T_β . Additionally, V_d is the displaced cylinder volume, and N is the number of revolutions per cycle, e.g., $N = 2$ for four-stroke engines.

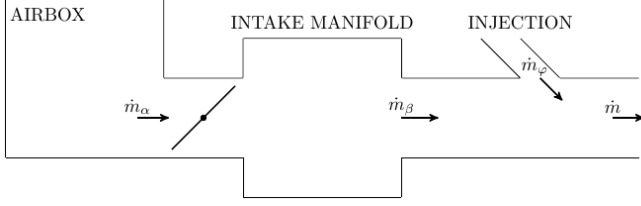


Fig. 2 Schematic diagram of the mass flow into the cylinder.

One can split the efficiency parameter into two main factors (multilinear formulation), namely a speed-dependent part $\lambda_{l,\omega}(\omega)$ and pressure-dependent part $\lambda_{l,p}(p)$, resulting in

$$(3) \quad \dot{m} = \dot{m}_\beta + \dot{m}_\varphi \approx \frac{p}{R_\beta T_\beta} \lambda_{l,\omega} \lambda_{l,p} \frac{V_d}{N} \frac{\omega}{2\pi}.$$

To become independent of fuel type, for the specific gas constant and temperature, we assume air instead of the unknown air-fuel mixture, for example, $R \rightarrow R_\beta$. Literature, e.g., [8], shows that this approximation results in an error of about 5% for pure gasoline. Obviously, for other fuels or fuel mixtures, it can be more significant.

Using the relationship between the air-fuel equivalence ratio λ and the actual AFR

$$(4) \quad \lambda = \frac{AFR}{AFR_{ST}}$$

where AFR_{ST} denotes the stoichiometric air-fuel ratio, for the air mass flow into the cylinder applies

$$(5) \quad \dot{m}_\beta = \dot{m} \frac{1}{1 + \frac{1}{\lambda AFR_{ST}}} = \dot{m} \tilde{\sigma}.$$

Furthermore, we assume the intake manifold to be a receiver, i.e., a fixed volume with constant thermodynamic states but dependent on time. With the simplifications or assumptions

- no changes in kinetic energy,
- no heat transfer via walls,
- constant volume,
- frictionless mass transport,
- no work brought in through the walls,

one can use the isothermal formulation of the ideal gas law to obtain

$$(6) \quad \frac{d}{dt}(p) = \frac{RT}{V_m} (\dot{m}_\alpha - \dot{m}_\beta)$$

suitable for lower speed or load torque. Parameter V_m denotes the manifold volume, R and T , the mixture gas constant, and temperature. Again, assuming pure air instead of the air-fuel mixture for simplification, for (6) applies

$$(7) \quad \frac{d}{dt}(p) = \frac{R_\beta T_\beta}{V_m} (\dot{m}_\alpha - \dot{m}_\beta).$$

The second central part of the provided control-oriented model deals with the mechanical part, i.e., the mechanical torque generation and engine speed. Literature, e.g., [8], shows that the mechanical torque is a highly nonlinear function of many variables,

e.g., fuel mass, air-fuel ratio (AFR), engine speed, ignition timing, etc., but not suitable for control purposes. To reduce the complexity, [8] suggests introducing the fuel mean effective pressure (FMEP)

$$(8) \quad p_\varphi = \frac{C_l \dot{m}_\varphi}{V_d}$$

where C_l is the lower calorific value of the fuel, and the brake mean effective pressure (BMEP) or mean effective pressure

$$(9) \quad p_e = \frac{4\pi T_{q,c}}{V_d}$$

where $T_{q,c}$ denotes the torque generated by the combustion process. With

$$(10) \quad \dot{m}_\varphi = m_\varphi \frac{\omega}{4\pi}$$

and

$$(11) \quad \lambda = \frac{\dot{m}_\beta}{AFR_{ST} \dot{m}_\varphi}$$

one can express (9) by

$$(12) \quad p_e = \frac{4\pi}{\lambda AFR_{ST}} \frac{C_l \dot{m}_\beta (t - \tau_{ips})}{V_d \omega (t - \tau_{ips})}$$

where τ_{ips} describes the time delay from fuel injection to ignition.

The relationship between theoretical mean fuel pressure and actual mean effective pressure is given by

$$(13) \quad p_e = e(\omega, \lambda, \zeta, \dots) p_\varphi$$

where e is the so-called efficiency constant, including all thermodynamic properties. Joining (8), (9), and (13), one obtains a formulation for the generated torque

$$(14) \quad T_{q,c} = p_e \frac{V_d}{4\pi} = e p_\varphi \frac{V_d}{4\pi} = e \frac{C_l \dot{m}_\varphi}{4\pi}.$$

Taking into account friction losses

$$(15) \quad p_{e,f} = (d_0 + d_1 \omega) \frac{4\pi}{V_d}$$

where d_0 and d_1 describes the friction coefficients and gas exchange losses

$$(16) \quad p_{e,g} = p_{exh} - p$$

with assumed constant exhaust manifold pressure p_{exh} , one obtains the mechanical moment available for use

$$(17) \quad T_q = (e p_\varphi - p_{e,f} - p_{e,g}) \frac{V_d}{4\pi} = T_{q,c} - T_{q,f} - T_{q,g}$$

where $T_{q,f}$ is the friction moment and $T_{q,g}$ is the gas exchange moment (losses). Usually, there are two adjusting screws, i.e., input variables, to influence the generated torque and speed or velocity. On the one hand, via a change in the air mass flow, i.e., the position of the throttle valve (throttle angle) u_α , and via the ignition timing. While the influence of the throttle valve is rather sluggish due to the dynamics of the air path (indirect input quantity), the change of the ignition angle Δu_ζ can directly influence the combustion and thus the mechanical torque. To incorporate the ignition angle delay, one splits the efficiency constant into a speed-dependent part e_ω and an ignition angle-dependent part e_ζ . Other thermodynamic properties are neglected due to simplicity. One can write

$$(18) \quad e \approx e_\omega \cdot e_\zeta = (\eta_0 + \eta_1 \omega) \cdot \left(1 - k_\zeta \Delta u_\zeta \left(t - \frac{\tau_{seg}}{2}\right)^2\right)$$

where η_0 , η_1 and k_ζ are model coefficients need to be estimated, and τ_{seg} describes the time constant for torque generation. Finally, assuming constant moment of inertia, one obtains

$$(19) \quad \frac{d}{dt}(\omega) = \frac{1}{J}(T_q - T_{q,L})$$

where J is the engine's moment of inertia and $T_{q,L}$ describes the external load torque.

Equations (7) and (19) describe the dynamic system behavior. By inserting the presented parts, one finally obtains a nonlinear model of the form

$$(20) \quad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{u}) \\ \mathbf{y} &= \mathbf{g}(\mathbf{x}, \mathbf{u}) \end{aligned}$$

with state vector $\mathbf{x}$, input vector $\mathbf{u}$, output vector $\mathbf{y}$, and vector fields $\mathbf{f}, \mathbf{g}$.

Neglecting time delays, for the mean value engine model applies

$$(21) \quad \begin{aligned} \dot{\mathbf{x}} &= \begin{pmatrix} -\frac{V_d}{V_m} \frac{\omega}{4\pi} \tilde{\sigma} \lambda_{l,\omega} \lambda_{l,p} p + \frac{RT_m p_a}{V_m \sqrt{2RT_a}} \alpha_0 \\ \frac{1}{J} \left(-(\beta_0 + \beta_1 \omega) - \frac{V_d}{4\pi} (p_{exh} - p) \right. \\ \left. + \frac{RT_m p_a}{V_m \sqrt{2RT_a}} \alpha_1 u_\alpha \right. \\ \left. + (\eta_0 + \eta_1 \omega) (1 - k_\zeta \Delta u_\zeta^2) \frac{C_l \dot{m}_\beta}{AFR_{ST} \lambda \omega} - T_{q,L} \right) \end{pmatrix} \\ \mathbf{y} &= \omega \end{aligned}$$

with state vector $\mathbf{x}^T = (p \ \omega)$, input vector $\mathbf{u}^T = (u_\alpha \ \Delta u_\zeta)$, and output $\mathbf{y} = \omega$. For a more detailed survey on mean value engine modeling, the kindly reader is referred to, e.g., [8].

Unknown model parameters have to be estimated using measurement data to fit the model to the real engine system. Depending on the form of the parameters in the equations, different methods are suitable. For example, parameters that occur linearly in the equations can be determined using least squares. A detailed survey about parameter estimation of continuous-time systems is given in [9]. For real-time application, Poisson Moment Functional (PMF) approach is suitable, e.g., [10].

3. Control Concepts

In general, speed control can follow arbitrary transient speed trajectories (not only stationary or step functions), with the significant advantage is that it becomes possible to fulfill the user's speed request and execute some fault monitoring applications. For example, it should be possible to follow any arbitrary transient speed trajectory, suitable for estimating specific parameters, maybe for fuel identification.

3.1. Equilibrium Point Linearization

The linearized model equations often describe the nonlinear model with sufficient accuracy for small deflections from a rest position or equilibrium position. According to this, it is possible to apply the sufficiently known and proven methods for analysis and synthesis, e.g., linear state controllers. One possible equilibrium state is the engine idle.

Assuming sufficiently small deviations $\Delta \mathbf{u}$ from $\mathbf{u}_s$ and $\Delta \mathbf{x}_0$ from $\mathbf{x}_s$, it applies

$$(22) \quad \begin{aligned} \Delta \dot{\mathbf{x}} &= \mathbf{A} \Delta \mathbf{x} + \mathbf{B} \Delta \mathbf{u} & \Delta \mathbf{x}(t_0) &= \Delta \mathbf{x}_0 \\ \Delta \mathbf{y} &= \mathbf{C} \Delta \mathbf{x} + \mathbf{D} \Delta \mathbf{u} \end{aligned}$$

where

$$(23) \quad \begin{aligned} \mathbf{A} &= \left. \frac{\partial}{\partial \mathbf{x}} \mathbf{f}(\mathbf{x}, \mathbf{u}) \right|_{\mathbf{x}=\mathbf{x}_s, \mathbf{u}=\mathbf{u}_s} & \mathbf{B} &= \left. \frac{\partial}{\partial \mathbf{u}} \mathbf{f}(\mathbf{x}, \mathbf{u}) \right|_{\mathbf{x}=\mathbf{x}_s, \mathbf{u}=\mathbf{u}_s} \\ \mathbf{C} &= \left. \frac{\partial}{\partial \mathbf{x}} \mathbf{g}(\mathbf{x}, \mathbf{u}) \right|_{\mathbf{x}=\mathbf{x}_s, \mathbf{u}=\mathbf{u}_s} & \mathbf{D} &= \left. \frac{\partial}{\partial \mathbf{u}} \mathbf{g}(\mathbf{x}, \mathbf{u}) \right|_{\mathbf{x}=\mathbf{x}_s, \mathbf{u}=\mathbf{u}_s} \end{aligned}$$

are the matrices of the linearized model.

3.2. Linear State Control (Fixed Setpoint Control)

Linear state controllers have been an essential tool in modern control for many years. In contrast to classical input/output controllers, the eigenvalues of the closed-loop dynamic matrix are specified by weighted feedback of all system states to achieve the desired dynamic.¹ In nonlinear models, these must be linearized around an operating point to design the control law around this operating point. Because all state variables are used in the control law, all system states must also either be measured or estimated by state observers.

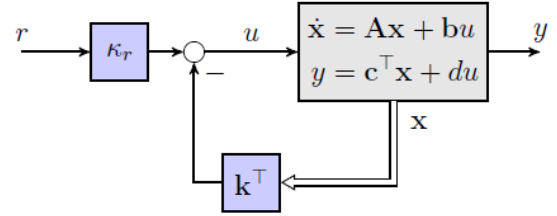


Fig. 3 Linear state control (SISO).

The linear state model for single-input single-output (SISO) reads

$$(24) \quad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{A} \mathbf{x} + \mathbf{b} u \\ \mathbf{y} &= \mathbf{c}^T \mathbf{x} + d u \end{aligned}$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{b} \in \mathbb{R}^{n \times 1}$, $\mathbf{c}^T \in \mathbb{R}^{1 \times n}$, and $d \in \mathbb{R}$. With the control law

$$(25) \quad u = -\mathbf{k}^T \mathbf{x} + \kappa_r r$$

one obtains

$$(26) \quad \begin{aligned} \dot{\mathbf{x}} &= (\mathbf{A} - \mathbf{b} \mathbf{k}^T) \mathbf{x} + \mathbf{b} \kappa_r r = \mathbf{A}_e \mathbf{x} + \mathbf{b}_e r \\ \mathbf{y} &= (\mathbf{c}^T - d \mathbf{k}^T) \mathbf{x} + d \kappa_r r = \mathbf{c}_e^T \mathbf{x} + d_e r \end{aligned}$$

where the feedback vector $\mathbf{k}^T = (k_0 \ \dots \ k_{n-1})$ is used to set the eigenvalues of the extended dynamic matrix $\mathbf{A}_e \in \mathbb{R}^{n \times n}$ properly. If the model is in controllable canonical form, i.e.,

$$(27) \quad \mathbf{A}_e = \begin{pmatrix} 0 & 1 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -a_0 - k_0 & -a_1 - k_1 & \dots & -a_{n-1} - k_{n-1} \end{pmatrix}$$

and

$$(28) \quad \mathbf{b}_e = \mathbf{e}_n = (0 \ \dots \ 0 \ 1)^T$$

one can quickly build the characteristic polynomial

$$(29) \quad p(s) = -a_0 - k_0 + (-a_1 - k_2)s + \dots + (-a_{n-1} - k_{n-1})s^{n-1} + s^n$$

and obtains a calculation rule for the choice of the feedback vector. If the model is not in control canonical form, it must be transformed. Provided that the system is fully reachable, i.e.,

$$(30) \quad \text{rank}(\mathbf{M}_e) = \text{rank}(\mathbf{B} \quad \mathbf{Ab} \quad \dots \quad \mathbf{A}^{n-1}\mathbf{b}) = n$$

the eigenvalues of the extended dynamics matrix can be placed arbitrarily, and the feedback vector can be calculated with Ackermann's formula, i.e.,

$$(31) \quad \begin{aligned} \mathbf{e}_n^T &= \mathbf{t}_1^T \mathbf{M}_e = \mathbf{t}_1^T (\mathbf{B} \quad \mathbf{Ab} \quad \dots \quad \mathbf{A}^{n-1}\mathbf{b}) \\ \mathbf{k}^T &= \mathbf{t}_1^T p(\mathbf{A}) = \alpha_0 \mathbf{t}_1^T + \alpha_1 \mathbf{t}_1^T \mathbf{A} + \dots \\ &\quad + \alpha_{n-1} \mathbf{t}_1^T \mathbf{A}^{n-1} + \mathbf{t}_1^T \mathbf{A}^n \end{aligned}$$

where $p(s) = a_0 + \alpha_1 s + \dots + \alpha_{n-1} s^{n-1} + s^n$.

To achieve stationary accuracy for step input $r = \sigma(t)$, i.e.,

$$(32) \quad y_s = \lim_{t \rightarrow \infty} y = r_s$$

for parameter κ_r applies

$$(33) \quad \kappa_r = -\frac{1}{(\mathbf{c}^T - d\mathbf{k}^T)(\mathbf{A} - \mathbf{b}\mathbf{k}^T) + d}.$$

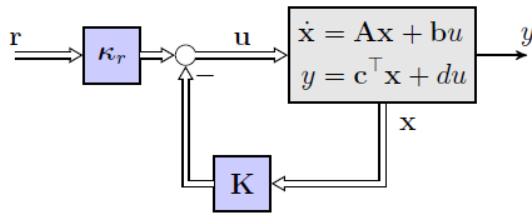


Fig. 4 Linear state control (MISO).

Equations (31) and (33) can be extended to multiple-input single-output (MISO) models

$$(34) \quad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{Ax} + \mathbf{Bu} \\ \mathbf{y} &= \mathbf{c}^T \mathbf{x} + d\mathbf{u} \end{aligned}$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, $\mathbf{c}^T \in \mathbb{R}^{1 \times n}$, and $d \in \mathbb{R}^{1 \times m}$. Using a dyadic control approach, e.g. [11], one introduces $\tilde{\mathbf{u}} \in \mathbb{R}$, $\mathbf{q} \in \mathbb{R}^m$, and substitutes

$$(35) \quad \mathbf{u} = \mathbf{q}\tilde{\mathbf{u}}$$

resulting in the equivalent SISO model

$$(36) \quad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{Ax} + \tilde{\mathbf{b}}\tilde{\mathbf{u}} \\ \mathbf{y} &= \mathbf{c}^T \mathbf{x} + \tilde{d}\tilde{\mathbf{u}} \end{aligned}$$

with $\tilde{\mathbf{b}} = \mathbf{B}\mathbf{q}$ and $\tilde{d} = d\mathbf{q}$.

The feedback vector $\tilde{\mathbf{k}}^T$ is computed using (31), and one obtains the feedback matrix for the MISO withⁱⁱ

$$(37) \quad \mathbf{K} = \mathbf{q}\tilde{\mathbf{k}}^T.$$

3.2. PI - State Control

To eliminate permanent (steady-state) deviations, the state control law can be extended by an integral component. Literature shows several approaches for the selection of the weights or the feedforward control gain. In [12], an approach is presented, making it possible to take over the existing control law and design only the integral part anew. This has the additional advantage of switching the integral component on and off in real-time. According to [12], the extended control law reads

$$(38) \quad \begin{aligned} \dot{x}_I &= y - r \\ u &= -\mathbf{k}^T \mathbf{x} - \kappa_I (x_I + \Delta \mathbf{k}^T \mathbf{x}) + \kappa_r r \end{aligned}$$

with

$$(39) \quad \Delta \mathbf{k}^T = -(\mathbf{c}^T - d\mathbf{k}^T)(\mathbf{A} - \mathbf{b}\mathbf{k}^T)^{-1}.$$

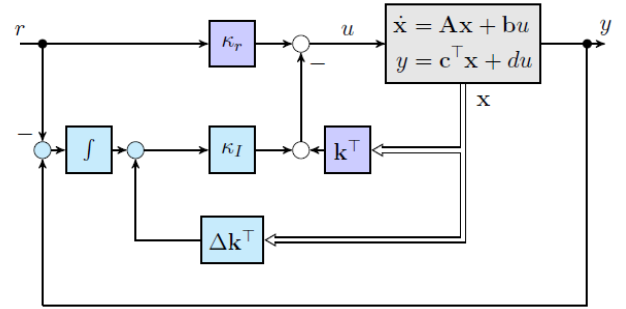


Fig. 5 Linear state control with integral part (SISO).

For a general multiple-input multiple-output (MIMO) system

$$(40) \quad \begin{aligned} \dot{\mathbf{x}} &= \mathbf{Ax} + \mathbf{Bu} \\ \mathbf{y} &= \mathbf{Cx} + \mathbf{Du} \end{aligned}$$

where $\mathbf{A} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times m}$, $\mathbf{C} \in \mathbb{R}^{n_y \times n}$, and $\mathbf{d} \in \mathbb{R}^{n_y \times m}$, one can extend the control law and end up with

$$(41) \quad \begin{aligned} \dot{x}_I &= \mathbf{y} - \mathbf{r} \\ \mathbf{u} &= -\mathbf{K}\mathbf{x} - \kappa_I (\mathbf{x}_I + \Delta \mathbf{k}^T \mathbf{x}) + \kappa_r \mathbf{r}. \end{aligned}$$

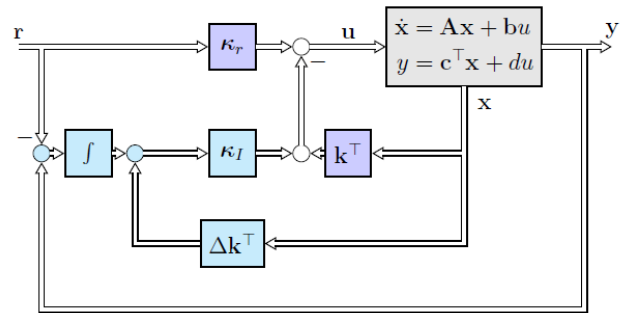


Fig. 6 Linear state control with integral part (MIMO).

Table 1: Mean value engine model parameters.

Abbreviation	Description
$\dot{m}_\alpha$	air mass flow through throttle valve
A_α	valve opening area (coefficients α_0, α_1)
p_a	ambient pressure
R, R_β	specific gas constant, β denotes fresh air
T_a	ambient temperature
$\dot{m}$	engine mass flow
$\lambda_i(p, \omega), \lambda_{i,\omega}, \lambda_{i,p}$	volumetric pump, efficiency parameters
$\dot{m}_\beta$	air mass flow into cylinder
$\dot{m}_\phi$	fuel mass flow into cylinder
p	(intake) manifold pressure
T_β	fresh air temperature
V_d	displaced cylinder volume
N	number of revolutions per cycle
ω	engine speed (model output)
λ	equivalence air-to-fuel ratio
AFR, AFR_{ST}	(stoichiometric) air-to-fuel ratio
V_m	(intake) manifold volume
p_ϕ	fuel mean effective pressure (FMEP)
C_l	Lower heating value
m_ϕ	fuel mass burnt per combustion cycle
p_e	brake mean effective pressure (BMEP)
$T_{q,c}$	torque generated by combustion
τ_{ips}	time delay from fuel injection to ignition
e, e_ω, e_ζ	thermodynamic efficiency constant (coefficients η_0, η_1, k_ζ)
$p_{e,f}/T_{q,f}$	friction losses pressure/torque (coefficients d_0, d_1)
$p_{e,g}/T_{e,g}$	gas exchange losses pressure/torque
p_{exh}	exhaust manifold pressure
T_q	mechanical torque
τ_{seg}	time constant for torque generation
u_α	throttle angle (model input)
Δu_ζ	ignition angle delay (model input)
$T_{q,L}$	load torque
J	moment of inertia (engine)

4. Results & Discussion

To obtain the equilibrium system states for linearization, the nonlinear model is simulated with arbitrarily chosen constant model inputs $\mathbf{u}_s$

$$(42) \quad u_\alpha = 2.3\% \quad \Delta u_\zeta = -20^\circ$$

resulting in rest position $\mathbf{x}_s$

$$(43) \quad p_s = 2.12 \cdot 10^4 \text{ Pa} \quad \omega_s = 118.74 \frac{\text{rad}}{\text{s}}.$$

Fig. 7 shows the simulation results of the SISO and MISO state controller without an integral component applied to the nonlinear model. Both controllers react to a sudden load torque at time $t = 2$ s, and equilibrium is reached. As expected, a stationary deviation remains due to the unknown load torque. Due to the faster intervention of the ignition angle delay, this is smaller with the MISO controller than with the SISO controller.

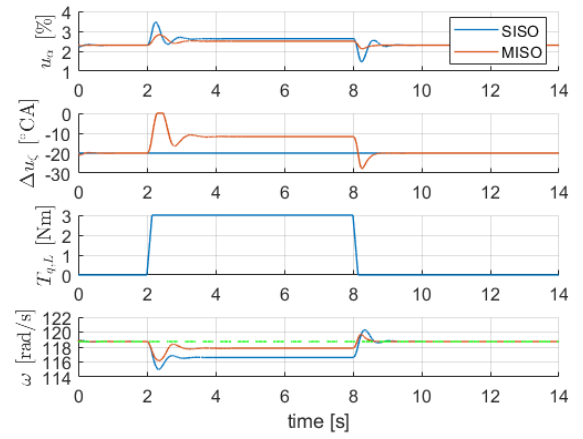


Fig. 7 Linear state control SISO vs. MISO. Operating point control with step-wise load change, where green-dashed is the setpoint.

If an integral component is added to the controllers, even these steady-state deviations can be controlled to zero, see Fig. 8.

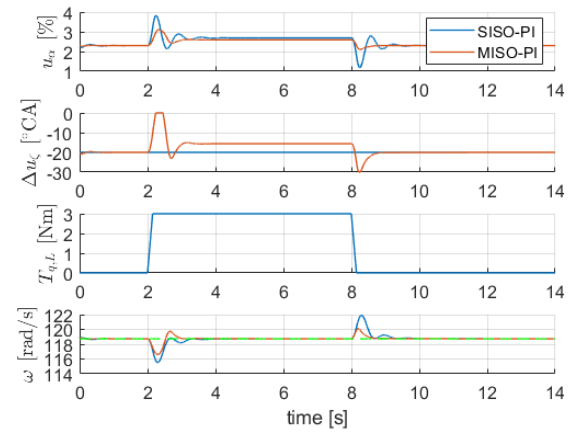


Fig. 8 Linear state control with integral part (SISO vs. MISO). Operating point control with step-wise load change, where green-dashed is the setpoint.

5. Conclusion & Future Work

In this work, on the one hand, the derivation of a second-order control engine model was shown. On the other hand, the operating point linearization and the concept of the linear state controller were explained. Simulation results show the functionality of the linear state controller on the nonlinear model, both for the single- and multi-variable case. Such control concepts are well suited for operating point control but not for the specification of arbitrary speed characteristics over an extensive speed range. This is because the linearized model is only valid in a small environment around the rest position. A change of the operating point is not trivial since the linearized model, and the state controller must be recalculated for each new operating point. Nonlinear flatness-based control concepts provide a remedy. With the help of exact linearization and a trajectory-following control, it is possible to specify arbitrary speed curves that can be followed precisely.

Other useful extensions of this work include implementing a wall film model, e.g., [5, 13], a multi-component fuel model, e.g., [5], and the exhaust path. By implementing the exhaust gas path, a lambda control can be implemented, for example. One can estimate specific characteristic fuel parameters (online) based on the introduced or planned control concepts with a fuel model, thus ensuring permanent engine tuning to the fuelled fuel, e.g., [7].

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ⁱ Please note, if not all system states are measured, the missing quantities must be determined or estimated otherwise. State observers, e.g. Luenberger observers, or Kalman filters are suitable for this purpose.

ⁱⁱ For practical implementation, for example, the Matlab command "place" is suitable.

Optimal design of an integrated 1st generation biodiesel / diesel supply chain based on solid waste management for energy efficiency improvement

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Abstract: The transport sector is a major consumer of diesel fuel, which ranks it among the main greenhouse gas (GHG) emissions generators. They can be reduced by gradually introducing biofuels into transport fuels and their share is expected to increase over the years. However, full sustainability can only be achieved by simultaneous consideration of all stages of the product life cycle with a tendency to close it, by utilization of solid waste by-products to improve the energy efficiency of considered biofuel production.

This study proposes an approach for optimal design of an Integrated Biodiesel/Diesel Supply Chain (IBDSC) based on 1st generation feedstock, taking into account the impact of the used feedstock for its energy efficiency improvement. It based on mathematical models of the environmental and economic impact of the considered IBDSC. The latter are included in an optimization problem for determination of optimal number, size and location of bio refineries and solid waste facilities; areas and quantities of raw materials needed for the production of biodiesel and mode of transport. Two optimization criteria are defined: environmental - minimum generated GHG emissions from IBDSC operation and economic - the total annual costs optimization criteria. The problem is solved if either at one of the two criteria, or at an integrated environmental and economic criterion. The approach involves an additional analysis of different feedstock as well as useful by-products. Based on this analysis, the sunflower has been selected as the most appropriate feedstock which can be used as a generator of a useful by-product - sunflower husks. The obtained optimal amount of sunflower husks generated in the production of tons of biodiesel is 0.431(t/t.). They are used to produce the required amount of heat in biorefineries, where there are plants for burning flakes and is 0.215(t/t.). The remaining amount of sunflower husks is used for the production of pellets. When using an integrated environmental-economic optimization criterion, the following results are obtained - 33.4% of sunflower husks are used for the production of pellets, and 66.6% for the production of heat in biorefineries. This would have a positive impact on the formation of the final price of biodiesel.

Keywords: INTEGRATED BIODIESEL/DIESEL SUPPLY CHAIN, OPTIMAL DESIGN, SUNFLOWER FEEDSTOCK, SOLID WASTE UTILIZATION, ENERGY EFFICIENCY IMPROVEMENT, PRODUCTION OF PELLETS, GHG EMISSIONS MINIMIZATION, TOTAL ANNUAL COST MINIMIZATION

1. Introduction

The transport sector is one of the largest consumers of fuels, mainly diesel, which ranks it among the main generators of greenhouse gas emissions. Improving the sustainability of this sector is at the heart of Directive 2009/28 / EC which imposes gradually introduction of biofuels, providing for an increase in their share over the years, as in 2020 it is 10%. Modern biodiesel production, however, is associated with large costs compared to fossil diesel, which hinders its widespread use. One of the ways to improve its economic indicators is to optimize all processes in the chain, from obtaining the raw materials for its production to distributing the products to the end user or applying the concept of so-called supply chains (SC). An additional effect for improving the sustainability has the inclusion in the SC for the production of biodiesel from raw materials of the 1st generation of the processes related to the utilization of the waste from the processing of the raw materials (biomass). The latter leads to improved energy efficiency of this type of production [1, 2] and is associated with optimal management of waste and by-products [3]. An example of such a process is the utilization of sunflower husk in the production of biodiesel sunflower. It can be used to generate steam and electricity for the production needs of refineries, as a substitute for fossil fuels and at the same time has a positive effect on the generated amounts of greenhouse gas emissions [4]. Therefore, the proper choice of raw material, from the point of view of the obtained by-product related to its production, is extremely important for increasing the sustainability of considered biodiesel SC.

This study proposes an approach for optimal design of an integrated 1st generation biodiesel/diesel supply chain from sunflower and rapeseed, using the sunflower husk in order to improve the energy efficiency of production. The approach includes consideration of the stages of the product life cycle, namely: growing the raw material, transporting it to the biorefineries, production of biodiesel and transport to the blending centers. The aim is to simultaneously minimize the amounts of greenhouse gas emissions during the operation of the production system and the total annual operating costs. The optimization is performed by including one of the criteria in the system of constraints and looking for the optimal values of the main criterion.

2. Mathematical Model

2.1. General Formulation of the Problem

The optimization model is formulated in terms of MILP and its solution is related to determining the optimal values of: (1) the number, sizes and locations of bio refinery and installations for the production of sunflower husk pellets; (2) the sites and amount of 1G feedstock; (3) the transportation plans of 1G feedstock, sunflower husk, fossil diesel, glycerine and biodiesel, (Fig. 1).

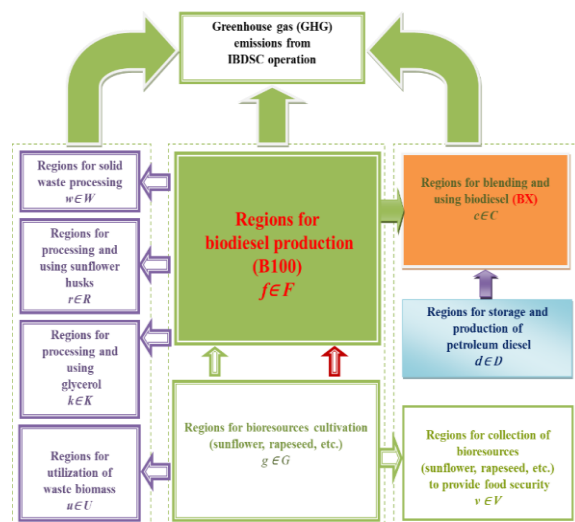


Fig. 1 Superstructure integrated biodiesel supply chain (IBSC).

2.2. Mathematical Description

MILP optimization model includes definition of constant parameters and decision variables; models of the environmental impact and the economic performance of IBSC. An objective function and constraints are also included. For the purpose of modelling the set of time intervals of the planning horizon $\tau =$

$\{1,2,...,T\}$ is introduced. The environmental, economic constants and continuous and binary variables are taken from [5].

2.3. Modeling of IBSC Environmental Impact

The environmental impact objective function is defined in terms of total GHG emissions $[\text{kgCO}_2\text{eq}]$ stemming from the supply chain activities as they are converted to carbon credits by multiplying them with the carbon price at the market. During formulation of the objective function the following life cycle stages of biodiesel production are taken into account: biomass cultivation, growth and acquisition; biomass transportation from source locations to facilities; transportation of biodiesel facilities to the demand areas; sunflower husk transportation from biodiesel facilities to utilization plants; local distribution of liquid transportation fuels in demand areas; emissions from biodiesel and fossil diesel usage. The objective function represents the total environmental impact of IBSC operation resulting in generation of GHG emissions for each time interval $\tau, \tau \in T$. These emissions are equal to the sum of the impact that each of the stages of life cycle has on the environment. The total GHG emissions are defined as follows:

$$(1) TEI_t = ELS_t + ELB_t + ELD_t + ETT_t + ESW_t + ESTRAW_t + ECAR_t + E_{RECYCLING_t}, \forall t$$

where:

TEI_t	Total environmental impact of IBSC operation, $[\text{kgCO}_2\text{eq}/\text{d}]$;
$\{ELS_t, ELB_t, ELD_t, ETT_t\}$	Environmental impact of life cycle stages, $[\text{kgCO}_2\text{eq}/\text{d}]$;
ESW_t	GHG emissions generated during sunflower husk recovery, $[\text{kgCO}_2\text{eq}/\text{d}]$;
$ESTRAW_t$	GHG emissions generated during residual straw utilization in the regions, $[\text{kgCO}_2\text{eq}/\text{d}]$;
$ECAR_t$	GHG emissions generated during the use of biodiesel(B100) & fossil diesel in vehicles, $[\text{kgCO}_2\text{eq}/\text{d}]$;
$E_{RECYCLING_t}$	GHG emissions from the disposal of unused sunflower husks.

2.4. Modeling of IBSC Economic Performance

The economic objective function is defined in terms of the total annual costs for IBSC design. It includes the biomass feedstock acquisition costs, the local distribution costs of final product, the production costs and the transportation costs of biomass, and final products. The production costs take into consideration both the fixed annual operating costs, which is given as a percentage of the corresponding total capital investment, and the net variable costs, which is proportional to the processing quantity. The transportation costs include both distance-fixed costs and distance-variable costs. The economic criterion includes total investment cost of biodiesel production facilities and IBSC operation:

$$(2) TDC_t = TIC_t + TIW_t + TPC_t + TTC_t - TL_t - TA_t - T_ENERGY_t - T_PELLETS_t + T_RECYCLING_t, \forall t$$

where:

TDC_t	IBSC total costs, $[\$/y]$;
TIC_T	Total investment costs for the production capacity of IBSC to the whole operating period and purchase of the plant, $[\$/y]$;
TIW_T	Total investment costs for IBSC facilities for the production of sunflower husk pellets to the whole operating period and purchase of the plant, $[\$/y]$;
TPC_T	Biodiesel(B100) production costs, $[\$/y]$;
TTC_T	Total IBSC transportation costs, $[\$/y]$;

TL_t	Costs associated with government incentives for biodiesel(B100) production and consumption, $[\$/y]$;
TA_t	Total costs associated with obtained by-products (glycerol, cusp), $[\$/y]$;
T_ENERGY_t	Price of sunflower husks for heat production in biorefineries $[\$/y]$;
$T_PELLETS_t$	Price of sunflower husks for pellet production $[\$/y]$;
$T_RECYCLING_t$	Price for utilization of unused sunflower husks $[\$/y]$;

2.5. Constraints

It is introduced a system of constraints on: 1.) Plants capacity; IBSC flow acceptability; 2.) Sunflower husk pellets plants capacity; 3.) Logical constraints; 4.) Transportation links; 5.) Total environmental impact; 6.) Mass balances between biodiesel plants & biomass regions; 7.) Mass balances between biodiesel plants & customers; 8.) Energy balances; 9.) Total network cost.

2.6. Economic Objective Function

The economic cost includes all IBSC operating costs, from the purchase of raw materials to the transport of the final product, as well as the investment costs of bio refineries and sunflower husk pellets facilities which are subject to minimization. The IBSC operating costs include: the raw materials prices, the transportation costs of raw materials to the bio refineries, the cost of conversion to biodiesel and the transportation costs of biodiesel to the blending regions. Economic objective function is represented in terms of the total annual costs for IBSC design:

$$(3) \text{ COST} = \sum_{t \in T} (LT_t TDC_t),$$

2.7. Environmental Objective Function

The environmental objective function represents the minimum total GHG emissions. It integrates the Eco indicator 99 method, taking into account the specific activities that are carried out in the IBSC operation. The cumulative environmental impact of the IBSC operation, is expressed by the equation:

$$(4) \text{ ENV} = \sum_{t \in T} (LT_t TEI_t),$$

2.8. Integrated Economic and Environmental Objective Function

The integrated economic and environmental objective function is formulated as follows:

$$(5) \text{ Int_COST} = \text{COST} + C_{CO_2} \sum_{t \in T} (LT_t \alpha_t TEI_t)$$

where α_t IBSC operating period for one year, $[\text{d}/y]$.

The total emissions are converted into carbon credits by multiplying with the carbon price C_{CO_2} on the market, where it has a value $[0.149 \$/\text{kgCO}_2\text{eq}/\text{d}]$.

3. Formulation of the Optimization Problem

The optimization problem is formulated and solved using either economic criterion - the total annualized cost for IBSC design or using the environmental ones such as: the total GHG emissions associated with its operation and the integrated economic and environmental criterion. The remainder criteria are defined as constraints. The aim is to be defined the optimal biodiesel facilities locations in the regions and their parameters. Formulated optimisation problems were solved using GAMS® optimization software-CPLEX solver [6].

4. Case Study

The model efficiency is approved on a case study from Bulgaria. Two main types of biomass resources are used - sunflower and rapeseed for the production of first generation biodiesel (B100).

4.1. Input Data

For the purpose of evaluation of the effectiveness of the proposed optimization approach, the 27 districts of Bulgaria were considered as searching areas. 5-year planning horizon (2016-2020) with an annual time step is considered. To estimate the quantity of the biodiesel required for these regions, data for the quantities of fossil diesel are taken from the National Statistical Institute of Bulgaria. For the considered time period (2016-2020) they are: 2016→2,050,000 t, 2017→2,219,000 t, 2018→2,401,000 t, 2019→2,583,000 t, 2020→2,775,500 t. In 4 districts in Bulgaria pellets production facilities can be installed (Region_12, Region_14, Region_18, Region_26), and in 4 other districts the glycerine produced can be sold at the plants located there. The search areas are provided with the required fossil diesel from 3 refineries (Region_2, Region_15, Region_20) or combined warehouses. In this study, when determining the optimal number of

bio refineries, it should be borne in mind that they are four types with different maximum capacity. The necessary investment costs for their building are as follows:

Size-1→8,500 t/y→3.8 M\$, Size-2→19,000 t/y →4.8 M\$,

Size-3→48,000 t/y →7.3 M\$, Size-4→74,000 t/y →8.9 M\$.

The pellets production facilities have a maximum capacity of 85,000 t/y and their installation price is 0.380 M\$. The main raw material that is a sunflower husks generator is sunflower. In the present work, the amount of sunflower husks that are generated in the production of tons of biodiesel is 0.431 t/t. They are used to produce the required amount of heat in biorefineries where there are plants for burning sunflower husks and is 0.215 t/t. The remainder amount of sunflower husks is used for the production of pellets. The study assumes that the price of sunflower husks for heat production is 80.00 \$/t, and for pellet production is 70.00 \$/t. The rest data related with the population, cultivated and free cultivated areas used for crops production are taken from [7].

4.2. Results and Discussion

The MILP models were solved using 2.5 GHz Intel Core-i7 Processor with 6 GB Memory. The obtained results are listed in Table 1, Table 2 and Figure 2.

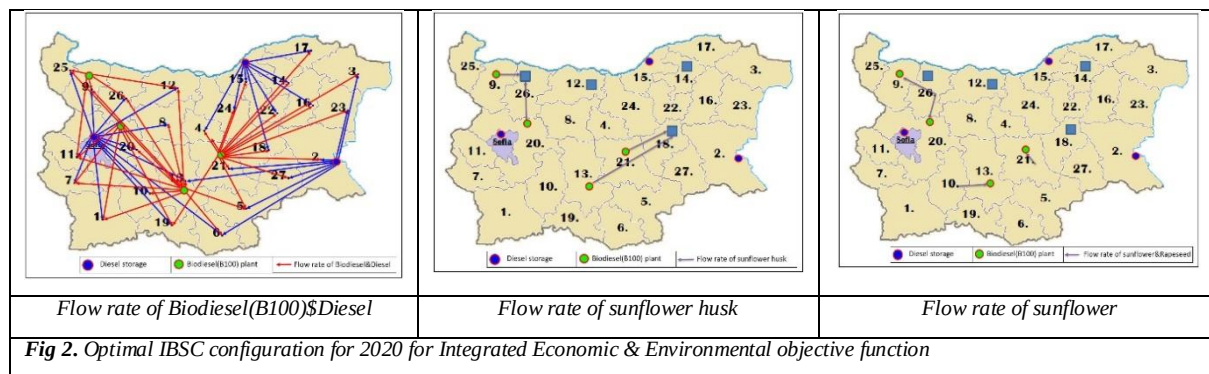
Table 1: Localization, optimal size and load for biodiesel production from sunflower and rapeseed.

	Installed biorefineries in the regions				Installations for the production of pellets	
Facility location	Region-9	Region-13	Region-20	Region-21	Region-18	Region-26
Biorefinery size	Size_4	Size_4	Size_4	Size_4	Size_W1	Size_W1
Production of biodiesel from sunflower [t/y]	67,960	73,727	53,244	73,924		
Rapeseed biodiesel production [t/y]	75	75	75	75	[t/y]	
Biodiesel produced by biorefineries [t/y]	68,035	73,803	53,320	74,000		
Sunflower for biodiesel production [t/y]	183,180	198,726	143,515	199,256		
Rapeseed for biodiesel production [t/y]	250	250	250	250		
Sunflower husks for pellets in plants [t/y]					31,879	26,166
Sunflower husks for heat in biorefineries [t/y]	29,290	31,776	22,948	31,861		
Sunflower husks for cake in biorefineries [t/y]	14,672	15,918	11,493	15,960		
Sunflower husks generated by biorefineries [t/y]	43,963	47,694	34,442	47,822		

Table 2: Results obtained for sunflower and rapeseed biodiesel production

Years > Biodiesel(B100) fossil diesel ratio	2016>6%	2017>7 %	2018>8 %	2019>9 %	2020>10 %
Objective function value (7) - >1302.642- [M\$]					
Objective function value (5) ->14.186 [t _{CO₂eq}] ⁶					
Cost for the whole period [M\$/y]	73.434	96.266	135.441	153.440	166.025
Investment for biorefineries [M\$/y]	1.786	2.679	2.679	3.572	3.572
Investment for pellet installations [M\$/y]	0.076	0.076	0.076	0.076	0.076
Total biodiesel production costs [M\$/y]	76.243	99.354	138.015	158.088	174.097
Costs of pellet production [M\$/y]	0.022	0.028	0.035	0.042	0.051
Transport costs [M\$/y]	5.645	6.910	8.875	9.960	11.735
Total sanction for CO ₂ -Ekv for the period [M\$/y]	13.813	17.583	22.466	26.747	31.243
Government incentives for biodiesel [M\$/y]	-10.193	-12.892	-15.968	-19.357	-23.147
Revenue from the sale of glycerin [M\$/y]	-10.032	-12.780	-16.315	-19.465	-22.782
Revenues from the use of flakes for heat production in biorefineries [M\$/y]	-2,038,636	-2,578,568	-3,193,708	-3,871,426	-4,629,534
Revenues from the use of pellet flakes [M\$/y]	-1.788	-2.008	-1.117	-2.234	-4.063
Total GHG emissions (t _{CO₂eq} /y)	547,683	698,040	892,804	1,063,371	1,242,622
Total quantities of biodiesel and fossil diesel produced per year [t/y]					

Total biodiesel(B100) [t/y]	118,525	149,916	185,680	225,082	269,159
Total fossil diesel [t/y]	1,945,321	2,086,596	2,237,010	2,384,211	2,537,784
Price for biodiesel (B100) production [\$ /t]	619	642	729	681	616
Distribution of available land [ha]					
Sunflower land for biodiesel [ha]	82,874	96,519	74,751	119,382	188,228
Rapeseed land for biodiesel [ha]	97	7,784	50,964	35,239	195
Sunflower land for food [ha]	1,063,531	1,157,169	1,388,851	1,464,935	1,464,935
Rapeseed land for food [ha]	400,668	336,161	613,987	432,521	1,464,935
Free arable land [ha]	1,997,379	1,952,153	1,423,924	1,508,037	1,508,688



5. Conclusion

The optimal arable area needed for growing sunflower and rapeseed, is concentrated in a small number of regions of the country (Region 10, Region 21 and Region 26). In order to obtain the optimal mix of 1G bio resources, using the target function "Minimum total annual costs", in 2020 it is necessary to use 2.39% of the agricultural land for sunflower cultivation and 0.00028% for rapeseed. For the case of the integrated target function (case 6) for IBSC, the average price of biodiesel (B100) for the considered period (2016-2020) is \$ 657 / t, while for case 5 of the minimum total GHG emissions, it is \$ 698 / t, therefore 16% higher. On the other hand, for case 5 of the environmental criterion used, the total GHG emissions are 9.6% lower than those obtained using the integrated economic and environmental criterion. With regard to the sunflower husks used when using the integrated target function (case 6), about 33.4% of sunflower husks are used for the production of pellets and 66.6% are used for the production of heat in biorefineries.

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Features of modeling of ultralow power electric fields

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Abstract: The article presents the results of modeling quasi-stationary ultralow power electric fields (the order of tens of nanowatts) and establishes ranges of rational values of parameters (average density of electric voltage, specific potential) of these fields. As a result of mathematical modeling (based on a system of Gaussian equations) and subsequent numerical experiment, it is shown that an instantaneous increase in the average electric density of a quasi-static electric field in 2 times in one part of the field leads to an increase in charge redistribution time from 34 ns (at an initial density of electric tension of $17 \text{ nN/Ku.}\mu\text{m}^3$) to 189 ns (at a density of electric tension of $145 \text{ nN/Ku.}\mu\text{m}^3$). This redistribution allows us to determine the range of rational values of the specific potential, which is $1.1 \dots 9 \text{ nV}/\mu\text{m}^2$. In this case, the maximum specific power that can occur in such a field is $0.5 \dots 0.77 \text{ nW}/\mu\text{m}^2$.

Keywords: ULTRALOW POWER ELECTRIC FIELD, MATHEMATICAL MODEL, GAUSSIAN EQUATION, ELECTRIC VOLTAGE DENSITY, SPECIFIC POTENTIAL

1. Introduction

The active growth of the number of products based on microelectronic devices and systems based on them is due to the significant technical and economic advantages of such devices, as well as technological advantages in the process of their manufacture [1]. However, further increase in the range and production of microelectronic devices and systems requires, in addition to expanding their functionality and operational capabilities, improving the technical and material base for their production, which primarily consists in the use of new composite materials and technologies of miniaturization and hybridization in manufacturing these devices. However, the miniaturization of electronic circuits, which is to reduce the size and distance between their components, along with the use of various mechanisms of electrical conductivity (conductors, semiconductors, dielectrics) and structural features (quantum dots, linear conductors, thin films, nanostructures, etc.) materials, as well as the operating parameters of these electronic circuits (voltage, frequency, etc.) leads to the emergence and accumulation in the materials of the components of these circuits as individual electric charges and electric fields created by them.

In this case, such electric fields, which is a necessary physical phenomenon that occurs for any electrical devices, in addition to providing the basic functions of electrical circuits, such as: electrical capacity, memory elements, etc., can cause adverse effects. on these schemes: the effect of electrostatic "sticking" of moving microelements of mechanisms, attraction of microparticles of atmospheric moisture and dust, which significantly reduces the cooling and conductivity of circuit components and the most dangerous – electrostatic breakdown, which causes electromechanical destruction of electrical devices and, as a consequence out of order.

A number of leading domestic and foreign scientists deal with the issues of measurement and research of electric fields in electronic devices, such as: S.V.Biryukov, V.V.Dovgusha, E.P.Dyakov, O.V.Masleeva, N.A.Shavrina, J.P.Booth, L.Cengel, F.Ollendorf, T.Vinh and others [2-4]. However, despite the scientific achievements of these scientists, the important issue of modeling electric fields of ultra-low power arising in microelectronic devices in order to establish limit values of the characteristics of these fields, exceeding which leads to electric breakdown.

Therefore, modeling of dynamic and quasi-stationary electric fields of ultralow power to determine the power and energy characteristics of such electric fields that occur in microelectronic devices, with the possibility of obtaining and visualizing the spatio-temporal distribution of these characteristics is an urgent task.

The purpose of the study: to increase the efficiency of determining the characteristics of dynamic and quasi-stationary electric fields of ultra-low power, which take place in microelectronic devices, by their mathematical modeling, which allows high-precision and adequate determinations and spatial-

temporal visualization of power and energy characteristics of these fields.

2. Characteristics, causes and propagation of ultra-low power electric fields

As is known [5], the electric field is one of the components of the electromagnetic field that exists around bodies or particles that have an electric charge, as well as in free form when the magnetic field changes (for example, in electromagnetic waves). In the case where the electric field does not change over time, it is called an electrostatic field. Accordingly, the electric field, the distribution of charge (and, accordingly, energy) in which it is variable in space over time - is called a dynamic electric field.

The electric field can be observed due to force and / or energy impact on charged bodies. The main quantitative characteristic of an electric field is its characteristic, such as intensity. At the same time, the energy characteristics are the voltage and potential of the electric field.

It should be noted that the relationship between the main characteristics of the electric field can be expressed by certain laws: [6], which proves the existence of a correlated relationship between these characteristics. This relationship greatly simplifies the calculation and modeling of electric fields and their characteristics, both in space and time.

The main sources of electric fields and electromagnetic radiation in a wide range are [7]: a variety of electronic devices and video display terminals (especially those running on cathode ray tubes) that accumulate static electricity on the surface of the monitor screen.

Mechanisms of electric fields. The electric field is a special state of matter, different from "classical" matter, consisting of material particles. Like other fields, the electric field is continuous, that is, it exists at every point in space and changes smoothly. If the source of the electric field moves, it generates changes in the field that propagate in it at the speed of light.

The electric field is a vector, that is, at each point in space it can be matched with a vector called the field strength (E), the length of which is proportional to the force with which the field acts on charged bodies, and the direction coincides with the direction of a single test charge.

If the electric field is static, or changes over time very slowly, it can be given through one scalar function - the potential U . In this case, the voltage and potential are related by the equation: $\vec{E} = -\nabla\varphi$.

In a homogeneous electric field (ie, one where the voltage is constant, for example, in the field between the capacitor wrappers) the voltage between two points is equal to: $U = -\vec{E} \cdot \vec{R}$, where R is the vector connecting the field points.

The electric field is created by charged bodies, in particular charged elementary particles. Such a field is potential. Its intensity

is determined by Coulomb's law. The lines of force of a potential electric field begin and end on charges or go to infinity.

According to the law of electromagnetic induction, the electric field is also created by an alternating magnetic field. Such an electric field is a vortex. The power lines of the vortex electric field are closed. In particular, the vortex electric field is a component of the electromagnetic wave. When the charge is moved along a closed curve in such a field, the work performed is not equal to zero

Thus, as a result of the analysis of the relevant information sources, it is established that the main characteristics of electric fields are as follows: voltage E , voltage U and potential ϕ . In this case, the established causes of these fields are: natural (eg, electric discharges, friction of dielectrics), artificial (mutual location in the space of conductors with electric current, sources of electromagnetic radiation) and others [8].

3. The mechanism of influence of electric fields of ultralow power on surface of materials and elements of electronic devices

Electrical stability of the material and electrostatic breakdown. The electrical stability of the material (we mean dielectric materials, usually insulators) depends on [9]: the shape of the electric field; type of voltage and polarity; voltage action time; dielectric homogeneity; electrophysical characteristics; temperatures, etc.

There are three types of breakdown of a solid dielectric [10]:

- 1) electric - at a voltage of 10^2 - 10^3 kV/mm;
- 2) thermal - at a voltage of 10 - 10^2 kV/mm;
- 3) aging - at a voltage of 10 kV/mm and less.

The strongest influence on the electrical strength of the material is carried out: the time of application of voltage, temperature, thickness. In general, the dependence of the breakdown voltage on the time of its application is called the volt-time characteristic (Fig. 1).

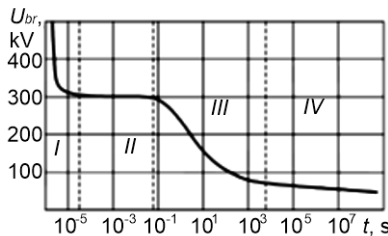


Fig. 1. Volt-time characteristics of the material (for example, porcelain):
I - electrical breakdown, delay in the development of the discharge channel;
II - electrical breakdown, $t < 0.1$ s, independent of temperature; III - thermal breakdown, $t > 0.1$ s, a sharp decrease in breakdown voltage over time;
IV - aging, breakdown voltage U_{br} changes little, the time to breakdown increases significantly

On the curve (Fig. 1) can be divided into four areas. Areas I and II correspond to the electrical breakdown (voltage application time $t < 0.1$ s). The sharp increase in the breakdown voltage in region I is due to the delay in the development of the discharge relative to the time of application of the voltage. Region III is characterized by a sharp drop in breakdown voltage, which indicates the predominant role of thermal processes. Area IV - slow decrease in breakdown voltage with increasing time of action, which is associated with slow aging and degradation of the material.

At the same time, the electrical strength of the dielectric E_{br} increases with decreasing thickness (especially rapidly in the region of micron thicknesses). This effect is used in the insulation of capacitors, conductors, inputs and other elements.

It is known [11] that the temperature also significantly affects the penetration stress of the material. Thus, from the dependence of the electrical strength of porcelain on temperature, Fig. 2, it can be seen [12] that up to a temperature of +75 °C the breakdown voltage

of porcelain E_{br} practically does not change (region A). A further increase in temperature leads to a sharp decrease in E_{br} (region B).

Under the influence of an electric field dielectric, the intensity of which is greater than some critical value E_{cr} , new physical phenomena occur in the dielectric, which are not peculiar to it, in particular [9]: partial discharges, accumulation of bulk charge, electroluminescence.

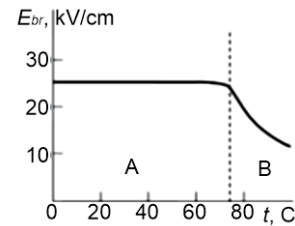


Fig. 2. Dependence of breakdown voltage on temperature for porcelain

At the same time, the phenomenon of partial discharges has the greatest influence [13]. Partial discharges are breakdowns of defects in the material, ie air infiltrations, layers of oil, the electrical strength of which is below the solid phase. Partial discharge leads to the breakdown of only the weakened part, not the entire dielectric gap.

The occurrence of partial discharges always indicates the local inhomogeneity of the dielectric. In this regard, the registration of the characteristics of partial discharges allows you to assess the quality of the material and detect local defects. The characteristics of partial discharges correlate quite well with the size and number of defects, ie allow to judge the degree of defect of the structure itself.

Partial discharge occurs when the electric field strength (the so-called intensity of the beginning of the partial discharge), which is much less than the breakdown voltage of the entire interval. Single partial discharges are practically not harmful for isolation, they arise at constant voltage. But at alternating voltage (for example, already at a frequency of 50 Hz), even one partial discharge for half a period leads to 100 discharges per second.

Thus, it is established that the main mechanisms of influence of electric fields of ultra-low power on the surface of materials of different electrical conductivity are accumulative and discharge [14]. At the same time, the combined nature of the electrical conductivity of most elements of electronic devices does not allow to determine a specific mechanism of action of the electric field on these elements. Therefore, the study of the effect of combined conductivity mechanisms on electricity is insufficient today. Therefore, conducting mathematical modeling of these mechanisms (especially the edge effects that occur in these elements) [15].

4. Modeling of ultralow power electric fields distributed on the dielectric surface and in space

To determine the spatial distribution of point electric charges, as well as complex electric fields with several sources, three main methods are used [16]: electrodynamic, energy, probabilistic.

Electrodynamic method. The electrodynamic approach to the description of electric fields (EF) is based on the solution of Maxwell's equations for known sources of the electric field. In this case, the medium in which these fields propagate is considered homogeneous and isotropic. The group signal that determines the EF at the observation point $P(x_0, y_0, z_0)$ can be found as their superposition from m separate mutually independent sources. The basic model of the EF source is an elementary electric emitter (Hertz dipole) [17], Fig. 3.

General expressions for EF (Hertz dipole) in a spherical coordinate system have the form:

$$\begin{aligned} \dot{H}_\varphi &= \frac{I_m \cdot l \cdot \beta^2 \cdot e^{-j\beta r}}{4\pi} \left[j \frac{\lambda}{2\pi r} + \left(\frac{\lambda}{2\pi r} \right)^2 \right] \sin \theta = \\ &= \frac{I_m \cdot l \cdot e^{-j\frac{2\pi r}{\lambda}}}{4\pi} \left[j \frac{2\pi}{\lambda r} + \frac{1}{r^2} \right] \sin \theta, \end{aligned}$$

$$\dot{E}_\theta = \frac{I_m \cdot l \cdot \beta^3 \cdot e^{-j\beta r}}{4\pi\omega\epsilon} \left[j \frac{\lambda}{2\pi r} + \left(\frac{\lambda}{2\pi r} \right)^2 - j \left(\frac{\lambda}{2\pi r} \right)^3 \right] \sin \theta = \frac{I_m \cdot l \cdot Z_w \cdot e^{-j\frac{2\pi r}{\lambda}}}{4\pi} \left[j \frac{2\pi}{\lambda r} + \frac{1}{r^2} + \frac{\lambda}{j 2\pi r^3} \right] \sin \theta,$$

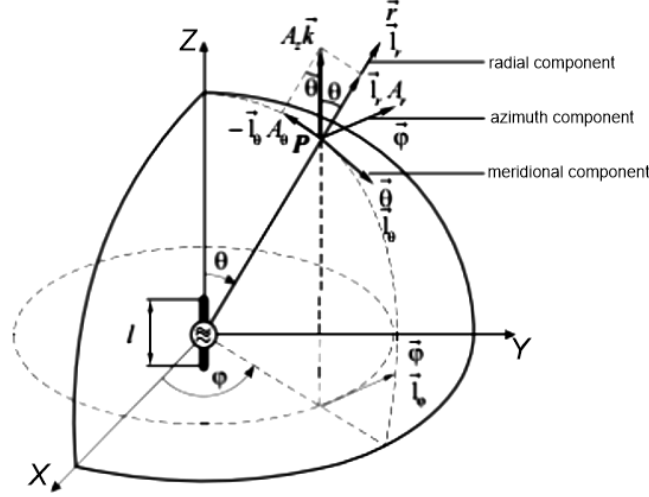


Fig. 3. Components of the electric field (Hertz dipole)

$$\dot{E}_r = \frac{I_m \cdot l \cdot \beta^3 \cdot e^{-j\beta r}}{2\pi\omega\epsilon} \left[\left(\frac{\lambda}{2\pi r} \right)^2 - j \left(\frac{\lambda}{2\pi r} \right)^3 \right] \cos \theta = \frac{I_m \cdot l \cdot Z_w \cdot e^{-j\frac{2\pi r}{\lambda}}}{2\pi} \left[\frac{1}{r^2} + \frac{\lambda}{j 2\pi r^3} \right] \cos \theta,$$

where I is the current in the emitter, l is the length of the emitter, r is the distance (dipole arm), $\beta = 2\pi/\lambda$ is the phase coefficient.

The presented formulas are written in such a way that the terms $(\lambda/2\pi r)^n$, where $n = 1, 2, 3$, characterize the components and depend on the ratio of wavelength and distance to the observation point r .

From these formulas it follows that under the condition: $r \ll \lambda/2\pi$ the component of lower degrees can be ignored and vice versa.

The distance $r_{cr} = \lambda/2\pi$ is called critical or limiting. If the observation point is located at a distance much less than r_{cr} , then the field is characterized by the near zone (induction zone), if $r \gg r_{cr}$, the far zone (radiation zone). The zone around r_{cr} is called the intermediate zone. Table 1 shows the formulas for the near and far zones of the electric emitter [18].

Table 1. Components of EF in the near and far zones for the electric emitter

Near zone	Far zone
$\dot{H}_\varphi = \frac{I_m \cdot l}{4\pi r^2} \sin \theta$	$\dot{H}_\varphi = \frac{I_m \cdot l \cdot \beta}{4\pi r} e^{-j\beta r} \sin \theta$
$\dot{E}_\theta = -j \frac{I_m \cdot l}{4\pi\omega\epsilon r^3} \sin \theta$	$\dot{E}_\theta = j \frac{I_m \cdot l \cdot \beta^2}{4\pi\omega\epsilon r} e^{-j\beta r} \sin \theta$
$\dot{E}_r = -j \frac{I_m \cdot l}{2\pi\omega\epsilon r^3} \cos \theta$	$\dot{E}_r = \frac{I_m \cdot l \cdot \beta}{2\pi\omega\epsilon r^2} e^{-j\beta r} \cos \theta$

Based on the formulas given in table 1, we can conclude that in the near zone the electromagnetic wave is not formed, which is why the near zone is called the induction zone or the guidance zone. Another feature of the near zone is that the impedance depends not only on the parameters of the medium, but also on the type of emitter: $Z_W^{el} = \frac{1}{j\omega\epsilon r}$, ie the field is high impedance.

In order to obtain a complete group signal at the point $P(x_0, y_0, z_0)$, which is created by a set of radiations from m independent sources, it is necessary to vector sum the EF voltages: $\vec{E}_\Sigma = \sum_{i=1}^m \vec{E}_i$.

For preliminary estimation of EF it is possible to use a technique of formal ordering of components of the concentrated noise, having arranged them in the form of hierarchical degrees. In

addition, the use of an electrodynamic approach to the description of EF is complicated by the fact that the distribution of currents by the volume occupied by the radiating system is not always known [19].

Energy method. To implement the energy method, it is advisable to separately identify the noise-focused interference and time-focused interference.

We define such interferences as an ensemble of n narrowband signals. Let's write the i -th narrowband signal as follows:

$$e(t) = E_i(t) \cos[\omega_{0i}(t) + \varphi_{0i}(t)],$$

where $E_i(t)$, $\varphi_{0i}(t)$ is the bypass phase and the phase of the radio wave field strength from the i -th source; ω_{0i} - circular frequency of the carrier.

In this case, the noise, concentrated in the spectrum, is represented by the formula:

$$e(t) = \sum_{i=1}^n E_i(t) \cos[\omega_{0i}(t) + \varphi_{0i}(t)].$$

If the number of components of the group signal is large, the definition of EF is quite complex. It is advisable to divide the components of the spectrum-concentrated interference into discrete energy levels, then the narrowband signal will look like:

$$e(t) = E_{mi} K_i(t) \cos[\omega_{0i}(t) + \varphi_{0i}(t)],$$

where E_{mi} is the amplitude value of the field strength of the i -th signal at the point of reception, $K_i(t)$ is a dimensionless factor that characterizes the law of change of the envelope.

According to Parseval's equation, the specific energy of the process:

$$W_i = \frac{1}{\pi} \int_{\omega_{1i}}^{\omega_{2i}} A_i^2(\omega) d\omega = \frac{60 P_i D_i}{\pi r_i^2} V_i^2 \int_{\omega_{1i}}^{\omega_{2i}} a_i^2(\omega) d\omega.$$

Assuming that the i -th signal is concentrated in the band $\Delta\omega_i = \omega_{2i} - \omega_{1i}$, within which the modulus of the normalized spectral function $a(\omega)$ is constant. Let's simplify the previous formula:

$$W_i = \frac{60 P_i D_i}{\pi r_i^2} V_i^2 a_i^2 \Delta\omega_i = \frac{1}{\pi} A_i^2 \Delta\omega_i.$$

Thus, the specific interference energy concentrated in the spectrum can be determined as follows:

$$W_i = \frac{60}{\pi} \sum_{i=1}^n \frac{P_i G_i}{r_i^2} V_i^2 a_i^2 \Delta\omega_i = \frac{1}{\pi} \sum_{i=1}^n A_i^2 \Delta\omega_i.$$

Interferences are divided into impulse and fluctuation [20]. The difference between them is in determining the duration of the installation of transients.

If the transients from the previous pulse do not overlap in time the transients from the next pulse, such interference is considered

pulsed. If the imposition of these transients creates a continuous random process, such interference is considered *fluctuational*.

The probability of exceeding the amplitude noise, which is time-concentrated and which contains the fluctuation and impulse components of some level x_0 , is determined by its integral distribution function. It looks like:

$$p(u) = (1 - \nu\tau) \cdot e^{-x_f^2 \frac{\alpha_f}{2a_f^2}} + \nu\tau \cdot e^{-x_p^2 \frac{\alpha_p}{2a_p^2}},$$

fluctuation component pulse component

where A is the instantaneous value of the amplitude of the interference; A_{ef} - effective value of the amplitude of the interference, determined and averaged by the narrowband receiver; A and a are Weibull distribution parameters; ν - average pulse rate, c^{-1} ;

r - average pulse duration, s.

The RMS value of the power of the noise, concentrated in time, allocated to the unit resistance:

$$p^2 = (1 - \nu\tau) a_f^2 A_f \Gamma\left(\frac{2}{\alpha_f} + 1\right) + \nu\tau^2 a_p^2 A_p \Gamma\left(\frac{2}{\alpha_p} + 1\right),$$

where $\Gamma(a)$ is a gamma function.

The values of $p(u)$ and p^2 depend on the specific conditions at a particular point in the definition.

Probabilistic method. The probabilistic method is also used to estimate the EF. Information about the real EF can be subjected to statistical processing.

The statistical characteristics of the EF depend on whether the EF is only under the influence of the field source or it is affected by a set of charges and interference. The idealized EF, which corresponds to the first case, can be taken as a reference, with which the real is compared. Thus, the real EF can be judged by comparing the statistical characteristics of the two sources. Thus it is possible to receive also a quantitative estimation of EF if to compare among themselves probabilities of excess of the set level by sources on an interval of supervision T .

The advantage of this method is that the evaluation of the EF is carried out on the response of a particular source to a change in charge, which indirectly takes into account all measures of both technical and organizational nature, aimed at providing a stationary EF.

In addition to the above, there are other methods and approaches to determining the EF. For example, the geometric representation of EF, and the approach based on elements of set theory, and so on.

Thus, the main methods and means of determining the characteristics of point electric charges and electric fields distributed over the dielectric surface and in space are analyzed. As the most promising method, which is chosen as the basic in the research, the energy method is chosen, as one that allows with higher accuracy and relative simplicity of software implementation to model electric fields in a wide range of values of their characteristics.

5. Discussion of simulation results

As a result of the numerical simulation performed by Matlab, the results of modeling of quasi-stationary electric fields of ultralow power (of the order of tens of nanowatts) are obtained and ranges of rational values of parameters (average electric density, specific potential) of these fields are established. Thus, Fig. 4 shows the calculated dependences of the change in the distribution of electric charge in the surface layer of the dielectric plate (silicon DSP/Ssp<100><111>).

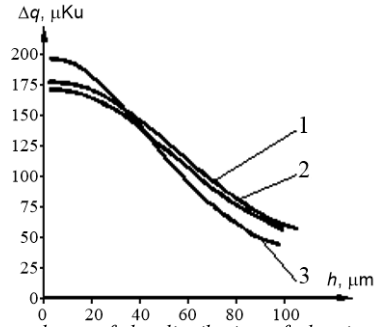


Fig. 4. The dependence of the distribution of electric charge Δq in the surface layer of a plate with a thickness of silicon DSP/Ssp <100> <111> at different values of the initial density of the electric field strength j_E : 1 - 17 nN/Ku μ m³; 2 - 81 nN/Ku μ m³; 3 - 145 nN/Ku μ m³

As can be seen from Fig. 4, the charge accumulated on the surface of the dielectric with increasing depth of the surface layer decreases significantly exponentially.

In fig. In Fig. 5 shows the dependences of the accumulated electric charge on the dielectric surface from the time of its redistribution.

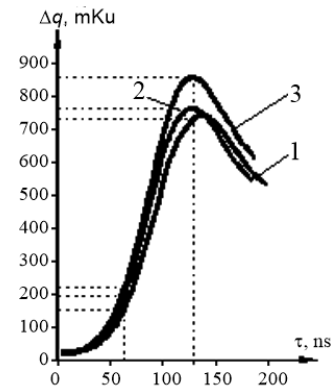


Fig. 5. Estimated dependences of the accumulated electric charge on the surface of silicon DSP/Ssp<100> <111> from the time of its redistribution at different values of the initial density of the electric field strength j_E : 1 - 17 nN/Ku μ m³; 2 - 81 nN/Ku μ m³; 3 - 145 nN/Ku μ m³

As a result of the calculations and the obtained dependences in the mathematical package Matlab determined that the maximum redistribution time of the electric charge on the surface of the silicon wafer DSP/Ssp <100> <111> is 189 ns (at a voltage density of 145 nN/Ku μ m³), then, as the minimum time is 34 ns (at an initial density of electric voltage of 17 nN/Ku μ m³).

6. Conclusion

Features of modeling of electric fields of ultralow power which is based on the decision of system of the analytical equations which are based on differential Laplace equations considering dynamics of change of EF and their sizes, and also influence of external factors (temperature, relative humidity, UV and gamma) are considered. radiation, mechanical deformation, surface friction, etc.).

Involvement of a modern mathematical processor MatLab allowed to develop a dynamic computer model of formation and redistribution of ultra-low power electric fields under the influence of external factors in space and time, which allows high accuracy (discrepancy between mathematical modeling data and experimentally obtained data does not exceed 5,6%) and in real time to visualize the distribution of EF, as well as to determine the ranges of power and energy parameters of EF, compliance with which does not lead to electrical breakdown.

It is established that the instantaneous increase of the average density of the electric voltage of a quasi-static electric field in one part of the field leads to an increase in the time of charge redistribution in the electric field from 34 ns (at the initial density of 17 nN/Ku μ m³) to 189 ns electrical voltage 145 nN/Ku μ m³). This

allows us to determine the range of rational values of the specific potential ($1.1 \dots 9 \text{ nV}/\mu\text{m}^2$) and the maximum specific power ($0.5 \dots 0.77 \text{ nW}/\mu\text{m}^2$) in such a field.

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Contact heat transfer in the foundry – Tunnel effect

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Abstract: Mathematical methods of quantum mechanics are needed to describe the contact phenomena of the boundary casting/mold. Apart from the macro-level, the contact phenomena are part of the technological processes first order phase transition and second order phase transition. Need for professional software for mathematical simulation at macro- and micro-level in foundry. Education in basic mathematics and mathematical physics is also required for engineers. The branch machine-building infrastructure must develop a mechanism for inclusion in the computing infrastructure of the micro-foundries.

Keywords: HEAT TRANSFER, COEFFICIENT CONTACT OF HEAT TRANSFER, TUNNEL EFFECT, SOFTWARES

1. Introduction – developing mathematical modeling gas pressing casting method

Crystallization in a high pressure casting process has a higher solidification rate; lower likelihood of suction than atmospheric pressure casting [1, 2 and 3]. The boundary condition at the mold work surface (B_{WS}) is:

$$-\lambda_C \nabla T_{C|B_{WS}} = \alpha_{B_{WS}}^{contact}(x, y, z, t)(T_{C|B_{WS}} - T_{M|B_{WS}}) = -\lambda_M \nabla T_{M|B_{WS}}, \quad (1)$$

where indexes C (casting) and M (mold); λ is thermal conductivity coefficient; $\alpha_{B_{WS}}^{contact}$ is Newton's heat transfer coefficient; $T_{C|B_{WS}}$ and $T_{M|B_{WS}}$ are the temperatures of the casting and the mold; $\nabla T_{C|B_{WS}}$ and $\nabla T_{M|B_{WS}}$ are the temperature gradients of the casting and the mold.

The influence of the high gas pressure P_{Gas} on the coefficient of contact heat exchange in eq. (1), which is a complex function. The more interesting question of the influence of gas pressure on the first order of phase transition (solidification) [8, 9, 10 and 16]:

$$\text{Liquid} \xrightarrow{\text{First order phase transition}} \text{Solid}, \quad (A)$$

and the casting final structure by the heat-treating [4 and 5] - second order phase transition:

$$\text{Solid} \xrightarrow{\text{Second order phase transition}} \text{Solid}. \quad (B)$$

The aim of this work is to show the need to use quantum mechanics in the evaluation of *contact heat transfer*.

2. Solid state physics

Works [9 and 11] complement each other very well methodologically [12] i.e. metal science is based on the physics of metals and the more general scientific field of solid state physics. The methodology encompasses all scientific knowledge [12] as new scientific fields are constantly emerging, which interact through mathematical logic and mathematics. As an example of work [12] here we accept works [13 and 16] and as an engineering necessity of quantum mechanics [14] and quantum physics [15].

3. Quantum mechanics and Quantum physics

M. Planck, L. de Broyle, W. Heisenberg, E. Schrödinger, M. Bourne, P. Dirac and others. There are two areas of quantum mechanics: *non-relativistic* studies motion with small velocities ($v \ll c$); *relativistic* quantum mechanics studying the motions of microparticles at high velocities ($v \approx c$) [14]. Quantum mechanics describes the behavior of microparticles; at distances of the order of $10^{-10} \div 10^{-15}$ m; new principles are introduced [14]; and quantum mechanics is a fundamental field of theoretical physics.

To refine the analysis of the contact heat transfer coefficient $\alpha_{B_{WS}}^{contact}$, the description [6] of: phonon transfer; thermal conductivity of free electron gas using the Schrödinger equation. In quantum mechanics, the closest phenomenon to an example is: the passage of an microparticle through a potential barrier [14] (see Fig.1). A stationary equation of Schrödinger is used, the form of which for the individual regions is as follows [14]:

Schrödinger equations and Solutions for regions 1 and 3

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0; \psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0; \psi_3(x) = A_3 e^{ik_3 x} + B_3 e^{-ik_3 x}, \quad (2)$$

Schrödinger equations and Solutions for region 2

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0; \psi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}. \quad (3)$$

where $\hbar = h/2\pi$ is Planck's constant; A_i and B_i are constants at $i=1; 2; 3$; particle energy is E , and U_0 is barrier energy; ψ_i $i=1; 2, 3$ are waves functions in every regions; $k_1 = \sqrt{2mE}/\hbar$ and $k_2 = \sqrt{2m(E - U_0)}/\hbar$ is imaginary number if $E < U_0$; m is particle mass. Then, we lay $k_2 = ik$, where $k = \sqrt{2m(U_0 - E)}/\hbar$, for the solution $\psi_2(x)$ we obtain [14]: Solutions 2 and 3 consist of two monochromatic waves propagating in two opposite directions 0X and -0X: such as wave on the 0X direction to the potential barrier is $A_1 e^{ik_1 x}$, and the reflected wave is in the -0X direction is $B_1 e^{-ik_1 x}$ [14]. $|A_1|^2$ determines the probability the move to the barrier, and $|B_1|^2$ is the probability the move in the opposite direction. The *reflection coefficient* of the barrier is called R the ratio [14]:

$$R = |A_1|^2 / |B_1|^2, \quad (4)$$

i.e. R is the probability that the microparticle will be reflected by the potential barrier. By analogy $A_2 e^{ik_2 x}$ and $B_2 e^{-ik_2 x}$ describe the motion of the particle in the two opposite directions in region 2 (see Fig. 1). Region 3 is from l to ∞ and therefore there is no wave reflected in it, i.e. $B_2 = 0$ and the solution for this region is of type $\psi_3(x) = A_3 e^{ik_3 x}$ and corresponds to the wave that has passed, propagating only in the positive direction 0X [14]. The ratio of the square of the amplitude of the wave passing through the barrier $|A_3|^2$ to the square of the amplitude of the incident wave $|A_1|^2$ is called the *barrier transparency coefficient* D :

$$D = |A_3|^2 / |A_1|^2. \quad (5)$$

Between R and D $\exists$ relations

$$R + D = 1: \quad (6)$$

and at $R = 1, D = 0 \Rightarrow$ we have the micro-particle reflection from potential barrier; at $R = 0$ and $D = 1 \Rightarrow$ the micro-particle has crossed the potential barrier [14]. Eq. (3) show that event at $E < U_0$

the micro-particle is likely to cross the potential barrier (i.e. to be in region 2 (Fig. 1)). This shows that the behavior of micro-particles considered in quantum mechanics is different that of particles in classical physics [14]. The condition of continuity of the wave function and its derivatives at the limit of the potential barrier of the solutions (2 and 3)

$$\begin{aligned} \psi_I(0) = \psi_{II}(0) \quad \text{and} \quad \psi_{II}(l) = \psi_{III}(l) \\ \frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx} \quad \text{and} \quad \frac{d\psi_{II}(l)}{dx} = \frac{d\psi_{III}(l)}{dx} \end{aligned} \quad \left(\begin{array}{l} \text{For } \psi \\ \text{boundary} \\ \text{conditions:} \\ \text{continuity,} \\ \text{derivatives} \end{array} \right)$$

are determined by the constants A_i and B_i . For the rectangular barrier (Fig.1) the coefficient D is determined by the formula:

$$D = D_0 e^{-2kl} = D_0 e^{-\frac{2l}{\hbar} \sqrt{2m(U_0 - E)}}, \quad (7)$$

where $k = \sqrt{2m(U_0 - E)}/\hbar$ (at $E < U_0$); $D_0 \approx 1$; m is microparticle mass. D depends on m , l and $(U_0 - E)$ as their probability of the microparticle passing through the barrier increases. Hence the conclusion: that for macrobodies quantum mechanics passes into the classical one: particles with large mass do not pass through the barrier.

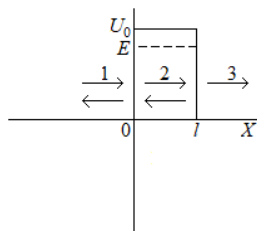


Fig.1 Free micro-particle motion through potential barrier: width l and height U_0 barrier energy; space is divided into three areas [14]: 1 ($x < 0$), 2 ($x \in (0, l)$) and 3 ($x > l$); direction of movement along the $0X$ axis; E is the total energy of a particle; the particle $E > U_0$ passes over the barrier, at $E < U_0$ it cannot pass through the barrier and reaches a height allowed by E . According to quantum mechanics, there is a probability $\neq 0$ ($E < U_0$) that the particle will cross the barrier and the motion is described by eq. (5, Schrödinger stationary equation).

The passage of a microparticle through a potential barrier is called the *tunnel effect*. This effect explains many phenomena in physics: cold emission of electrons from metals (separation of electrons from the surface of a metal under the action of an external electric field); α -decay of radioactive nuclei; contact phenomena at the boundary between solids etc. The tunnel effect is specific quantum phenomenon and is observed only at a very small width of the potential barrier (of the order of the size of atoms 10^{-10} m) [14].

Quantum physics tries (should) answer two fundamental question are being sought [15]: **What are the elementary components of matter? AND What are fundamental forces controlling their behavior?** In [15] the scientific disciplines related to these questions are presented as: I. Basic task of physics; II. Particle physics; III. Quantum physics: III.1 Open questions of physics; III.2 Basic task of physics. [15]. The scale of the considered processes and phenomena in physics are [15]:

$10^{-34} 10^{-30} 10^{-26} 10^{-22} 10^{-18} 10^{-14} 10^{-10} 10^{-6} 1 \text{ m} 10^6 10^{10} 10^{14} 10^{18} 10^{22} 10^{26}$

Quantum physics unites: quantum mechanics; quantum field theory applied in particle physics, nuclear physics, high energy physics, solid state physics, astrophysics and many other branches of Physics. The particle physics gives many important answers of the two questions, which are relevant to all physics; in particular, our interest in material science and in all knowledge. An important result for unification in physics is the standard model in elementary particles [15 and 17]. The main interaction in nature are: strong, weak, electromagnetic and gravitational. The standard model combines strong, weak and electromagnetic [15 and 17].

4. Materials Science – Contact Phenomena

First order phase transition (A) and second order phase transition (B) are the two fundamental processes of the material science.

In [18] the connection between the classical and quantum penetration barrier is shown as the length of the potential barrier is of the order of the de Broglie wavelength. The type of barrier potential is trapezoidal [18]. Some particles cross the barrier due to "strong fluctuations in the quantum mechanical potential". Other particles cross the barrier due to thermal fluctuations [18]. The tunnel effect is presented in lectures in courses for students such as one of the mysteries of quantum mechanics [19]. Contact phenomena of the macro level at the first order phase transition is eq. (1); but contact phenomena have in the same process of casting formation; metal glass production by quenching. In the second order phase transition contact phenomena is interest in the quenching process.

5. Multiscale Modelling – Material Science

Multiscale mathematical modeling: The need for the physical problem to be considered simultaneously hierarchical scales ($10^{-34} \div 10^{26}$) [14 and 15]; Choice from the area of macro-scales ($10^{-6} \div 10^{26}$) for example casting volume of kg/m^3 ; choosing for the specific task the necessary „fundamental level: crystallization theory “this can be the size of a micro-particle or an atom, (or micro-particles with atom), (or micro-particles with atoms in nucleus). It follows that the field of consideration may be ($10^{-14} \div 10^{-10} \div 10^{-6}$) i.e. use of mathematical fields and the parent methods created in them. In conformation of a multi-scale approach for us are the works [6, 8, 13 and 16].

In work [20] a scientific project is considered of Max-Planck-Institute für Eisenforschung GmbH Düsseldorf, Germany on the topic: Modeling of Materials: Development with Simulation – Discoveries through Simulation with participants F. Roters, T. Hickel, J. Neugebauer, M. Friak, C. Tasan, M. Diehl, D. Raabe. Complex alloys are an essential response to the challenges of sustainable societies [20]. Application of modeling and simulation in the design of complex materials from nano-level in real-world conditions to atomic scales [20]. Scientific mission: complex materials in real environments [20].

5. Quantum Chemistry – Physics Solids

Quantum chemical methods are shown on Fig.2 [26]:

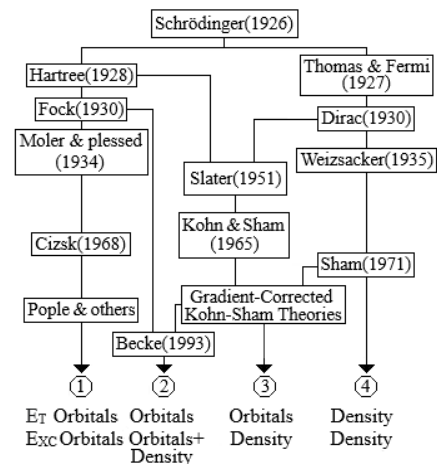


Fig.2. Evolution and classification of quantum chemical methods [26]. E_T is kinetic energy of the electrons; E_{XC} is exchange functionality.

It is well known that quantum mechanics was created to describe the properties of metals (metal physics) and is quite naturally applied in solid state physics [21, 11, 6].

Properties [22] of binary aluminum alloys Al – TM (TM = Ti, Zr and Hf) energy of alloying, formation enthalpies, intermetallic layers, lattice parameters, elastic properties are calculated with methodology is on the base: 1. CALPHAD thermodynamic calculations modeling for phase stability, phase transformation kinetics in complex systems with multicomponent alloys [22]; 2. Ab initio or first-principles methods based upon electronic density-functional theory (DFT) [22].

Powerful applications of quantum physics are professional software science products [27], for example CASTEP [7], VASP [22].

6. Multiscale Modelling – Creating Software

In [23], a combination of the finite size scaling method is proposed. A procedure for obtaining quantum critical parameters for a quantum system has been created. Results for the Yukawa potential were obtained by the finite element method [23]. The finite size scaling method is used to determine critical system parameters [23]. In work [24] criterion is derived for the determination of parameter domains of first order phase transitions in quantum mechanical tunneling models. This criterion [24] is tested by models for the study of spin tunneling in macroscopic particles. Preliminary heuristic identification domains are sought, with which agreement is sought in each case [24].

7. Conclusions - Materials Science of Macro- and Meso level

Overview of macroscopic quantum tunneling and quantum-classical phase transition of the evacuation rate in large spin system ideas are introduced by simple calculations [25]. Base ideas [25] path integral (PI), path integral formulation (PIF) or (FPI): 1. Original form PIF of quantum mechanics using the orthonormal position and momentum basis [25]; 2. The FPI with imaginary time (Euclidian) with application for particle tunneling in a forbidden region is applied to the tunneling in the potential of double wells [25]; 3. The PIF of single-molecular magnets (spin system) is required: the use of nonorthonormal spin coherence states in a $(2s+1)D$ Hilbert space, the coordinate-independent and coordinate-dependent shape of PI of the coherence state of spine are derivatives. These two (equivalent) forms of the coherent PI of rotation of the state are applied to the tunneling of single molecular magnets through a magnetic anisotropic barrier[25]; 4. Tunneling suppression: half-odd integer spin (*spin-parity effect*) at zero magnetic field is derivative on the base of the both forms of spin coherent state PI and is shown that (*spin-parity effect*) is independent of the choice of coordinate [25]; 5. They are presented experimental and theoretical result at zero magnetic field: is from the oscillation of tunneling splitting as a function of the applied magnetic field applied along the spin hard anisotropy axis direction [25]; 6. Tunneling in a model of dimeric antiferromagnetic exchange is considered [25]; 7. The formalism of the PI of the spin of the coherent state is a semiclassical method: an alternative exact mapping of the Hamiltonian of the spin to the Hamiltonian of a particle with potential field (effective potential method) is derived [25]. The methods from 1 to 7 in [25] are applied in different models of spin.

Here it is important to know that research is divided into two parts: 1. Basic research based on complete fundamental knowledge in mathematics; mathematical and theoretical physics; with 1.1 Fundamental experiments; 2. Applied research: based on the results of 1. And 1.1; Duration of research: the history of science and especially of the 20th century has shown [12] that the duration is almost the same, i.e. (Duration of studies 1. And 1.1) $\approx$ (Duration of studies 2.); 3. Research funding: Fundamental research is funded by the state; Applied research is funded by industry. The ideal lattice [21 and 20] is without defects and at the macro level is a mono crystal. A real lattice [21 and 20] has defects and at the macro level is a polycrystalline. The defects are [21 and 20]: dislocation;

polycrystalline grain formation (surface); precipitates; phases, cracks.

CASTEP is professional software introduced in BOVIA Materials Studio 2020 • CASTEP Guide [7]. Task in CASTEP: Single-point energy calculation; Geometry optimization; Molecular dynamics; Elastic constants calculation; Transition state search; Transition state confirmation. Mathematics and mathematical physics [14 and 15] must need of engineers [13], i.e. the curricula of the Faculties of Mathematics and Physics of Sofia University must also be curricula and for engineers [1, 2, 3, 4 and 5] to have maximum orientation in the methodology of science [12].

1. Contact phenomena are important part of macro- and micro-level of casting process.

2. Tunnel effect is describing by quantum mechanics.

3. To use professional software requires supercomputer resources with very good computing infrastructure.

4. Multiscale mathematical modeling is becoming a basic approach to work in fundamental and applied research as well as production skills to any company.

5. Mathematical provision of micro-foundries: inclusion in *the computing infrastructure* through the Machine Building.

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Newtonian mechanics inertial conception of microeconomical systems

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Abstract: *The study of the activities of microeconomic systems always remains a very important task of quantitative description of these systems. The proposal of new methods of study over time takes place in the emergence of new integrative scientific platforms such as econophysics which is a modern platform based on the description of economic phenomena by the application of classical and modern theories of physics. The microeconomic system of goods in general is characterized by the possession of some quantity of goods that is a potential for the revenues generating as the result of customer demands. The quantity of goods evolves over time as if it is a "trajectory" according to the theory of classical mechanics. This trajectory in economic terms is called the trend.*

The system "moves" on this trajectory and the movement takes place under the action of the forces acting on the system. This study delimits the following names of the forces acting on the microeconomic system. The first type of the force acting from the customers is called the driving force F_m . For the stable efficient continuation of the system over time, it is necessary both the permanent insurance with goods from the distributors and the payments in the form of salaries and other various taxes, all being expenses that are generally categorized in assets and liabilities. And they will be called in economic terms with a general term friction forces F_f . These friction forces stop the numerical increase of the revenues in general.

A special case belongs to the movement on a constant trend (case of uniform rectilinear movement). This case occurs when the driving force of customers is equal to all types of resistance force (all types of the payments in the form of various taxes and salaries). It should be noted that when all the free financial resources that come from the sale are all spent on new goods from distributors as well as other taxes and wages then it really seems that the system seems to be "in the rest state" ("does not move") This is Newton's first law, the respective speed and the acceleration is zero..

The mechanical conception of the description of the activity of microeconomic systems allows understanding deeply the mechanisms of the generation of bankruptcy as well as the special conditions necessary for income generation by the application of the physics language of Newtonian mechanics movement.

Keywords: MICROECONOMICAL SYSTEM, ECONOPHYSICAL MASS, GROSS PROFIT, ASSETS AND LIABILITIES, MOTOR FORCES, FRICTION FORCES, NEWTONIAN MECHANICS, ACCELERATION, INERTIA, FIRST LAW OF NEWTON

1. Introduction

Technical and scientific progress involves an integrational development of various scientific fields in order to solve new major goals and proxies in the field of medicine, economy, pharmaceutical industry, high modern technologies, social processes and the Human being in the new life conditions taking into account the evolution of climatic and ecological conditions. Also new philosophical conceptions about Life imply a widespread application of knowledge from different fields of science and eventual their application into new integrative scientific fields such as: biophysics, bioinformatics, econophysics, bioeconophysics etc.

Econophysics is an interdisciplinary research field, applying theories and methods originally developed by physicists in order to solve problems in economics, usually those including uncertainty or stochastic processes and nonlinear dynamics. Some of its application to the study of financial markets has also been termed statistical finance referring to its roots in statistical physics. [1]

Econophysics was started on 1990s by several physicists working in the subfield of statistical mechanics. Unsatisfied with the traditional explanations and approaches of economists – which usually prioritized simplified approaches for the theoretical models to matching financial data sets, and then to explain more general economic phenomena.

The worldwide scientist Harry Eugene Stanley is one of the pioneers of interdisciplinary science and is one of founding fathers of econophysics. Stanley has developed the term of econophysics for the description of the large number of papers written by physicists in the problems of markets and presented in a conference on statistical physics in Kolkata in 1995 and first appeared in its proceedings publication in Physica A 1996.[1, 2]

The multidisciplinary field of econophysics uses theory of probabilities and mathematical methods developed in statistical physics to study statistical properties of complex economic systems consisting of a large number of complex units or population (firms, families, households, etc.) made of simple units or humans. [3] Consequently, Rosario Mantegna and Eugene H. Stanley have

proposed the first definition of econophysics as a multidisciplinary field, or "the activities of physicists who are working on economics problems to test a variety of new conceptual approaches deriving from the physical sciences". Econophysics is a sociological definition, based on physicists who are working on economics problems. [4] Another, more relevant and synthetic definition considers that econophysics is an "interdisciplinary research field applying methods of statistical physics to the problems in economics and finance". [5]. Unquestionably, in the second half of the 19th century, physics significantly accelerated the development of economics by providing a necessary methodological framework. [6], [7]

The term "econophysics" [8] was introduced also by analogy with similar terms, such as astrophysics, geophysics, and biophysics, which describe applications of physics to different fields. Originating from physics as a quantitative science, econophysics emphasizes quantitative analysis of large amounts of economic and financial data, which became increasingly available with the massive introduction of computers and the Internet. Econophysics distances itself from the verbose, narrative, and ideological style of political economy and is closer to econometrics in its focus. Two major directions in econophysics are applications to finance and economics, statistical distributions of money, wealth, and turnover among interacting economic agents.

Econophysics that is a new branch of the study of economy includes not only proper sense of econophysics as usual but also physical economics [9] that explains the economical processes by the application of physical phenomena and has a large priority to choose the adequate physical model for the quantitative description of the processes of pharmaceutical marketing. [10]

Physics studies the general laws of nature and explains phenomena with appropriate patterns using mathematical methods. The traditional question of physics is: why does this phenomenon happen? And the answer is given according to the appropriate model. The development of physics has reached such limits that it is now becoming interdisciplinary. The human being always at different historical stages is accustomed to observing phenomena in nature and studying them in detail, to explain why these phenomena

occur and the cause of their defense. So, namely physics is called science that deeper insight studies the essence of all things in the Nature. Logically, we can ask ourselves in the following way, since physics explains the essence of all things, then it really does explain everything like: historical evolution of society and eventually statistical repetition of some historical processes, economic phenomena, periodical physics-statistical variations of some social and economical processes, market processes described by analogical physical laws, etc.

It is worth noting that many now-famous economists were originally educated in physics and engineering. The well known Italian scientist Vilfredo Pareto that is considered as a parent of modern science of econophysics earned a degree in mathematical sciences and a doctorate in engineering at the ends of 19th century. Working as a civil engineer, he collected statistics demonstrating that distributions of turnover and wealth in a society follow a power law [11]. Nowadays the Pareto's principle also has become a popular area of focus in the world of business and management and the statement of this principle is: 80 percent of effects always come from 20 percent of the causes. Pareto first observed this ratio when he realized that 80 percent of land and wealth in Italy was owned by 20 percent of the population. He then went on to observe the same phenomenon in his garden: 80 percent of peas came from 20 percent of pea pods. [11] Since he published these findings, the magical ratio of 80:20 (or the "80-20 rule") has been found to be scattered throughout society and nature. The 80 percent of any company's profits come from 20 percent of their best products, 80 percent of traffic comes from 20 percent of roads, 80 percent of food production comes from 20 percent of the best crops. The ratio is everywhere and frequently even tipped to a 90-10 or 95-5 division.

The Pareto principle is applied largely and it is combined with ABC analysis for supply management purpose both in medicine and economics. [12, 13] Therefore the effective supply management ensures uninterrupted availability of quality approved, safe and effective products. The econophysical studies that include the principle of Pareto were reflected in [10] which shows that each stock article of pharmaceutical products is characterized by so-named econophysical temperature and this term of econophysical temperature is the capacity of the generating power of turnover (revenues) during one day of one stock article and respectively for each rating marketing groups A, B, C, X, Z of the stocks these values of temperatures are $K_A=21$; $K_B=13$; $K_C=8$; $K_X=5$; $K_Z=3$ that coincide with the numbers of Fibonacci which stay on the basement of so-named "Golden ratio" of Nature's structures and economical structures [10, 14]. The Fibonacci sequence is applicable for various kinds of the stocks.

The econophysical studies presented in [10] apply the physical model of the "ideal gas" of the pharmaceutical stocks and this model is related to the marketing state of hyper competition. The sold and reserve inventory of stocks is described by the equation of marketing state of the microeconomical system [10]: $\langle P \rangle_p N_{tot} = N_{art} \cdot K$; here $\langle P \rangle_p$ is the average price of one pharmaceutical product; N_{tot} - total amount of products of the inventory; N_{art} - total amount of the names of articles; K - the value of econophysical temperature and for the full ensemble of stocks this value is $K = 5,65$ which is calculated on the base of $K_A=21$; $K_B=13$; $K_C=8$; $K_X=5$; $K_Z=3$ by the consideration of the peculiarities of ABC analysis and this value $K = 5,65$ is a worldwide constant that is independent on national currencies [10].

Similar expression like (1) is described in the paper [15]. The difference is that the econophysical temperature is the volatility in [15]. The greater is the volatility, then the greater is the opportunity to sell the stocks at high prices. [16] Otherwise, the higher the econophysical temperature K described by expression (1), the greater the opportunity to sell the stocks at high prices.

Generalizing the introductory information, then the definition of econophysics could be given as follow:

Econophysics is a multidisciplinary philosophical scientific integrative system that studies the general laws of the evolution of economical and social processes by the application of physics - mathematical and statistical methods of philosophical, social and economical sciences.

According to the point of view described in the paper [15] the equilibrium and crises in economies are explained well by phenomenological conception of econophysics.

Logically, the first chapter could be mechanics. Historically, classical mechanics emerged first and is originated with Isaac Newton's laws of motion in the paper [17] "Philosophie Naturalis Principia Mathematica".

Classical mechanics describes the general laws of the motion of macroscopic material bodies.

Microeconomics is the study of individuals, households and firms, behaviour in decision making and allocation of resources. It generally studies the markets of goods and services and deals with individual and economic issues [18]. It is focused on the study deals with what choices people make, what factors influence their choices and how their decisions affect the goods markets by affecting the price, the supply and demand [19].

The behaviour of the activity of the markets of stocks is studied last time not only by classical theories of economics but also by modern integrative means of interdisciplinary branches of sciences like statistical mathematics and theory of probabilities, and modern statistical integrative science that is called econophysics. [20-22].

The chapter of kinematics of microeconomical system of stocks has studied the movement of the systems of stocks without any considerations of the reasons of the apparition of the movement [23]. Simply, it studies the behavior over time of the activity states of microeconomical system of stocks. The states of the microeconomical systems are of two types: the rest state and the movement state. The reason of the transition of the system from the rest state into a movement state is the aim of study of this research. Of course, the motor force of the movement of the systems is the torrents of customers with their capacity of the buying of the goods and services. They are as the analogical mechanical forces that are acting upon the material bodies causing their movement. The kinematics theory of phenomenological mechanical econophysics describes very well the movement of the systems and the quantitative expressions are fitting satisfactory to the real results. Logically, it is obviously that the reason of the apparition of the movement must be studied. The theory of Newton's classical mechanics will be applied for the development of the conception of the mechanical dynamics of phenomenological econophysics. Analogically to the classical mechanics where the material bodies posses the masses, the microeconomical systems of stocks posses also the mass. The conception of the mass of this system is developed by the consideration of the difference of the prices of the selling and the prices of distributors, or by the terms of economy is the gross profit meaning the prices of sales minus the cost of goods. [1, 9]

The laws of Newton were for the first time used in the paper of Adam Smith (1723-1790), a Scottish economist and philosopher [7]. Adam Smith took Newton's conception of nature as a law-bound system of matter in motion as his model when he represented society as a collection of individuals pursuing their self-interest in an academic order governed by the laws of supply and demand [7].

Namely, the supply-demand processes are the basement of the application both to Newtonian classical mechanics and the socio-economical processes.

2. First law of Newton. Application of first law of Newton to microeconomical systems of stocks. The law of inertia and its application to these systems

Newton's laws of motion are three physical laws that, together, laid the foundation for classical mechanics. They describe the relationship between a body and the forces acting upon it, and its motion in response to those forces.

The first law of Newton is formulated as follow:

In an inertial frame of reference, an object either remains at rest or continues to move at a constant velocity, unless acted upon by a force. [24, 25]

This formulation is represented schematically on the Fig. 1

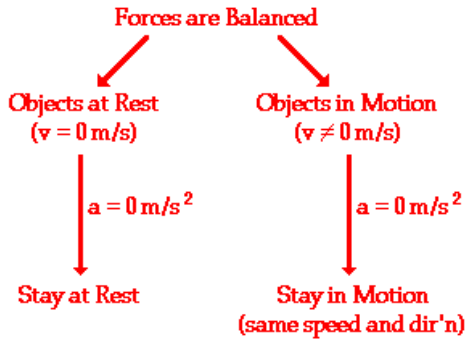


Fig. 1 The classical mechanics statement of the first law of Newton [26]

According to this Figure 1 the material body will stay in the rest state if the velocity is zero and the respective acceleration is zero. The material body does not move because all forces acting on this body have the resultant force equals to zero. Another moment is that this body could move with the constant speed all time and the respective acceleration is zero. The condition of unchangeable speed of the movement takes place only in the case when the resultant of all forces that are acting upon this body is zero. The forces that are acting upon the body during its movement (Fig. 2) are the motor force $\vec{F}_m$ for the movement of this body with physical mass m , friction force $\vec{F}_{fr}$ or the resistance force that appears as the result of the movement of this body on the contact surface of the support, gravitational force $\vec{m} \cdot \vec{g}$; $\vec{g}$ is the gravitational acceleration and for the Earth is $9.8 \text{ (m/s}^2\text{)}$; $\vec{R}$ - reaction force is the force that is acting from the surface contact. According to the first law of Newton, the body moves with the constant speed $\vec{v} = \text{const}$, when $|\vec{F}_m| = |\vec{F}_{fr}|$ and respectively $|\vec{R}| = |\vec{m} \cdot \vec{g}|$

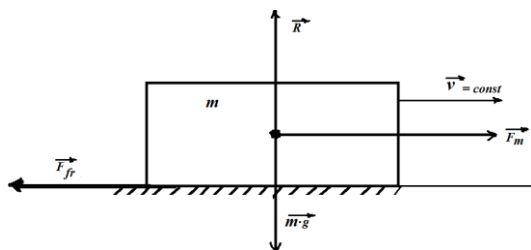


Fig. 2. Schematical representation of the forces acting upon the body in the state of the movement

Velocity (speed) is a vector quantity which expresses both the object's speed and the direction of its motion. Therefore, the statement that the object's velocity v is constant is a statement that both its speed and the direction of its motion are constant.

The first law can be stated mathematically when the mass is a non-zero constant, as:

$$\sum F = 0 \Leftrightarrow \frac{dv}{dt} = 0 \Rightarrow v = \text{const} \quad (1)$$

This expression (1) is known as the uniform motion. Loosely translated and applied to business, it means that the marketing plan will continue to deliver the same results unless something changes.[27]

Another scientific report regarding the first law of Newton [28] and applied for the stock market states that "simply put, the stock market is going up because it has no reason not to. It will remain in the uptrend until acted upon by an outside force". Here the explanation is of such order that if the socio-political laws and the rules of marketing are no changeable over time then the activity of the stock market is adapted well to these conditions and the respective business also is adapted unless an outside force acts upon it, i. e. the socio-political laws and the rules are changed under the influence of this outside force.

The application of the first law of Newton to the microeconomical system of stocks can be explained as follow. The microeconomical system can be considered as the "vehicle" or "car" that is moving on the trajectory. This trajectory is the reserves inventory evaluating over time. Analogically to the mechanical movement, the following forces are acting upon this system: 1) motor forces of the customers F_m , which means the buying capacity of the customers to purchase the goods. These types of the forces are able to produce the revenues in the form of the free financial resource; 2) the resistance or friction forces that are related to the payments of assets and liabilities. They are of two types: proper friction force F_{fr} and the force of the restoring of new stocks from the dealers (restore of the initial level of stock reserve) - $F_{s,r}$. The expenses of the assets are related to the restoring of the new stocks from distributors, but the liabilities are related to the various bills, bank accounts overdrafts, income taxes, salaries, etc. These friction forces every time have the tendency to reduce those free financial resources that are obtained from the revenues. In the case when the motor forces of the customers are compensated by the friction forces, then the result is null (finally, there are no free financial resources). It seems that the microeconomical system is situated into a "critical" state exactly similar like as the initial starting time. This "critical state" is such a state when all financial resources from the revenues are expensed for all types of expenses and the result is that there are no any more free financial resources. These "critical" states could also have the tendency of the critical default trend.

The similar trajectory as that shown on the Fig. 2 can be represented for the microeconomical system with the econophysical mass M on the Fig. 3. The trajectory ΔZ represents the amounts of products of the inventory of the system that is a sequence of the values of the amounts of products of the inventory ΔZ over time.

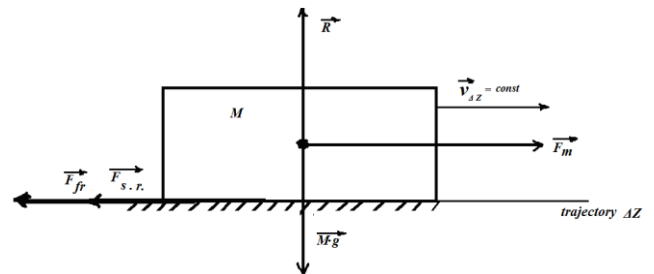


Fig. 3 The forces that are acting upon the microeconomical system of stocks with the econophysical mass M

The econophysical gravitational acceleration in this case g has another meaning and another numerical value that is different of the physical one. The reaction force R has the meaning of the force that maintains the microeconomical system on the trajectory ΔZ due to of the payments that are related to the assets and liabilities. When the friction forces and the forces that are related to the restoring of the stock reserve are absent, then $R=0$ and the microeconomical system is falling down (similar to the free gravitational falling in

mechanics). This situation could be the case of the liquidation of the full reserve inventory by special discounts before of the stopping activity of the systems due to of the default criteria.

That mentioned above the moment of "critical state" can be explained also by kinematical point of view. The dependence of the sold inventory expressed in terms of the amount of products $\Delta Z(t)$ is represented on the Fig. 4. The situation when the friction forces is equal to the motor forces of the customers leads to the continuous slow increasing till the critical value of sold inventory ΔZ_{cr} and then this value ΔZ_{cr} is unchangeable for a long time. Such critical state could be reached as the result of the decreasing of the torrents of customers. The decreasing of the torrents of customers leads to the decreasing of the revenues and finally such state is reaching when the financial free resources are equalized to the friction forces.

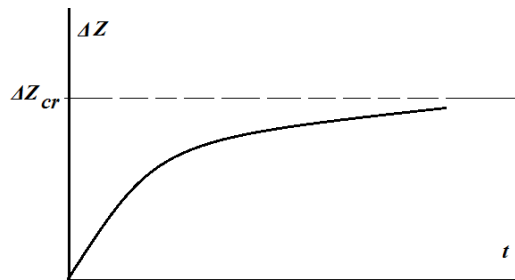


Fig. 4 The situation of the critical state of the sold inventory

Generalizing all the above described the formulation of Newton's first law for the microeconomic systems can be given as:

The microeconomic system is situated into a critical state of the rest when the financial resources from the revenues of the stocks and services equals to the all the types of the expenses that are expected.

The first law also is named the law of inertia. The first law of Newton in fact is a statement of a property of matter called inertia. Matter maintains its state of the rest or the uniform motion and a net force (resultant) is required to change its state. The resistance to change in velocity is called inertia. The inertia of a body is directly proportional to the mass of the body. The more mass an object has, the greater is its inertia and then it resists more to the change in velocity. In other words, the mass of an object is a measure of its inertia. [26] This short formulation of inertia is pure physical one.

The conception of inertia could be developed for the microeconomical system. It is necessary to define the notion of econophysical mass of microeconomical system. The profound logical analysis allows suggesting about the econophysical mass of the microeconomical system of stocks as the gross profit of the reserve inventory which is the difference between the selling price and the cost from the distributors.

It is necessary to differentiate the econophysical mass and the physical mass. The physical mass is the usual mass that is measured in grams, kilograms, etc., but the econophysical mass is measured in the values of the respective financial currencies and according to that mentioned above this econophysical mass is the gross profit. The co-relation between physical and econophysical mass is necessary to be established. Usual practice of the markets shows that as greater is the quantity of the goods that is sold then the lower is the price. The expression of microeconomical state of the stocks could show this relation between the physical mass and econophysical one. The respective expression of microeconomical state is: $\langle P \rangle_p \cdot N_o = K$. The amount of products N_o of the respective article could be expressed by the quantity of molecules of the substance N_{mol} as follow: $N_o = C \cdot N_{mol}$, where C is the proportional coefficient. As bigger is the amount of products N_o , then as bigger is the respective amount of molecules N_{mol} . The value N_{mol} could be expressed by the number of Avogadro and quantity of moles as:

$$\nu = \frac{N_{mol}}{N_A} = \frac{m}{M_o}; M_o \text{ is the molar mass of the respective chemical}$$

substance and m is the physical mass of the product.

Then, the value is

$$N_{mol} = \frac{m}{M_o} \cdot N_A; \Rightarrow N_o = C \cdot \frac{m}{M_o} \cdot N_A;$$

$$\Rightarrow \langle P \rangle_p \cdot N_o = \langle P \rangle_p \cdot C \cdot \frac{m}{M_o} \cdot N_A = K;$$

Finally, the respective average price of one product is:

$$\langle P \rangle_p = \frac{K \cdot M_o}{C \cdot m \cdot N_A} \quad (2)$$

As higher is the average price of one product $\langle P \rangle_p$ then higher is the econophysical mass M .

So: $M \sim \frac{1}{m}$. So, the important semi-quantitative expression is

obtained that as bigger as is the physical mass m then the econophysical mass M is smaller and the respective average price of one product $\langle P \rangle_p$ is smaller.

The force is the analogy of the purchasing power of customers and is nothing else but the amount of money that is paid to buy one product, i. e. money paid for one product. As bigger is the price of one product, then bigger is the econophysical mass of this product and respectively the corresponding force that is applied upon this product is bigger. According to these mentioned statements it could be formulated the following definition of inertial econophysical law: **As bigger is the econophysical mass of one product then as bigger is the force that is applied upon it.**

Such suggested econophysical formulation of the law of inertia has deeper meaning. The force according to this statement is not only the money paid for one product, but it is also a decision making (a decision thinking effort) of the customers. The question how faster or slower is the decision making can be given by the supply - demand processes of microeconomics. Forever, when the demand is high for one product then the price of one product has the permanent increasing. More demand products are quickly purchased nevertheless that they have high prices, and slowly demanded products have small prices. Such specifications on the demand are based on the special ABC marketing analysis combined with Pareto distribution. According to ABC marketing analysis, the stock is differentiated into "A", "B", "C", "X", "Z". The biggest profits that have the biggest prices of products have the segments A, B, C which together consists 20% of the articles of inventory. Pareto distribution states that 20% of the articles give 80% of revenues. The ratio 20/80 of Pareto distribution is observed for very great interval of time in major cases like several years depending on the type of the activity and the type of microeconomical systems. Namely, the first segment ABC gives this 80% of revenues. The products of A, B, C segments have highest prices, the respective demands are highest and their econophysical masses are biggest. The values of the rating coefficients of the stock K serve as the criteria of the decision making. The respective values of K are highest for A stocks and smallest for Z stocks.

The notion of inertia has deeper meaning. When we say that something or some idea is performed very slowly with very slow result, then this idea is very inertly. Transposing to pure physical phenomena we know that the bodies with bigger physical masses are very inertly. It is necessary a great physical force to make its starting of the movement. Applying to the stocks it means that the bigger physical masses have the stocks Z and the smallest physical masses have the stocks A. It means that the stocks Z are very inertly and the stocks A are slowly inertly. According to these statements it would be necessary the reformulation of the econophysical law of inertia of microeconomical systems of the stocks as follow:

The lower is the physical mass of one product then the higher is its demand.

This formulation has deep sense and it is observed for many real cases, for example in the cosmetics and the souvenirs shops. The customers have high demand for the products with small masses and respective small volumes, aesthetically and beautifully comfortably packed as the gifts for the large trips. These cases are used almost everywhere for the almost all types of the microeconomic systems. The manufacturers' designers analyze well the products purchasing processes and their designs and the volumes of products are changed periodically.

Also the ***econophysical mass of ensemble*** of stocks can be applied and described by the application of the principles of *ABC* analysis. As the *ABC* stocks consists only 20% of the articles then the econophysical mass of this *ABC* segment is smaller in comparison with the segments *XZ* which consists 80% of others.

Then, especially in this case of the **ensemble** the more inert is XZ as it is regarded as an **ensemble**, and less inert is ABC .

The research [29] appreciates by the application of Newton's laws that the small business and enterprises are more efficiently, nevertheless that they are of small sizes and their respective econophysical masses of ensembles are small. They are less inert and any other changeable factors of socio-political characters are adapted more quickly to these systems than in comparison of big ones, or they could be very sensible to any changes of socio-political factors than of big systems.

Results and discussion

The good activity of one microeconomical system is based on everyday reports as the form of table represented below which shows the values of stock reserves, cash desk, revenues and expenses and the net profits that are checked everyday from the cosmetical shop and could be calculated automatically by the complex manners of mathematical and logical operations of maths functions of Excel soft. (Fig. 5)

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Fig. 5. The balance of expenses-revenues of the microeconomical system of stocks (example of cosmetical shop). All revenues and expenses are expressed by BGN currency

The table of the Fig. 5 shows every days activity and first fourteen days is a good example of the demonstration of the first law of Newton. The sum of all expenses equals to the sum of all revenues. The reserve inventory from the table every day is almost the same. It means that the system moves on the almost straight line (Fig.6). This case is indeed a good example of first law of Newton.

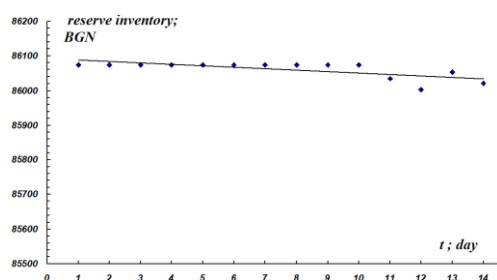


Fig. 6. The “movement” of the microeconomical system on the straight line (straight line trend)

The columns of the table with the values of the revenue and expense show well this example which illustrates the validity of Newton's first law. Expenses and revenues are almost the same, which indicates that the driving force of customers F_m (revenue) is equal to the friction force F_f (expenses). In order to see better that the friction force is equal to the driving force, then the cumulative values of the revenues and of the expenses are calculated and the dependency graph $R_{cum}=f(E_{cum})$ is represented.(Fig.7)

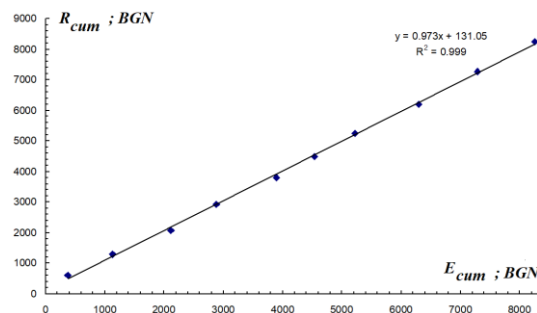


Fig. 7. The equality of the cumulative revenue and of the cumulative expenses of the validity of the first law of newton

The econophysical speed as a measure of the generating of free financial resources shows that these resources are almost not generating within fourteen days. The starting total cash is almost constant all time (it is similar to the rest state) (column 7 of the Table). It means that there is no any speed of “movement”. The speed in general is considered also the degree of the change of stock inventory, but there is no any change of the stock inventory and therefore the speed is zero.

In general we can say that the activity of the microeconomic system is described by the applying of the language of physics. In this way it can be concluded that the trend can have variations only when the driving force of the customers differs a lot from that of the resistance and finally the system will possess a speed.

Conclusions

The study which is described in this paper with the application of the language of physics of Newtonian mechanics is a fine and profound study. The trend, which is a qualitative description of the activity of microeconomic systems, gives an appreciation about the generation of financial resources. The speed that is the measure of the variation of the stock inventory is zero for the case of rectilinear trend with zero slopes which denotes a full coincidence with Newton's first law.

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Example of an accident reconstruction with Virtual Crash software and the mathematical simulation of this accident situation at intersection.

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Abstract: The paper presents an example of an accident situation using Virtual Crash software in the reconstruction of a high-speed side-impact accident of two vehicles at intersection. The simulation allowed estimating the velocity of the vehicles at the moment of collision and the determination of the location of the vehicles. We also focus on the result of the mathematical simulation of this accident situation at intersection when two vehicles and two pedestrians take part in this collision.

Keywords: ACCIDENT INVESTIGATION, ACCIDENT RECONSTRUCTION, UNCERTAINTY ANALYSIS, SIMULATION MODELS.

1. Introduction

The purpose of traffic accident reconstruction is to estimate the velocity of the vehicles at the moment of collision. Other objective of the reconstruction is the determination of the location of the vehicles in the cases when evidence is insufficient to estimate their positions and orientation at the moment of impact.[1]

The velocity of a vehicle in an accident can be determined using possible tire marks left on the road surface, or by measuring the amount of deformation caused during impact. In mapping the accident site, debris scatter analysis and driver and eye-witness statements are also utilized. Nowadays, substantial use is made of computers in traffic accident analysis. Crash analysis computer programs serve investigators in determining the relative velocity between the two vehicles prior to impact - an essential piece of information in most accidents.[2]

We will analyze an accident situation in its three phases through mathematical simulation and its modeling through the Virtual CRASH computer program which performs car collisions and 3D simulation trajectories, also represents the speed of vehicles in the positions before contact, at the moment of collision and after the collision. We will examine an accident situation when two vehicles (Alfa Romeo 147 and Audi A2) and two pedestrians participate in a crash. As a result of the collision of the two vehicles, the collided vehicle hits the two pedestrians as well.

1. Accident Description

Research is based in a road accident where was involved two vehicles and two pedestrians who were crossing the white lines and as a result of the collision of these two vehicles, one of the collided vehicles hits and two pedestrians. The mass of the Alfa Romeo was assumed to be 2080 kg, and the mass of the Audi A2 was assumed to be 890 kg. The accident happened during daylight at the intersection, in heavy traffic. The road surface was in favorable conditions with no precipitation. The common restitution coefficient was set equal to 0.25, which is a probable number in case of high-speed collisions of automobiles.[3]

2. Computer simulation

PC-Crash - performs 3D collisions & 3D trajectory simulation. Provides vehicle speeds, at pre-impact, collision, and post-impact positions. It has 3D road tool for constructing or importing 3D scenes and automatic calculation of secondary impacts including sustained contact.[4]

The vehicles involved in the accident are present with blue color (Alfa Romeo 147) and with red color (Audi A2). Collision process between vehicles happened while they was movements in different directions with vehicle at angle about 90° (Figure 1).

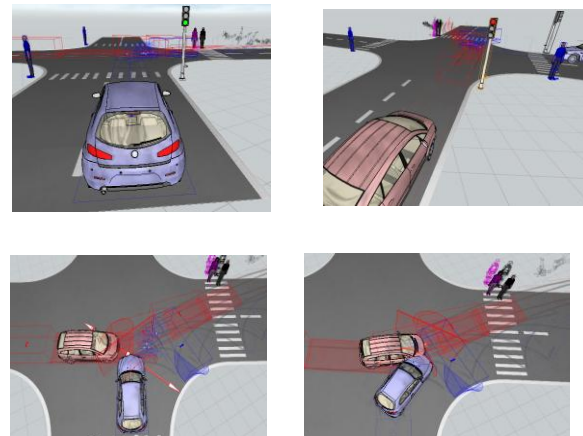


Fig. 1 Virtual Crash simulation of "Alpha Romeo" - "Audi".

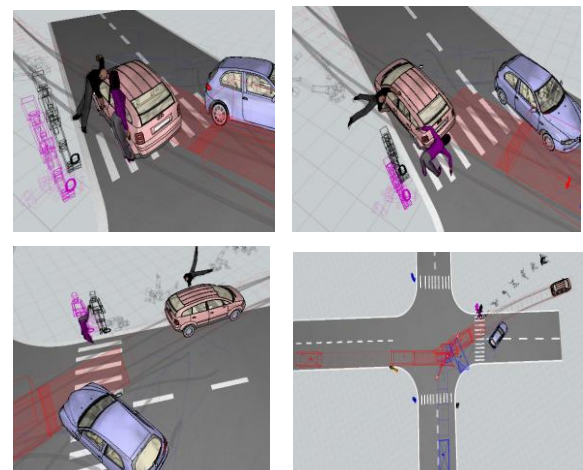


Fig. 2 Virtual Crash simulation after crash moments.

3. Mathematical simulation of this accident situation at intersection.

We need to calculate the speed and movements of the vehicles involved in the accident. Then it is possible to evaluate the spins and linear movements under which the two vehicles have gone under in the movement from the first contact location on to the final location.[5]

Spins and displacement (centre of importance) provided as follows:

$$\alpha_1 = 137^\circ = 2,4 \text{ rad} - \text{rotation of Audi A}_2 \text{ (running clockwise)}$$

$\alpha_2 = 107^\circ = 1,9 \text{ rad}$ - rotation of Alpha Romeo (running anti-clockwise)

$S_1 = 7.90 \text{ m}$ - linear displacement of the center of importance of Audi A₂

$S_2 = 7.40 \text{ m}$ - linear displacement of the center of importance of Alpha Romeo.

To calculate the velocity, we apply the general momentum equations. The task of the reconstructionist is to determine how the vehicles came together from the evidence. These are: the point of impact, pre-collision angle of each vehicle, post-collision angle of each vehicle, weights of each vehicle, post-collision velocity of each vehicle.[6]

Note: m_1 - measures of Audi A₂ with two people on board, m_2 - measures of Alpha Romeo with two people on board, v_1, v_2 - the velocities of vehicles before the collision, v'_1, v'_2 the velocity of the vehicles after the collision, q_1 - the angle formed by the vector v_1 , q_2 - the angle formed by the vector v_2 , θ'_1 - the angle formed by the vector v'_1 , θ'_2 = the angle formed by the vector v'_2 .

Then

$$m_1 = \frac{2.080 + 1.40}{9.81} = \frac{2.220}{9.81} = 226 \text{ kg m}^{-1} \text{ s}^2$$

$$m_2 = \frac{890 + 140}{9.81} = \frac{1.030}{9.81} = 105 \text{ kg m}^{-1} \text{ s}^2$$

$$\theta_1 = 0 \text{ and } \cos 0 = +1,00, \theta_2 = 111^\circ \text{ and } \cos 111^\circ = -0.36$$

$$\theta'_1 = 4^\circ \text{ and } \cos 4^\circ = +0,99, \theta'_2 = 16^\circ \text{ and } \cos 16^\circ = +0.96$$

We see that after the collision velocities – listed with v'_1 and v'_2 - can be determined primarily on the theoretical route by considering only linear displacements S_1 and S_2 by the formulas:

$$v'_{10} = \sqrt{2g f S_1} = \sqrt{2 \times 9.81 \times 0.40 \times 7.90} = 28 \text{ km/h}$$

$$v'_{20} = \sqrt{2g f S_2} = \sqrt{2 \times 9.81 \times 0.40 \times 7.40} = 27 \text{ km/h}$$

Also, for the first and second vehicle we calculate:

$$v_{*1} = \sqrt{g f p \alpha_1} = \sqrt{9.81 \times 0.45 \times 2.54 \times 2.4} = 19 \text{ km/h}$$

$$v_{*2} = \sqrt{g f p \alpha_2} = \sqrt{9.81 \times 0.45 \times 2.39 \times 1.9} = 16 \text{ km/h}$$

Now we obtain the velocity after collision:

$$v'_1 = v'_{10} + v_{*1} = 28 + 19 = 47 \text{ km/h}$$

$$v'_2 = v'_{20} + v_{*2} = 27 + 16 = 43 \text{ km/h}$$

Equations for the velocities before collision are:

$$v_1 = \frac{v'_1 m_1 \cos \theta'_1 + v'_2 m_2 \cos \theta'_2 - v_2 m_2 \cos \theta_2}{m_1 \cos \theta_1}$$

$$v_2 = \frac{v'_1 m_1 \sin \theta'_1 + v'_2 m_2 \sin \theta'_2}{m_1 \sin \theta_2}$$

Then $v_1 = 80 \text{ km/h}$, $v_2 = 70 \text{ km/h}$.

4. Conclusion

Modern methods of analyzing accidents allow for a rather precise reconstruction. Such reconstruction is based on the precise specifications of the forensic evidence. Among the most basic of these are tracks and marks left at the place of the accident, damage to the respective vehicles, and objects (including persons involved), and their mutual positions occupied after the accident. With regard to such source data and material, we can determine the impact speed very precisely. To evaluate the accident, we also have to determine the speed of the involved vehicles at the time of the reaction of the drivers. It is only possible to determine this in accidents at light controlled intersections if the signal plan of the intersection is implemented into the accident scenario.[7]

At the presented paper the values found for the speed of movement of two vehicles show:

a. for the vehicle Audi A₂, an overcoming speed with 60% related to the allowed norm (50 km / h) which is known in the waiting area of widely hazard warning and situation of countries (Article 141 and 142 of the Highway Code).[8]

b. for the vehicle Alpha Romeo, failing to stop at the Stop located at the exit from the road crossing the, because if it was given the rest to reach the crash at a speed of 70 km / h = 19.4 m/s in the confined space of $S = 6.50$ meters should have won an acceleration $a = v^2 / 2S = 19.4^2 / 13 = 29 \text{ m/s}^2$. In a time of $t = v/a = 19.4 / 29 = 0.7 \text{ s}$ (violation of Article 5,139 and 143 of the Highway Code of Albania). While not stop at Stop and instead taking a crossing speed of 19.4 m/s to reach Stop the crash of traversing 6.50 meters has occupied a time $t = s/v = 6.5 / 19.4 = 0.3 \text{ s}$. Value that gives an idea of the overcoming speed on this situation.

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Highly efficient stochastic approaches for multidimensional integrals in biology for access control

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ABSTRACT: Monte Carlo methods have become popular computational device for problems in biology. In this work we implement and analyze the computational complexity of the Latin hypercube sampling algorithm. We compare the results with Importance sampling algorithm which is the most widely used variance reduction Monte Carlo method. We show that the Latin hypercube sampling has some advantageous over the importance sampling technique.

KEYWORDS: MONTE CARLO ALGORITHMS, MULTIDIMENSIONAL INTEGRALS, LATIN HYPERCUBE SAMPLING, IMPORTANCE SAMPLING, COMPUTATIONAL BIOLOGY

1 Introduction

Monte Carlo (MC) methods always produce an approximation to the solution of the problem or to some functional of the solution, but one can control the accuracy in terms of the probability error [4]. An important advantage of the MC methods is that they are suitable for solving multi-dimensional problems [3], since the computational complexity increases polynomially, but not exponentially with the dimensionality. Another advantage of the method is that it allows to compute directly functional of the solution with the same complexity as to determine the solution. In such a way this class of methods can be considered as a good candidate for treating innovative problems related to modern areas in quantum physics and finance and security. The MC methods for multidimensional integrals can be used in problems where the data is taken in randomized way such that some applications in computational biology. Multidimensional numerical quadrature are of great importance in these areas.

The crude MC method has rate of convergence $O(N^{-1/2})$, which is independent of the dimension of the integral, and that is why MC integration is the only practical method for many high-dimensional problems. Much of the efforts to improve Monte Carlo are in construction of variance reduction methods which speed up the computation. Importance sampling (IS) is probably the most widely used MC variance reduction method, [1]. One use of importance sampling (IS) is to emphasize rare but important events, i.e., small regions of space in which the integrand is large [5]. One of the difficulties in this method is that sampling from the importance density is required, but this can be performed using acceptance-rejection. It is also known that IS can greatly increase the variance in some cases, [10]. In Hesterberg (1995, [6]) a method of defensive IS is presented; when combined with suitable control variates, defensive IS produces a variance that is never worse than the crude MC variance, providing some insurance against the worst effects of importance sampling. Defensive IS can however be much worse than the original importance sampling. Owen and Zhou (1999) recommend an IS from a mixture of m sampling densities with m control variates, one for each mixture component. In [10] it is shown that this method is never much worse than pure IS from any single component of the mixture.

The layout of the rest of this paper is as follows. The next Section 2 discusses the problem that we are considered in this paper. Section 3 describes the Latin hypercube sampling algorithm (LHS). The numerical experiments and results are given in Section 4. Finally, some conclusions have been made concerning the advantages and disadvantages of the algorithms studied.

2 Description of the problem

Consider the problem of approximate integration of the multiple integral:

$$\int_{[0,1]^d} f(x) dx = \int_0^1 dx^{(1)} \int_0^1 dx^{(2)} \dots \int_0^1 dx^{(d)} f(x^{(1)}, x^{(2)}, \dots, x^{(d)}),$$

where

$$x = (x^{(1)}, \dots, x^{(d)}) \in [0, 1]^d.$$

For small values of d , numerical integration methods such as Simpson's rule or the trapezoidal rule (see Davis and Rabinowitz [2]) can be used to approximate the integral (1). These methods, however, suffer from the so-called curse of dimensionality and become impractical as d increases beyond 3 or 4. The Crude MC method has rate of convergence $O(N^{-1/2})$, where N is the number of samples, which is independent of the dimension of the integral, and that is why MC integration is the only practical method for many high-dimensional problems.

3 Latin Hypercube Sampling

The main problem of some of the widely used MC methods such as IS is that a sample that is very close to another does not provide much new information about the function being integrated. One powerful variance-reduction technique that addresses this problem is called stratified sampling. Stratified sampling works by splitting up the original integral into a sum of integrals over sub-domains. In its simplest form, stratified sampling divides the domain G_d into N sub-domains (or strata) and places a random sample within each of these intervals. A quantity of interest is the variance of the obtained approximation, considered as a random variable. It can be shown that stratified sampling can never result in higher variance than pure random sampling [11]. If $N = 1$, we have random sampling over the entire sample space (see [12]).

The Latin hypercube sampling (LHS) was described by McKay in 1979 [8]. If we wish to ensure that each of the input variables x_i has all portions of its distribution represented by input values, we can divide the range of each x_i , in our case the interval $[0, 1]$, into M strata of equal marginal probability $1/M$, and sample once from each stratum. In the case of integral approximation, we must simply divide the interval $[0, 1]$ into M disjoint intervals, each of length $1/M$ and to sample one point from each of them. Let this sample be X_{kj} for dimensions $k = 1, \dots, d$, $j = 1, \dots, M$. Those of them having first index k ($k = 1, \dots, d$) are the different components for the k -th dimension of the random points that are used for the integral's approximation. These components are matched at random. Thus the maximum number of combinations for a Latin Hypercube of M divisions and s variables (i.e., dimensions) can be computed by the formula $(M!)^{d-1}$. In the context of statistical sampling, a square grid containing sample positions is a Latin square if (and only if) there is only one sample in each row and each column. Thus following the described algorithm, we obtain a set of points with positions forming a Latin square. Note that this

sampling scheme does not require more samples for more dimensions (variables); this independence is one of the main advantages of LHS scheme. In LHS one must first decide how many sample points to use and for each sample point remember in which row and column the sample point was taken. Note that such configuration is similar to having N rooks on a chess board without threatening each other. There are examples of random, stratified and Latin hypercube samplings with 16 points in [7]. A Latin hypercube is the generalisation of this concept to an arbitrary number of dimensions, whereby each sample is the only one in each axis-aligned hyperplane containing it. To prove that the variance of the LHS is smaller than the variance of IS we use a theorem proved in [8].

Generally, the time complexity of the algorithm depends on the integrand. However, it follows easily that the computational complexity of the Latin hypercube sampling is linear, we will have only a constant number of additional operations compared to the regular Crude MC method and it is easy to show that the computational complexity of the crude Monte Carlo is linear.

4 Numerical example

We want to compute the following 7 dimensional integral that can be used to describe random process in biology:

$$\int_{[0,1]^7} e^{1 - \sum_{i=1}^3 \sin(\frac{\pi}{2} \cdot x_i)} \cdot \arcsin \left(\sin(1) + \frac{\sum_{j=1}^7 x_j}{200} \right) \approx 0.7515.$$

We will use the IS algorithm with probability density function

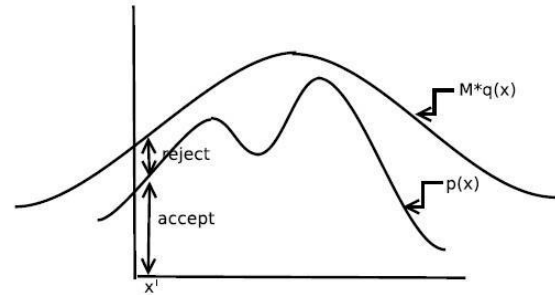
$$f(\vec{x}) = \frac{1}{\eta} e^{1 - \sum_{i=1}^3 \sin(\frac{\pi}{2} \cdot x_i)}.$$

The value of η must be found separately. It is equal to the value of

$$\int_{[0,1]^3} e^{1 - \sum_{i=1}^3 \sin(\frac{\pi}{2} \cdot x_i)}.$$

We evaluate the last integral with Crude Monte Carlo method for a number of samples $N = 10^5$. After that we use the

method of selection (the acceptance-rejection method). The idea of the method is given by the following graphic:



We choose density $q(x)$, and constant M , such that $f(x) \leq M \cdot q(x)$, then we generate a random variable with density $q(x)$ and its value x_0 is accepted with probability density function $p(x_0)$. In our realization we use the probability density function $q(x) = 1$ and constant $M = e/\eta$. We are also using two quasi-Monte Carlo methods just for a quick comparison. The detailed comparison between Sobol algorithm and Lattice rule based on Fibonacci numbers will be an object of a future study. We obtain the following graphics given below for the relative error and the total amount of time for performing each of the algorithms- see Figure 1 and Figure 2.

As we expected LHS outperforms IS by far. The results are given in the tables below. Each table contains information about the MC approach which is applied, the obtained relative error, the needed CPU time and the number of points. It can be seen that the CPU time for the Latin hypercube sampling and crude MC method is equal, while importance sampling method needs much higher time. It can be seen that for large number of samples the LHS outperforms the importance sampling. Therefore the Latin hypercube sampling is definitely better from the Importance sampling method for computing multidimensional integrals.

Table 1 presents the results for the multidimensional integral under consideration for a fixed number of random samples, while Table 2 presents the obtained relative errors for a fixed computational time.

Table1. Relative error for 7 dimensional integral for given number of samples

N	Crude	time	LHS	time	IS	time
1000	7.28e-2	0.15	2.46e-3	0.13	6.61e-3	3.1
5000	2.71e-2	0.75	9.03e-4	0.71	3.35e-3	15.8
10000	5.92e-3	1.52	4.43e-4	1.50	1.09e-3	30.2
25000	3.73e-3	3.51	1.10e-4	3.27	7.51e-4	74.5
100000	1.62e-3	13.8	7.26e-5	14.02	5.41e-4	315
1000000	8.02e-4	104	6.26e-6	110	2.53e-4	3056

Table2. Relative error for 7 dimensional integral and equal execution times

time, sec.	Crude	LHS	IS
0.1	2.38e-2	2.37e-3	5.51e-2
1	8.87e-3	3.37e-4	2.31e-2
5	5.16e-3	1.38e-4	8.05e-3
10	1.28e-3	8.78e-5	4.91e-3
20	2.03e-3	6.87e-5	2.58e-3
100	8.61e-4	7.01e-6	7.18e-4

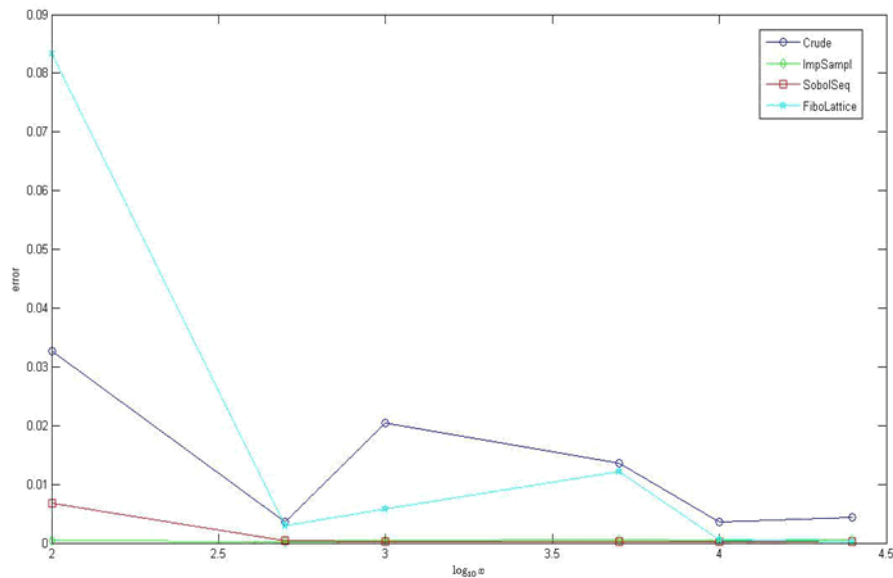


Figure 1. Relative error for 7 dimensional integral with importance sampling and crude method.

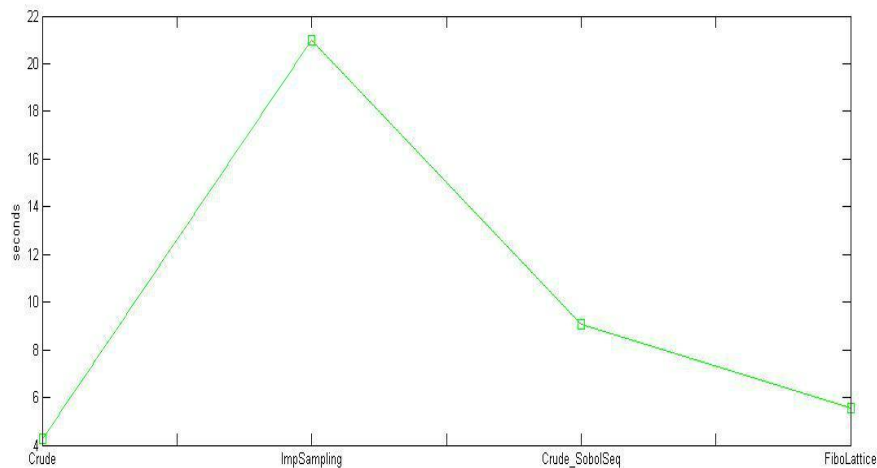


Figure 2. The total amount of time for the importance sampling and crude method for the 7 dimensional integral.

It is important to say that the numerical experiments demonstrate the fast convergence of the algorithms. While Crude Monte Carlo approach is by definition one of the fastest stochastic approach, one can observe that the presented Latin hypercube sampling algorithm has the same speed. The probabilities under consideration can be connected to correct identification on the face, auricle, papillary lines on the fingers, iris picture. All these can be biometric data that are used in access control systems. The multidimensional integral under consideration can be connected with probabilities when accessing a person by only one biological feature (ear, face, fingerprint). In total multidimensional integrals like this can be used in programs where all biometric data is already running according to Monte Carlo highly efficient approaches. The presented stochastic approach demonstrates that the big data processing even for large dimensions can be very fast.

5. Conclusion

In this numerical study we present and study the Importance sampling and Latin hypercube sampling algorithms. We compare the results with crude Monte Carlo method. The developed Latin hypercube sampling algorithm shows the best results and can be used in various problems in science where multidimensional integrals are needed. Such kind of multidimensional integrals can be used in probabilistic representations of biological data that is used in access control systems by significant features (ear, face,

fingerprint). The Importance sampling algorithm requires higher computational time than the crude Monte Carlo method, but we show that for a fixed computational time it gives closer accuracy to the crude Monte Carlo method. However, Latin hypercube sampling is far better than the Importance sampling in terms of lower relative error and shorter computational time. One should have use the Latin hypercube sampling algorithm instead of Importance sampling algorithm in evaluating multidimensional integrals arising in different areas of science. Clearly, the progress in the area of computational biology, is closely connected with the progress in reliable algorithms for multidimensional integration.

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