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Естественные науки
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This publication assembles papers given at the conference for young scientists «Presenting Academic Achievements to the World» which was held in March 29-30, 2010 at Saratov State University. The articles present the results in such fields of natural sciences as Physics, Chemistry, Geography, Geology and Information Technology.

Редакционная коллегия:

Н.И. Иголкина (отв. редактор), Е.Л. Стеркина, С.В. Пыжонков, Ю.В. Пиввуева, Л.В. Левина (отв. секретарь)

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Stochastic systems and processes are characterized by the mixing effect in the phase space. This effect leads to finiteness of time of predictability of the evolution. The fundamental result of the theory of dynamical systems is the metric entropy of a dynamical system introduced by Kolmogorov (Kolmogorov, 1959). It was strictly proved that in a chaotic system the Kolmogorov entropy is characterized by a finite positive value that denotes the correlations decay in time and finiteness of time of predictability of dynamics in a chaotic regime. For a random process, (white noise, for example) the metric entropy is infinite that denotes the absence of any predictability.

From the point of view of the strict Kolmogorov theory, dynamical systems can have stable regular regimes with a zero-value entropy and chaotic regimes with a finite entropy value. In the case of presence of noise in a system the entropy is infinite. The last case seems to be the most interesting one from the practice point of view because the overwhelming number of physical systems function in the presence of unavoidable noise influence. In (Anishchenko, 2007) and (Anishchenko, 2008) the term «relative metric entropy» was introduced and substantiated for estimatig quantitatively the external noise influence on the mixing degree in noisy systems. The applicability of the method was illustrated by a number of examples. In this paper the mixing influence of noise on a nonlinear system using the relative metric entropy approach is studied.
In a regular system the mixing can be introduced by an external stochastic or chaotic forcing only. However, the degree of their influence on a system may be different.

Let us consider two interacting regular oscillators each of which oscillates at a certain frequency. If the coupling is weak and the natural frequencies of the oscillators are close, the synchronization phenomenon can take place. In the absence of synchronization the system dynamics is characterized by two time scales that correspond to a two-dimensional ergodic torus in the phase space. When synchronization appears, only one time scale remains in the system and corresponds to a limit cycle. The latter case intuitively seems to be less complicated. However, the entropy of a regular system (including the relative metric entropy) remains zero-valued in transitions from an asynchronous regime to synchronization and back.

Now we add noise to one of the oscillators. The relative metric entropy of the system would grow monotonously when the observation precision increases. We assume that the relative metric entropy would decrease in the synchronization regime for a fixed precision value. To verify this assumption we consider a system of two interacting van der Pol oscillators where the first one is subjected to white Gaussian noise:

\[
\begin{align*}
\dot{x}_1 &= y_1, \\
\dot{y}_1 &= -\omega_1 x + (\alpha - x^2) y + \gamma(y - y_1) + \sqrt{2D}\xi(t), \\
\dot{x}_2 &= y_2, \\
\dot{y}_2 &= -\omega_2 x + (\alpha - x^2) y + \gamma(y - y_2).
\end{align*}
\]

(1)

Here \(x_{1,2}, y_{1,2}\) are the dynamical variables, \(\omega_{1,2}\) are the basic frequencies of the first and the second oscillators, respectively, \(\alpha\) is the nonlinearity parameter, \(\gamma\) is the coupling coefficient, and \(\xi(t)\) is the white Gaussian noise source with intensity \(D\). In such a system the effect of mutual synchronization is realized through the frequency locking inside the region presented in fig. 1.

Let us study how the relative metric entropy is varied when moving through the synchronization region on the parametric plane. The graph of the relative metric entropy is presented in fig. 2 versus the natural frequency \(\omega_2\) of the second oscillator. As it has been assumed, \(\hat{K}_2\) has a significantly smaller value inside the synchronization region than outside it.

Now we consider a more complicated case. We insert an external harmonic force with amplitude \(C_0\) and frequency \(\omega_{ex}\) in the second equation of system (1):
The bifurcational analysis of the synchronization phenomenon in this system for $D = 0$ has been carried out in (Anishchenko, 2009) by using the phase approach.

\[
\begin{align*}
\dot{x}_1 &= y_1, \\
\dot{y}_1 &= -\omega_1 x_1 + \left(\alpha - x_1^2\right) y_1 + \gamma(y_2 - y_1) + C_0 \cos(\omega_{ex} t) + \sqrt{2D} \xi(t), \\
\dot{x}_2 &= y_2, \\
\dot{y}_2 &= -\omega_2 x_2 + \left(\alpha - x_2^2\right) y_2 + \gamma(y_1 - y_2).
\end{align*}
\]

The bifurcational analysis of the synchronization phenomenon in this system for $D = 0$ has been carried out in (Anishchenko, 2009) by using the phase approach.
It has been shown in (Anishchenko, 2009) that the saddle-node bifurcation is connected with the frequency locking. The result enables one to obtain the bifurcational diagram for system (3) that is presented fig. 3. Three types of regions can be distinguished in fig. 3. In region $B$ the spectrum of oscillations includes three main peaks which correspond to the frequencies of each oscillator and the external harmonic force. In region $C$ two main peaks are presented in the spectrum. This corresponds to the natural frequency locking of one of the oscillators by the external force or to the mutual synchronization of the oscillators. In region $D$ both oscillators are synchronized with the external harmonic force and a single peak is observed in the spectrum.

![Fig. 3. Synchronization if system (2): region $B$ denotes three-frequency oscillations, region $C$ corresponds to the fundamental frequency locking of one oscillator by external harmonic force or to the mutual synchronization of both van der Pol oscillators with the asynchronous external harmonic force, $D$ denotes the region where both oscillators are synchronized with the external harmonic force (single-frequency oscillations).](image)

If our assumption is correct, then when the external forcing frequency increases from 9.9 to 10.1 the relative metric entropy would increase (in $C\rightarrow B$ transition), then decrease ($B\rightarrow C$) and further decrease until the minimum ($C\rightarrow D$). Afterwards, the relative entropy would start to grow ($D\rightarrow C$, $C\rightarrow B$) until its local maximum and then it should decrease ($B\rightarrow C$). The numerical results of the relative metric entropy calculation are presented in fig. 4. Indeed, the maximal values are located in regions $B$ and the minimal value is in $D$.

Thereby, using the relative metric entropy we show that the mixing effect of noise on a regular system depends on the dimension of the corresponding limit set in the phase space in the absence of noise (the greater the dimension, the stronger the effect). Besides, if to compare the results presented in figures
we can conclude that a cycle lying on the surface of a two-dimensional torus which lies on the surface of a three-dimensional torus (fig. 4, region $D$) is more affected by noise than a cycle lying on the surface of a two-dimensional torus which lies on a plane (fig. 2, synchronization region). A similar situation is observed for tori. In the case of a two-dimensional torus lying on the surface of a three-dimensional torus (fig. 4, region $C$) the noise induces a higher degree of mixing than in the case of a two-dimensional torus lying on a plane (fig. 2, outside the synchronization region).

Another interesting phenomenon that can appear in a nonlinear system in certain conditions is the effect of stochastic resonance (Anishchenko, 1999). The stochastic resonance consists in a significant amplification of a weak signal when the noise intensity increases. It has been shown in (Anishchenko, 1999) that in the vicinity of stochastic resonance the dynamical entropy and the Kulbak entropy decrease. It seems that the relative metric entropy should behave in a similar way.

Let us consider a model of the overdamped bistable oscillator:

$$\dot{\phi} = - A \cos(\Omega + \phi) + \sqrt{2} \xi(t), \quad (3)$$

where $A$ and $\Omega$ are the amplitude and the frequency of an external signal, respectively, $\xi(t)$ is a source of the white Gaussian noise with intensity $D$. We fix the control parameters at the following values: $\Omega = 0.1$, $A = 0.05$, $\varphi = 0$. The relative metric entropy of this system versus the noise intensity is presented in fig. 5. At first $\hat{K}_2$ grows. Then the relative entropy decreases until its minimum for $D \approx 0.13$ (that corresponds to the maximum of the signal to noise ratio presented in (Anishchenko, 1999) for the same parameters). If
the noise intensity further increases, $\hat{K}_2$ grows unlimitedly. Hence, a noisy nonlinear system shows the relative metric entropy decrease until a certain minimum at the stochastic resonance. This result approves the conclusion made in (Anishchenko, 1999): the stochastic resonance increases the order degree in a system.

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References:

LITOGEOGRAPHIC-PETROPHYSIC CHARACTERISTICS
OF THE BOBRIKOVSFKIAN TERRIGENOUS RESERVOIR ROCKS
IN THE NORTHEASTERN PART
OF THE UST-CHEREMSHANSKIJ TROUGH

S. Astarkin

Saratov State University

Lithology-petrophysical investigations, terrigenous reservoir, Bobrikovskian horizon

The Bobrikovskian beds occur widely over the Samara Trans-Volga Region; the deposits are regionally oil-and-gas bearing. No lithologic structur of their composition has, however, been made for over three decades, either in the Samara Trans-Volga Region or over the Middle Volga Region as a whole. At present, hydrocarbon materials are mostly acquired by means of developing numerous complicated and low-permeable reservoirs. Such reservoirs are peculiar for various degrees of structural non-uniformity caused by diverse lithologic and facies sedimentation settings. This results in high scatter of the reservoir properties and petrophysical parameters, which emphasizes the need of extensive examinations of reservoir rocks with regard to the lithologic parameters affecting the petrophysical ones. The filed lies in the area of the Samara Region and in the near-border northeastern zone of the Ust-Cheremshanskij trough, conjugated with the southwestern slopes of the South-Tatar swell.

In the Bobrikovskian reservoir rocks from the Ivanovskoye field in the northeastern part of the Ust-Cheremshanskij trough, complex examinations of the core have made it possible to distinguish three lithologic-petrophysical rock types (LPT). In the study area, rocks of that age have been encountered in the interval 1392 – 1410 m. The core of the interval is represented by sandstones, with solitary thin (0.05-1.5 m) argillite intercalations in the horizon top and bottom layers. The sandstones are quartzy, inequigranular, unsorted, massive, with subhorizontal gradational stratification caused by alternating interlayers of different fractional compositions. Secondary mineralization is frequently developed in the sandstones; this is associated with generation of the postsedimentation, mostly sulfate cement. The cement is non-uniformly mottled, mostly anhydrite, more rare – gypsum and dolomite. Pore- and poikilitic-type cementation is observed. More rarely, clayey kaolinite material occurs as pore and pore-film cement. The sandstone texture is subhorizontally thin-layered, lenticular-stratified, disturbed by bioturbation in some sites and interlayers. Besides, intensely pyritized interlayers of clayey-coaly composition occur in the uppers part of the horizon. Argillites in the horizon top and bottom layers are dark gray, non-uniformly silty, horizontally thin-layered, intensely pyritized.

LPT definition was based on lithotype recognition in the section from a complex of lithologic characteristics (structure, texture, mineral composition)
and subsequent analyses of the reservoir properties and the petrophysical parameters of the recognized lithotypes. Each type is described from common lithologic and petrophysical parameters. LPT recognition is highly specific for every field.

Examinations have shown the mineral compositions of the clastic portions in all the recognized LPT to be quartzy, and the mineral compositions of clays to be hydromicaceous-kaolinitic. The differences consist in the following: in the I rock type, the cement is clayey (makes 20-25%), of basal-pore type, represented by the following association of clay minerals: hydromica, kaolinite and chlorite admixture. Hydromica is isometrically tabulate, degraded; kaolinite is rounded and clastic. Those are minerals of allothigenous origin. Admixture of authigenic magnesium-iron chlorite testifies to certain changes of the original clayey cement, ceased upon oil invasion into the layer. The textures are subhorizontally interruptedly thinly and lenticular-disrupted laminated, bioturbated in some sites and interlayers, the porosity ratios (Rp) make 2-8%, the permeability ratios (Rpr) <500 mD.

In the II rock type, the secondary cementation is either non-characteristic or irregularly manifested, the texture is massive, Rp=12-23%, Rpr>500 mD. Reservoir properties of the II type sand rocks are described from the absence of primary cement and, consequently, common occurrences of intergranular pores, 0.08 up to 0.75 mm large. The pores are diversely shaped (isometric, slot-like, with processes) and are regarded as primary ones. Throat-like pores occur frequently (with the length-width ratios of up to 1:10), therefore many pores in the slide planes interconnect and fringe the grains that have no contacts and are kind of “floating” in emptiness. The channels connecting the porous areas are 0.01-0.02 mm wide.

In the III type, the cement is clayey (up to 10%), of the filmy-contact type, contains authigenic minerals; kaolinite, hydromica, chlorite and mixed-layered aggregates like montmorillonite-hydromica with minor admixtures of authigenic sodium montmorillonite. The cement is altered, secondary. Sporadically, mottled anhydrite cement of the basal-pore and poikilitic types (1-5%) is observed, the texture is obliquely laminated, massive, Rp=2-6%, Rpr<100 mD. Developing anhydritization process is among the peculiarities of the II type sandy reservoir rocks. According to X-ray mineralogical analyses, anhydrite contents in sandstones vary from 0.5 to 27%. Precipitation of heterocrystalline anhydrite in void spaces leads to volume reduction and structure complication due to the pore size reduction, complete “healing” and narrowing of the openings in the connecting channels. Irregular development of that process leads to formation of dense areas of various shapes and sizes, with the pores totally “healed” with anhydrite. This is obviously one of the reasons of lacking clear functional relation between the Rp and the Rpr values (r=0.46) in the Bobrikovskian sandy reservoir rocks, which is non-characteristic of terrigenous rocks. The other reason lies in domination of poorly sorted
varieties, peculiar for more complicated structures of the void spaces due to the wide range of the pore sizes and of the connecting channel sections. The results of the granulometric analyses make it possible to recognize three types of reservoir rocks; each one is peculiar for the ratio distributions of its own and corresponds to the recognized LPT.

Calculation of the statistic values designated as granulometric indices is among the ways of presenting the results of granulometric analysis. The statistic indices – median, sorting, asymmetry, excess – calculated from the granulometric analysis results make it possible to recognize three intervals, each one described from the values of the indices distribution. In type I, the values of median, asymmetry, sorting and excess are indicative of the medium-to fine-grained composition, poor sorting of the sediment, highly positive asymmetry and the excess values of 0.5 to 1. In the second type the values of the statistic indices are indicative of the medium-grained composition, medium, fairly good sorting of the sediment, positive asymmetry and the excess values of above 1. In type III, the deposits are peculiar for very fine-grained composition, moderate sorting, positive asymmetry and the excess values close to zero.

Several factors are known to determine the rock reservoir properties; the granulometric factor is among those. The following granulometric parameters were found to influence formation of the sandstone reservoir properties: shift of the granulometric equilibrium towards the increased contents of the coarse fractions is directly reflected in improvement of their reservoir properties. The curves of porosity, permeability, granulometric fractions and the median sizes over the section are roughly duplicate, with the correlation between the median and the reservoir properties in the second type being positive and varying from 0.75 to 0.93. The sediment sorting degrees influence porosity and permeability, as well: reservoirs composed of more uniform grains over the section possess better reservoir properties and vice versa. The correlation coefficient between median, asymmetry, sorting, excess, porosity and permeability in type II has been determined as positive with the value of $R=0.67-0.94$. The reservoir rocks in the same interval have the best reservoir properties: porosities make 12-23%, permeabilities are above 500 mD. It should be noted, that in the first and in the third intervals, with the correlation coefficients between the statistic parameters, porosities and permeabilities below 0.5 and occasionally negative, the sandstones have inferior reservoir properties (porosities of 2-8%, permeabilities below 500 mD in the first interval and below 100 mD in the third one). It should be noted, that improved reservoir properties are also observed in the second interval of the section, with the excess values of above one.

Analyses of the core petrographic examinations show that the I and the II types comprise sandstone varieties with higher clay contents (type I) and sandstones with the void spaces substantially confirmed by cementation
with secondary carbonate and poikilitic anhydrite (type III). Depending on the amount of clayey cement, the highest permeabilities are observed in the rocks with the filmy and the contact cement types (type III). The basal and the pore cement types make a rock practically impermeable (type I). The second group consists of sandstones of the II type, with the secondary cementation of the void space either non-characteristic or manifested irregularly and slightly. Substantial variations of the Rpr values in the varieties with close Rp values are accounted for by both, different cementation degrees and primary structural-textural features of the rocks. Availability of sandstones with variously sorted clastic materials, massive and layered varieties, has caused availability of reservoir rocks with diverse morphostructures of the void space (variable relationships of diversely sized pores and connecting channels, degrees of the pore interconnection, pore-channel morphology). All this taken together has substantially affected the observed variations of the reservoir properties and, consequently, called forth diverse types of the porous-type reservoirs.

Among sandstones, porous reservoirs of the I-III classes, according to A.A. Khanin (Khanin, 1969), dominate (77% of the samples); those are peculiar for very high (>1000 mD), high (500-1000 mD) and medium (1000-5000 mD) permeabilities. The share of the I class reservoirs may be up to 40% high and corresponds to the lithologic-petrophysical type II; about 30% of the II and III type reservoirs correspond to the lithologic-petrophysical type III. Only 23% fall within the porous reservoirs of the lithologic-petrophysical type I, with reduced (Rpr=10-100 mD), low (Rpr=1-10 mD) and very low (Rpr<1 mD) permeabilities.

Thus, the investigations made by the authors have demonstrated the influence of the reservoir-rock mineral compositions and the structural-textural features on the petrophysical and reservoir properties. Lithologic heterogeneity is not always recognizable from petrophysical parameters. Therefore, petrophysical examinations should be preceded by mineralogic-petrographical ones, that may provide the grounds for predicting reservoir properties and their variations depending on granulometric compositions, fracturing degrees and cavernosities. First, lithotypes are distinguished, then, the rock lithologic-petrophysical types. It is impossible to create petrophysical models of complicatedly structured reservoirs without due regard to the lithologic features of their structures.

References:

SOLUTION OF THE PROBLEM OF PHOTONIC CRYSTALS
MODELING WITH THE USE OF HIGH-LEVEL ALGORITHM
PARALLELIZATION TOOLS

D. Atmakin, P. Shilovsky, I. Khvatov

Saratov State University

Phonotic Cristals modelling, parallel computing, concurrent programming, Grid technology, integral equation

Recently, due to the progress of nanotechnology, has increased interest in the one-dimensionally periodic (1D), two-dimensionally periodic (2D) and three-dimensionally periodic (3D) artificial magneto-dielectric structures – periodic inclusion body of different nature in a homogeneous dielectric. Such structures are used in optics, and are called Photonic Crystals.

While such structures have long been used and there are large number of works on the modeling of their properties, but as a rule, most of the results are approximate character. Rigorous electrodynamic modeling for analysis of 2D and 3D Photonic Crystals began to be applied only in recent years. Davidovich M.V. proposed a universal approach to modeling of 1D, 2D Photonic Crystals[1].

On the basis introduced in the paper the Green’s functions are formulated various integral and integro-differential equations. Consider the integral equation only for the dielectric inclusions in a dielectric base

\[ E(r) = E_{in}(r) + j\omega\varepsilon_0 \int \Gamma_{ee}(r - r')(\varepsilon(r') - \hat{n})E(r')dV', \]

where \( \Gamma_{ee}(r - r') = (j\omega\varepsilon_0\varepsilon)^{-1}(\nabla\nabla\cdot + k_0^2\varepsilon\hat{1})G(r - r') \) and \( E_{in} = 0 \).

This equation can be interpreted as a Fredholm equation of the first kind with an additional singularity \( \delta(r - r') \). The most effective method of the solution of integral equations – is replacing the integrals by finite sums and to solving systems of algebraic equations [2]. Quadrature method relates to approximation methods. He is widespread in practice, because it is universal principle of constructing algorithms for solving both linear and nonlinear equations. The method is based on quadrature formula:

\[ \int_{c}^{b} \varphi(x)dx = \sum_{j=1}^{n} A_j\varphi(x_j) + e_n[\varphi]. \]

Bottleneck of this method lies in the process of solving systems of algebraic equations. Linear algorithm of solving the large systems of algebraic equations may require really a lot of CPU time and memory resources.
There is no methods for optimization calculation of systems algebraic equations in the single-process programming pattern. We can reduce the runtime of the program by using technology of parallelization. In this case, independent pieces of program code will run in the same time on the different processors. Number of independent pieces of code of the program which can be run in the same time depends on the algorithm of the program and on number of available processor kernels.

Optimally, the speed-up from parallelization would be linear – doubling the number of processing elements should halve the runtime, and doubling it a second time should again halve the runtime. However, very few parallel algorithms achieve optimal speed-up. Most of them have a near-linear speed-up for small numbers of processing elements, which flattens out into a constant value for large numbers of processing elements.

The potential speed-up of an algorithm on a parallel computing platform is given by Amdahl’s law, originally formulated by Gene Amdahl in the 1960s. [3] It states that a small portion of the program which cannot be parallelized will limit the overall speed-up available from parallelization. Any large mathematical or engineering problem will typically consist of several parallelizable parts and several non-parallelizable (sequential) parts. This relationship is given by the equation:

\[ S = \frac{1}{1 - P}. \]

Where \( S \) is the speed-up of the program (as a factor of its original sequential runtime), and \( P \) is the fraction that is parallelizable. If the sequential portion of a program is 10% of the runtime, we can get no more than a 10× speed-up, regardless of how many processors are added.

Parallel programs are more difficult to write than sequential ones, because concurrency introduces several new classes of potential software bugs, of which race conditions are the most common. Communication and synchronization between the different subtasks are typically one of the greatest obstacles to getting good parallel program performance. For elimination common problems in the pattern of concurrent programming, some high-level programming languages provide special constructions for synchronization intermediate results of calculation and memory control. These can generally be divided into classes based on the assumptions they make about the underlying memory architecture – shared memory, distributed memory, or shared distributed memory. Shared memory programming languages communicate by manipulating shared memory variables. Distributed memory uses message passing. POSIX Threads and OpenMP are two of most widely used shared memory APIs, whereas Message Passing Interface (MPI) is the most widely used message-passing system API.

Program which implements MPI technology has one important advantage – opportunity of using processors placed on different computers linked over
network. But implementation of MPI technology in present time exists only for some programming languages, such as: C++, Fortran and Python. For getting advantages of distributed parallel computing on the different processors which linked over network in programs which based on shared memory paradigm, was invented Grid technology.

Grid computing is the most distributed form of parallel computing. It makes use of computers communicating over the Internet to work on a given problem. Because of the low bandwidth and extremely high latency available on the Internet, grid computing typically deals only with embarrassingly parallel problems.

Most grid computing applications use middleware, software that sits between the operating system and the application to manage network resources and standardize the software interface. The most common grid computing middleware is the Berkeley Open Infrastructure for Network Computing (BOINC). Often, grid computing software makes use of «spare cycles», performing computations at times when a computer is idling.

Automatic parallelization of a sequential program by a compiler is the holy grail of parallel computing. Despite decades of work by compiler researchers, automatic parallelization has had only limited success.

Mainstream parallel programming languages remain either explicitly parallel or (at best) partially implicit, in which a programmer gives the compiler directives for parallelization. A few fully implicit parallel programming languages exist–SISAL, Parallel Haskell, and (for FPGAs) Mitrion-C.

The article discuss common approaches to solving the problem of performance algorithm of Fredholm integral equation first kind, which underlies one of the problems associated with modeling of Photonic Crystals on the base of high-level parallelization tools.

References:

PULSES OF THE FORMING SYSTEM «ARTIFICIAL LINE (AL) OF THE SECOND INITIAL FORM – PULSE TRANSFORMER (PT)»

M. Balakin

Saratov State University

Artificial line, pulse transformer, pulses

An electric circuit made up of inductance-capacitance network with characteristics similar to those of a long line is called an artificial transmission line. The artificial line has the following properties:

1. Ability to store a large amount of energy in electric field of condensers.
2. Ability on a load to return stored energy quickly and generate short voltage or current pulses with steep edges of rectangular flat-top waveshape.

These properties allow to apply artificial lines as mile-microsecond pulse technique to store energy of electric field and to form high-power short pulses of a rectangular shape.

To increase the load voltage in powerful microsecond pulse generators a step-up pulse transformer (PT) is attached between an artificial line (AL) and load (e.g. magnetron) [1,2].

Mutual influence of the AL and the PT on the output pulse leads to the idea of the whole «AL – PT» system analysis to consider all factors that contribute to the deterioration of the pulse shape.

Fig. 1. Circuit diagram of forming artificial line of the first initial form with the pulse transformer

1) Method of calculation

To analyze the studied circuit we use a state variable method [3]. Instant values of voltage on capacities and currents through inductance are called state variable of a circuit. These variables are the unknown components of the equation to be calculated. This role of the state variables is defined by two factors.

First, they explicitly define an energy stored in a circuit at any moment. Therefore, for example, if for any reason the input signal stops traveling, the
process in a chain goes on due to the sufficient amount of energy stored, that is determined by values of state variables. Second, any other voltage and current in a circuit can be estimated through the state variables provided that they are involved in Kirchhoff’s equations or Ohm’s law.

If each of branches contains only on one reactive component the quantity of unknown variables of a status subject to definition is equal to number of branches. In this case the same number of state variable equations are to be made up following the same rules as for the branch current method. In case some branches contain both inductance and capacity the number of unknown variables is doubled.

The acquired system of the differential equations can be solved numerically on the computer. To do this, equation should be solved for the first derivative. Such differential equation system contains the first derivative of one of the state variables in the left part of each equation, and all other components (without derivatives) in the right part.

The physical values being components of these differential equations should be normalized [4]. The choice of normalizing bases is made in respect to record convenience of acquired normalized equations, components and simulation curves. The additional requirement to base values is their constant character within a particular designed task as they define scale of transition from normalized sizes to absolute values. Normalising allows to receive the generalised curves. Considering that on one hand base values only serve for scale (or level) change of circuit parameters and elements and on the other hand normalizing does not change the interconnection between them, which defines a course of physical process, any elements of the circuit is available to be a base elements, provided that the elements correspond to noted general requirement.

In the present work we estimated influence of PT parasitic parameters, such as leakage inductance \( L_s \) and capacity \( C_s \), on the pulses shape \( AL \) of the first initial form. Results of calculation of relative overshoot and ringing of top, absolute and relative front-edge time of formed pulses for various normalized values \( l_s \) and \( c_s \) are shown in charts 1, 2, 3 respectively. Under the received data corresponding dependences \( \Delta u/u = f (c_s) \) (fig. 1), \( \Delta u/u = f (l_s) \) (fig. 2), \( \tau_f = f (c_s) \) (fig. 3), \( \tau_f = f (l_s) \) (fig. 4), \( \tau_f / \tau_{in} = f (c_s) \) (fig. 5), \( \tau_f / \tau_{in} = f (l_s) \) (fig. 6) have been plotted.

Capacity \( c_s \) influences relative overshoot and ringing of top, increasing the first maximum and reducing \( \Delta u/u \) to certain minimum value. From fig. 1 it can be seen that dependence \( \Delta u/u = f (c_s) \) has a maximum which size decreases with increase of leakage inductance \( l_s \). After reaching maximum size \( \Delta u/u \) with increase of \( c_s \) monotonously decreases. From fig. 3, 5 it can be seen that \( c_s \) negligibly influences pulse front-edge time. Dependences \( \tau_f = f (c_s) \) and \( \tau_f / \tau_{in} = f (c_s) \) have a minimum after which achievement with growth \( c_s \) pulse front-edge time monotonously increases.

In addition influence of PT leakage inductance \( l_s \) on relative overshoot and ringing of top (fig. 2) and front (fig. 4, 6) has been considered. \( l_s \) monoto-
nously smoothes the first maximum and reduces $\Delta u/u$ to some minimum value which negligibly depends on PT dynamic capacity $c_s$. Fig. 4, 6 illustrates that $l_s$ changes front.

Fig. 1. Dependence of relative overshoot & ringing of formed pulses top on PT dynamic capacity $l_s$

Fig. 2. Dependence of relative overshoot & ringing of formed pulses top on PT leakage inductance $l_s$
Fig. 3. Dependence of front-edge time of formed pulses on $c_s$

Fig. 4. Dependence of front-edge time of formed pulses on $l_s$

Fig. 5. Dependence of relative front-edge time of formed pulses on $c_s$
The present paper deals with the analysis of «an artificial line of the second initial form – the pulse transformer» system that has not been described before in literature.

Normalized curves of output pulses in such a circuit are calculated. The mutual influence AL and PT as a uniform system on the output pulse shape is studied. Some preliminary results are obtained:

1. Contribution of transformer equivalent circuit to the pulse front edge time and shape, overshoot on the pulse top that determines its deterioration
was quantitatively estimated to be necessary to design high-voltage pulse generators.

2. The studied system was shown to form pulses of a satisfactory quasi-rectangular shape ($\tau_f = 1.14$, $\Delta u/u = 3.037\%$).

References:


LOW-COHERENCE INTERFERENCE MICROSCOPY
OF RED BLOOD CELLS

E. Bogolyubova

Saratov State University

Interference microscopy, red blood cells

Application of full-field low-coherence interference microscopy for erythrocytes investigation in dry blood slide is discussed. The two-dimensional tomograms and images of erythrocytes, taken during the experiment, are presented. The method is proposed to measure thickness and radius of dry erythrocytes and restore erythrocytes shape using the tomograms.

Surface analyses could be made by different techniques, such as electron microscopy, confocal microscopy, X-ray diffraction analyses, low-coherence interferometry (LCI) and etc. During electron microscopy study the sample is fixed by chemical reagent and slicked, i.e. samples are destroyed. Resolution of X-ray diffraction analysis is high (~ 1 Å), however, this technique is highly invasive too. The confocal microscopy is time-consuming method, because it based on point-by-point scanning.
The above considerations show that, investigation method should realize two main features – high resolution (of about tenth micrometer) and noninvasive and noncontact principle of operation. Full-field low-coherence interferometry proposed in this work meets all these requirements.

An analysis of literature shows that last years, biological liquid is investigated by different optical devices very active. Red blood cells (RBC) are investigated especially active, because we can identify disease knowing erythrocytes shape or erythrocytes optical characteristics. Erythrocytes investigation works concerned with optical coefficients measurements and detecting osmolarity depend on optical coefficients using spectral analysis [1], obtaining mechanical information of RBCs by instantaneous spatial light interference microscopy [2] and confocal diffraction phase microscopy [3], detection of red blood cell agglutination using spectrophotometric analysis [4] etc. Dry biological liquid also used in experiments.

Fifteen whole blood slides of three patients were investigated in this work using low coherence interference microscopy system. The blood slides were prepared during haemanalysis at different time after in-vivo introduction of glucose.

Figure 1 shows the fragment of dry blood slide. This picture was taken by microscope. Erythrocytes on this photograph seem to be red and green. Blood slide and thin film are very much alike and in both interference is observed. Interference fringes are many-colored by reason of white light illumination and they are the same color if film thickness is constant (fringes of constant thickness). Rely on said, we can make a preposition that erythrocytes thicknesses are different.

In our experiment we compare erythrocytes thicknesses and radiiuses from one blood slide with erythrocytes thicknesses and radiiuses from one another.

The full-field white-light interferometer used in this study is developed
based on the optical scheme of the Linnik interferometer. Interferometer has two modes of operation: interference and microscopic. In microscopic mode interferometer works like inverted reflection microscope; in interference mode reference wave reflected from the mirror is added to object wave reflected from the sample surface. At the output of interferometer interference of these two waves is observed. The object under study was placed on the stepper motor microstage, which allowed moving the sample along the optical axis of interferometer. During the scanning the sample moved along the optical axis of interferometer and CCD camera recorded the monochrome microimages (Fig. 2) of sample fragments every 0.156 μm.

![Fig.2. Left: Erythrocytes microimage was taken in microscope mode; center and right: microimages of the same erythrocyte were taken in interference at different position of the sample](image)

After scanning we have a “layer cake” being composed from microimages, subsequently cross-section of this stack depicts 2D tomogram of erythrocyte (Fig.3). Operations described above were done at the sample fragments having erythrocytes in center. Ten erythrocytes from everyone dry blood slide were investigated and based on it sample statistics and patient statistics were formed.

![Fig. 3. Interferometric 2D cross-section of erythrocyte](image)
Erythrocytes shape and thickness were determined using interferogram. Erythrocytes thickness estimate method based on distance estimate between the interference fringe corresponding to plasma and position of the same order interference fringe corresponding to point of interest. We fix seven coordinates on the interferogram as shown in the Figure 4, which are restored the erythrocytes shape, and recorded the data in it (x, y coordinates).

![Fig. 4. Erythrocytes shape](image)

Erythrocytes radius were estimated in two orthogonal directions, because it could have oval shape. In addition difference between two radiuses was determined too.

We made statistic diagrams, using the results obtained during the experiment (Fig. 5). Figure 6 shows: left top angle – circle center coordinate conforms to distance between 1(7) and 4 coordinates, circle radius equals distance dispersion in one blood slide; right top angle – circle center coordinate conforms to distance between 2(6) and 4 coordinates, circle radius equals distance dispersion in one blood slide; left lower angle – circle center coordinate conforms to distance between 3(5) and 4 coordinates (if erythrocytes is bulging, then coordinate is positive; if erythrocytes is concave, then coordinate is negative), circle radius equals distance dispersion in one blood slide; right lower angle – circle center coordinate conforms mean erythrocytes radius, circle radius equals difference between two orthogonal radiuses in one blood slide.

We can noticed, that 4th and 9th samples erythrocytes are approximate equal and they have practically round shape, erythrocytes in sample number 11 have distance between 1(7) and 4 coordinates equal distance between 2(6) and 4 coordinates and practically plane shape, 12th and 14th samples erythrocytes have more bulging and more concave shapes then other, respectively, using the diagrams.

In this work experimental results of morphological parameters of red blood cells in whole blood slide study are presented. These results are obtained using low-coherence interference microscopy. This method is perspective in biological tissues internal structure investigation with micron and submicron resolution. Interference microscopy with extensive white light source has advantages over most related methods, such as high spatial resolution and
nondestructive probing principle. These properties of method are very important for biological tissues investigation.

Use of low-coherence interference microscopy made possible to detect number of differences of red blood cells topology in dry whole blood slide produced by glucose level changes.

Figures 6 and 7 show erythrocytes shape changes for every patients after glucose introduction. We can noticed, that red blood cells shape changes movement are different for every patient.

The data presented in this work agrees well with results obtained using other methods, including cytometry. However, interference microscopy method suggested gives an opportunity to obtain more information from the sample. This method can provided us with information about erythrocytes topology, erythrocytes optical structure. Cause of changes in these parameters may be different. Thereby, this method could be considered as one of the most perspective cardiovascular diseases diagnostic method based on erythrocytes morphometric characteristic changes.

Fig. 5. Statistic diagram obtained during investigation
Fig. 6. Top: Erythrocytes center height in comparison with plasma height away from erythrocytes; Lower: Erythrocytes center height in comparison with plasma height near erythrocytes.

Fig. 7. Top: Erythrocytes center height in comparison with erythrocytes border height; Lower: Plasma height away from erythrocytes in comparison with plasma height near erythrocytes.
MULTIPARAMETER ANALYSIS OF NANOPARTICLES PROPERTIES

O. Chichvarina, Y. Karsakova

Saratov State University

Nanoparticle, density, analysis, method, impedometry, topology, parameter, core, dependence

Nanoparticles (NP) can be indicated by a great number of different parameters and the most significant among them is their core-shell structure. Recently, a
considerable interest has been drawn to the creation of methods that could provide the ability of reliable and nondestructive detection of the topology of NP [1]. Particularly, the identification of the shell thickness $l$ and core diameter $d$ is of interest. However, there is a difficulty conditioned by the fact that the models of NP are a priori unknown and, moreover, their properties can differ from the properties of solid material. That is why it seems reasonable to use several independent methods which permit to confirm the applicability of the proposed model, to check if the findings are reliable and to obtain more specific data in case of need. So this study presents a determination of the oxide layer thickness and the diameter of the core in core–shell iron NP using three independent methods. The first of them is based on elemental composition of NP, the second one relies on NP density and the last is grounded on frequency impedometry.

In the majority of possible cases when the shell is generated due to the oxidation process the usage of X-ray analysis data permit to find a concentration ratio $\frac{N_{Fe}}{N_{O}}$ (for instance, for the iron NP):

$$d = D \left[ A \frac{N_{Fe}}{N_{O}} - C \right]^{1/3} \left[ A \frac{N_{Fe}}{N_{O}} + B - C \right]^{1/3}, \quad A = \frac{\rho_{FeO} \cdot M_{O}}{(M_{FeO})^2}; \quad B = \frac{\rho_{Fe}}{M_{Fe}}; \quad C = \frac{\rho_{FeO} \cdot M_{Fe}}{(M_{Fe})^2},$$

where $M_{FeO}$ and $M_{Fe}$ are the molecular weights; $\rho_{Fe}$ and $\rho_{FeO}$ are the densities.

A single particle density is connected with the values of its sizes by means of the following correlation:

$$\rho = \frac{\rho_1 d^3 + \rho_2 (D^3 - d^3)}{d^3 + (D^3 - d^3)},$$

where $\rho_1$ and $\rho_2$ are the core and the shell densities, respectively.

Connecting experimental density $\rho_e$ with referred $\rho$, we have got the expression for the core diameter $d$:

$$d = D \left[ \frac{\rho_e + \rho_2}{\rho_1 + \rho_2} \right]^{1/3}, \quad l = (D - d) / 2.$$

Iron and silicon powder samples were investigated using scanning electron microscope (SEM). After respective calculations it was found that the shell thickness $l$ founded with ECM virtually coincide with PDM thickness (Table. 1). Calculating error amounts to 1.25nm, which confirms the validity of the proposed methods.

For the realization of this method the formula for the effective permittivity obtained by V. D. Buchelnikov, D. V. Louzguine-Luzgin et al. [2] was applied:
Calculation results

<table>
<thead>
<tr>
<th>Methods</th>
<th>$D$, nm</th>
<th>$d$, nm</th>
<th>$l$, nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ECM</td>
<td>50</td>
<td>25</td>
<td>12,5</td>
</tr>
<tr>
<td>PDM</td>
<td>50</td>
<td>28</td>
<td>15</td>
</tr>
</tbody>
</table>

$$
\begin{align*}
\rho \zeta \frac{\varepsilon_2[3\varepsilon_1 + (\zeta - 1)(\varepsilon_1 + 2\varepsilon_2)] - \varepsilon_{\text{eff}}[3\varepsilon_2 + (\zeta - 1)(\varepsilon_1 + 2\varepsilon_2)]}{2\alpha \varepsilon_{\text{eff}} + \beta \varepsilon_2} + \\
(1 - p\zeta) \frac{\varepsilon_g - \varepsilon_{\text{eff}}}{\varepsilon_g + 2\varepsilon_{\text{eff}}} &= 0
\end{align*}
$$

where

$$
\zeta = \left(\frac{R_2}{R_1}\right)^3 = (1 + l)^3 ; \quad \alpha = (\zeta - 1)\varepsilon_1 + (2\zeta + 1)\varepsilon_2 ;
\beta = (2 + \zeta)\varepsilon_1 + 2(\zeta - 1)\varepsilon_2 ; \quad l = \frac{R_2 - R_1}{R_1}.
$$

In our experiment the iron spherical core-shell particles were in the similar way randomly distributed in a dielectric matrix – paraffin. Firstly, 10% and then 20% composite was located between two glass slices coved with the conductive layer of InxSnyOz and this set up was fulfilling the role of the capacitor. Due to the plot conductivity-frequency of NP an approximating line was drawn and the slope of this line $n$ was determined (Table. 2). The same value of $n$ was predicted by Landau L.D. and Livshits E.M. [3]

Approximation results

<table>
<thead>
<tr>
<th>q</th>
<th>n</th>
<th>$\sigma, (\Omega \cdot m)^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,1</td>
<td>1,99</td>
<td>4,63</td>
</tr>
<tr>
<td>0,2</td>
<td>2,16</td>
<td>5,15</td>
</tr>
</tbody>
</table>

Thereby, it was found that the conductivity of NP changes under the following law: $\sigma = \sigma_0 \cdot \omega^n$.

The parameters of NP were processed with MathCAD program. As a result of modeling it was established that real $\text{Re}(x)$ and imaginary $\text{Im}(x)$ parts of the complex permittivity of NP depend on the shell thickness. For instance, the variation of the thickness within 0,5 and 4 nm produce changes of the real part from 100 to 20 (Fig.1).
Over a various range of values the dependences of $\text{Re}(x)$ and $\text{Im}(x)$ on and on $l$ are essentially different. Such relations make possible the determination of such parameters of NP as their thickness $l$, conductivity and its frequency dependence (Fig. 2).

Fig. 2. $\text{Re}(x)$ versus the core thickness $l$ and $z$

Fig. 3. $\delta$ versus the core thickness $l$ and $z$
\[ \delta = \arctg \left( \frac{\text{Im}(x)}{\text{Re}(x)} \right), \quad z = \frac{\sigma}{\omega}. \]

The methods stated in the study mutually supplement each other. The most informative is a method which permits to receive the data not only about the interior sizes of NP, but also about a number of physical properties of particles, their dependence on frequency and changes produced by various influences. The most informative is a method which permits to receive the data not only about the interior sizes of NP, but also about a number of physical properties of particles, their dependence on frequency and changes produced by various influences. Obviously, such results can be obtained only using the measurements of the impedance frequency dependences of NP. More simple methods based on the elemental structure of NP and their density can serve for the data acquisition. These data are to facilitate appreciably the inverse solution of the multiparameter analysis based on the frequency dependence of complex permittivity.

References:


**ELECTROMAGNETIC WAVES TRANSMISSION THROUGH STRATIFIED STRUCTURES WITH THE KERR NONLINEARITY**

*D.M. Doronin, M.V. Davidovich*

*Saratov State University*

Tunneling effects, waves, nonlinearity, the model of Kerr, resonance tunneling, band-stop filters

**Abstract**

The stiff differential equations are solved for the transmission of electromagnetic waves through a planar structure with a linear and nonlinear (Kerr nonlinearity) complex permittivity. The existence of resonance tunneling and the possibility of band-stop filters creating are shown.
Introduction

One of the topical questions of modern electronics is a development of devices, operating in the millimeter and optical wavelength range, on the base of tunneling effects of electromagnetic wave through a stratified structure. Tunneling effects are not sufficiently investigated when the potential barrier is a nonlinear medium [1]. Such effects are studied in this research work.

When an electromagnetic wave falls on a planar structure with nonlinear dielectric permittivity, a wide range of physical phenomena are observed. On this base different functional devices (such as band-stop filter, limiters of the power, photonic fibers, etc.) can be constructed.

Mathematical model

An electromagnetic waves transmission through an one-dimensional planar medium with permittivity are described by the equation (1):

$$\frac{d^2 E(z)}{dz^2} + k_0^2 \varepsilon(E(z)) E(z) = 0,$$

where $\varepsilon$ – the complex functions of a space coordinates, $k_0$ – wave number.

The task of an electromagnetic waves tunneling is solved numerically for the plane with Kerr nonlinearity ($\varepsilon(E) = \varepsilon^{(0)} + \varepsilon^{(2)} E^2$). To solve (1) analytically it’s necessary to write expressions for the fields in regions I, II and III and staple conditions on the boundaries.

In the case of $\varepsilon^{(2)} > 0$, for example, low-amplitude approximation can be used, as it was done in [1]. Using this, analytical solution for small amplitudes can be obtained. But without any approximations and simplifications, this task can not be solved analytically, and numerical methods for solving it have stringent requirements for solutions stability [2].
\[
\begin{align*}
\frac{dE(z)}{dz} &= X(z); \\
\frac{dX(z)}{dz} &= -k_0^2 \varepsilon(E(z))E(z).
\end{align*}
\]

At the numerical solution of the Cauchy task (2) difficulties come due to the stiffness of the system (the solution contains components with widely different scales of variables). To solve the stiff set of equation computational algorithms having increased stability margin are used. Therefore orientation to A-stable methods \([3, 4]\) was chosen. Among them implicit multistep methods, such as Gear's method and the method of Adams-Beshforts-Moulton, are well known.

This task is solved in the reverse direction (the boundary conditions are given) and in the forward direction (self-consistent problem).

The solution made in a forward direction requires knowledge of the field amplitude and its derivative on the left margin. But since the coefficients of reflection \(R\) and transmission \(T\) are unknown methods of optimization must be used to minimize the residuals of the boundary conditions at the right edge, given by follow equation:

\[
\left| E(l) + jk_0 \frac{dE(z)}{dz} \right|_{z=l} \rightarrow \min.
\]

In this case a multivariate optimization of four parameters \((\text{Real}[E(0)], \text{Image}[E(0)], \text{Real}[\frac{dE(z)}{dz}]_{z=0}, \text{Image}[\frac{dE(z)}{dz}]_{z=0})\) can be reduced to the optimization of two parameters \((\text{Real}(R), \text{Image}(R))\).

Computational modeling

As a result of numerical simulation the space distribution of the field amplitude in the medium was obtained (Fig. 2, 3). The reason of the field amplitude oscillations in the area \(z \in (-\infty; 6)\) is the interference of incident waves with the wave reflected from the boundaries of the structure (\(k_{0L} = k_{0R} = 1\)).

Nonlinear cases described in \([1]\) \((\varepsilon^{(0)} = -0,21, \varepsilon^{(2)} = \pm0,40333 / \pm0,80666)\) were considered. The change schedules dependence \(|T| = |T(A_0)|\) under the influence of the coefficient of nonlinearity \(\varepsilon^{(2)}\) is shown on Fig. 4.

Effects generated by Kerr nonlinearity were researched. The effect of resonant tunneling is well known as an effect when the incident
Fig. 2. The distribution of wave amplitude along the spatial coordinate $z$ for $\varepsilon(E) = \varepsilon^{(0)} > 0$

Fig. 3. The exponential decay of wave amplitude inside the barrier along the space coordinate $z$ for $\varepsilon(E) = \varepsilon^{(0)} = -1 < 0$
electromagnetic wave does not “see” single-layer structure and passes through without reflections. Physics of this phenomenon allows using this effect in the construction of micro- and nanodevices (so-called Resonant Tunneling Devices). On the base of researching model, this effect is obtained and studied (fig. 5). The incident electromagnetic wave don’t “see” a structure with the linear complex dielectric permittivity in the case when backward-wave field is absent on the left part of the structure (4).

![Graph showing transmission coefficient initial wave amplitude relation](image)

**Fig. 4.** Transmission coefficient initial wave amplitude relation $|T(A_0)|$. Curves 1, 2, 3, 4 are marked for $\varepsilon^{(1)} = -0.21$, $\varepsilon^{(2)} = -0.80666; -0.40333$ and $\varepsilon^{(2)} = 0.40333; 0.80666$

![Diagram of the resonant tunneling zones](image)

**Fig. 5.** Diagram of the resonant tunneling zones for $\varepsilon = 9$, $d = 22$, $|T| = 0.999$
\[ A_R + A^- = 0; \quad A_R + \frac{TA}{2} \left( 1 - \frac{k_0}{k} \right) e^{-j(k_0 + k)d} = 0; \quad d = \frac{j}{k_0 + k} \ln \frac{2\sqrt{1 - |T|^2}}{T \left( 1 - \frac{k_0}{k} \right)}; \quad (4) \]

Due to the existence of band gap it’s possible to create band-stop filters, as it was described in [6]. The dependences of transmission and reflection coefficients from the frequency of signal (Fig. 6) were calculated. The results indicate an increasing of filter stop band with increasing of the dielectric layers number used.

Fig. 6. Frequency dependence of the reflection and transmission coefficients and power balance for the three-layer medium with a linear dielectric permittivity \( \varepsilon = 9 \) and the total length \( L = 1.5 \)

Fig. 7. Frequency dependence of the reflection and transmission coefficients and power balance for the three-layer medium with a linear dielectric permittivity \( \varepsilon = 9 \) and the total length \( L = 1.5 \)
As it is indicated in [6] the application of photonic crystals today is done on the industrial level. For example, it is used for manufacture of photonic-crystal fibers, which operation is based on the usage of photonic band gaps instead of the total internal reflection phenomenon.

Conclusion
Thus, we have solved the system of stiff differential equations in the forward and reverse directions of the wave traveling. Nonlinear physical effects that occur in stratified structures with nonlinearity by the model of Kerr have been described using numerical calculation. It’s shown that stratified structures of nonlinearity can be used for the band-stop filters development.

References:
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THE METHOD OF HIGH-ORDER OPTIMAL DESIGN OF EXPERIMENT DEVELOPMENT ON THE BASE OF REGULAR SIMPLEX

*D.Doronin, A. Savin*

*Saratov State University*

Simplex-Sum Design, active experiment, regression analysis, properties of optimality

The results of optimal Simplex-Sum Design of experiment development for the numerical or physical experiments modeling are presented. Using developing method, design of experiments, that possess the properties of symmetry, orthogonality, rotatability, D-optimality and contains a small number of experiments, were made.

The development of high-power microwave devices supposes mathematic modeling of waveguide systems (WS) and processes of electron
beams interaction with electromagnetic fields of the WS, computation of characteristics of individual parts using models as well as an optimization of the whole device in order to achieve the required output parameters [1].

At the modern stage of computer modeling techniques the development of simulation of electrodynamics characteristics (EDC) of WS can be done quite accurately by the field methods based on Maxwell's equations for boundary conditions presented. Due to it’s an awkward task to do the optimization of WS with loss and deterministic inhomogeneous, taking into account. Also, at the process of moving in the short-wave range it’s difficult to account the manufacture inaccuracies and quality of the surface of WS, that has a significant influence on their parameters.

One of the ways of solving these problems is to use a polynomial regression models of EDC or parameters of equivalent circuit (for WS), constructed according to the numerical or physical designing experiments data and to take into account the implications of the above factors [2].

In this case a mathematical model can be represented by the following expression [3]:

$$\eta = f(x_1, x_2, \ldots, x_k),$$

where $$x_k$$ – independent variable (factor) – for example, the sizes of the WS,
$$\eta$$ – simulated electrodynamics parameter of the WS,
$$f(x_1, x_2, \ldots, x_k)$$ – polynomial of required order.

The problem of the adequate regression equation (1) construction using experimental data (i.e. solving of the task of coefficients determining in regression equation) is possible only under certain stringent requirements: design of the experiment should be symmetric, orthogonal, should ensure the minimum error of the regression coefficients dispersion (D-optimal), etc. [2]

The theory of design of experiments [2-8] offers different ways of optimal design searching by various criteria. Often, the complete factory experiment, in which all possible combinations of factor levels are implemented. It’s fractional replicate are widely used. But high complexity and unsuitability of this method is conditioned on a necessary number of experiments increasing with the number of factors taken into account addition. Therefore, all efforts of the design theory of experiments aimed at improving its efficiency by reducing the number of experiments with the model adequacy saving. In [10] the methods for constructing second-order Design, that available to reduce the number of experiments and improve the dispersion characteristics of the experimental data, are presented.

In [10] on the Traveling-Wave Tube Slow-Wave Structures EC modeling regression models were constructed according to the physical experimental data. The experiment was done on the base of second-order Simplex-Sum Design. The error of dispersion characteristics calculation by this model does not exceed 3% and the coupling resistance – 10%. Further reduction of the
error of models could be achieved by using data from experiments that were
done using designs of higher orders.

We propose the method for constructing high order composite designs of
experiments on the base of simplex. These designs possess the properties of
symmetry, orthogonality, rotatability, D-optimality and contain a small number
of experiments. It will be used for EC of WS modeling using a high-order
regression polynomial.

1. The design of experiments
   on the base of a regular simplex and its properties

Many principle single-factor experiments replaced by one multiple-factor
[4] suggest to use the experimental data, which belong to different single-
factor dependence in single-factor experiments, for cross-averaging. For that
purpose the allocation of experiments in the factors space must be performed
in a special way, called the optimal design of experiment. One of the optimal
design properties is that it does not only reduce the number of experiments,
but also provides less dispersion of averaged results variance than in separate
single-factor experiments.

Rotatable composite designs [5] are often used in the practice of the
experiments designing and besides points of the first-order design contain extra
hyper sphere were suggested for a polynomial regression.

In [7] correct simplex was proposed to use as a design of experiments,
which is defined as the set of \( k+1 \) equidistant points in a \( k \)-dimensional space.
In one-dimensional space it is a line segment. For two factors the simplex is an
equilateral triangle, for three – a tetrahedron (Fig. 1), etc. This design allows to
approximate the required characteristics with the help of a first order polynomial.

The matrix of a simplex in the \( k \)-dimensional space can be expressed by
the follow equation [6]:
where \( Q_j = \sqrt{\frac{j}{2(j+1)}} \) and \( q_j = \sqrt{\frac{1}{2j(j+1)}} \) — radiiuses of the round and inscribed in the -dimensional simplex spheres \((j = 1, \ldots, k)\), respectively.

The matrix \( X \) is the design of the \( m = k + 1 \) initial experimental series. The rows of the matrix \((k\)-dimensional vector \( \tilde{x}_j, i = 1, \ldots, m \)) are the coordinates of vertices of the regular simplex in \( k \)-dimensional factor space. The columns presents the varied factors. This design allows to approximate the required characteristics using a first-order polynomial.

The matrix \( X \) of simplex-design of experiment has the following properties:

- relative to the experiment center symmetry — the vector-column elements sum of each factor is zero:
  \[
  \sum_{i=1}^{m} x_{ji} = 0 \quad \forall j = 1, \ldots, k; \quad (3)
  \]

- normalization — constancy of the second-order moments:
  \[
  \sum_{i=1}^{m} x_{ji}^2 = \text{const} \quad \forall j = 1, \ldots, k; \quad (4)
  \]

- orthogonality — the sum of every two design matrix column-vectors termwise product is equal to zero, respectively, all parameter estimation are independent:
  \[
  \sum_{i=1}^{m} x_{ji} x_{il} = 0 \quad \forall (j, l) = 1, \ldots, k \quad \land j \neq l; \quad (5)
  \]

- rotatability — points in the design matrix are chosen so that the accuracy of the response prediction values does not depend on the direction and same at equal distances from the experiment center [7]:
  \[
  X_j^T M^{-1} X_j = f(\rho) \quad \forall j = 1, \ldots, k, \quad (6)
  \]

where \( M = X^T X \) — the matrix of variance-covariance,

\( X_j \) — column in the matrix of design \((2)\);

\( \rho \) — distance from the center to any point of the design.

- D-optimality — errors minimizing in the coefficients of regression estimating [6]. The D-optimality statistical interpretation implies minimizing of the regression coefficients disperse, considered as a vector, i.e. it is a parameter estimating scattering ellipsoid minimum. From the algebraic point of view D-optimality means the minimum of the disperse-covariance determinant:
  \[
  \min \det M^{-1}. \quad (7)
  \]

In [8] it was proposed to use a regular simplex \((2)\) as a basis for development of composite designs for the second-order polynomial. In addition,
these designs can satisfy the requirements of symmetry, normalization and orthogonality, and also possess the properties of rotatability and D-optimality.

2. Algorithm of n-th order simplex-sum design of experiment construction

Composite high order designs of experiment can be constructed by adding (summing) regular simplexes turned at a certain angle to the original design (2).

Turn of the regular simplex (2) can be achieved by turning on a certain angle of all vertices of the simplex – k-dimensional vectors \( \bar{x}_i, \ i = 1, \ldots, k + 1 \). Angle of rotation is determined by the required order \( n \) of design and equal to \( \varphi_r = \frac{r \cdot \pi}{n} \ \forall r = 1, \ldots, n - 1 \). The number of turns equal to \( n - 1 \). The central point in design must be added to ensure uniform. By that the conditions for optimality (3) – (7) are executed. The number of points in the constructed design is \( m = n(k + 1) + 1 \), that allows to determine the coefficients of a partial \( n \)-order polynomials in \( k \)-dimensional factor space.

Block-diagram of algorithm, implementing this method, is shown in fig. 2.

To construct a design the dimension of the factor space \( k \) and the order of the design \( n \) (see Fig. 1) must be specified. Coordinates of the simplex vertices which are the basis of this design, are calculated by incoming data and matrix (2) and then are stored in memory.

According to the order \( n \) the original simplex design is consistently turned in the factor space on the corner \( \varphi_r = \frac{r \cdot \pi}{n} \ \forall r = 1, \ldots, n - 1 \) and then added to the design stored in memory. The turning of simplex, that is carried out within the loop by the method of Givens rotations [9], which represents the rotation through an angle \( \varphi_r \) around the \( k \)-dimensional unit vector \( \bar{y}_p, \ \forall p = 1, \ldots, k \), passing through the center of the design and simplex edges. Depending on the number of current iteration output of the Simplex-Summed Design matrix \( i = n - 1 \) or going to the next iteration \( i < n - 1 \) are performed.
The program implementing the above-described algorithm was developed in the graphical programming environment LabVIEW 8.5.

![Block-diagram of the algorithm for constructing \( n \)-th order Simplex-Sum Design of experiment (dash-dotted line highlights the part of the algorithm based on Givens rotations)](image-url)

Fig. 1. Block-diagram of the algorithm for constructing \( n \)-th order Simplex-Sum Design of experiment (dash-dotted line highlights the part of the algorithm based on Givens rotations)
As an example the third-order design in the three-factor space of experiment, built on the above proposed algorithm, is presented on fig. 2. It satisfies the conditions for optimality (3) - (7) and contains 13 points.

Fig. 2. The third-order Simplex-Sum Design of experiments on the base of a correct simplex in the three-dimensional factor space.

Conclusion
In the course of the work method of high order Simplex-Sum Design of experiments constructing has been developed. The algorithm of method is implemented in the graphical programming environment LabVIEW 8.5. Developed Design is proposed to be used in EDCs modeling and for the parameters of equivalent circuits of Slow Wave Structures.

References:
PROGRAMMING THE DEBUG UNIT OF MICROCONTROLLER HCS12 ON EDUCATIONAL PLATFORM ELVIS II BY NATIONAL INSTRUMENTS

I. Druginin

Saratov State University

USB bus, debugging, HCS12 microcontroller

Now, when the universal serial bus (USB) became so popular that has superseded many other computer interfaces, it is difficult enough to ignore it in sphere of computer education. Till now at teaching of computer specialities, in particular within the course of the organization of peripheral devices, as the main communication facility with the personal computer the asynchronous serial interface or the COM-port working under standard RS-232 was used. Possessing enough low throughput and noise immunity, it nevertheless approaches for the majority of educational tasks. However, due the trend of refuse motherboard manufacturers to install the COM-port connectors, and sometimes controllers, it is difficult to organize group practical training in computer classes.

USB-bus is devoid of the above deficiencies. As a result was carried out software engineering of the debug unit of CSMB12 application module by AXIOM corporation (see fig. 1), a part of an educational platform for educational designing and creation of system prototypes ELVIS II by National Instruments company. Development was carried to receive the convenient interface of communications with the microcontroller, except of dependence on presence of the asynchronous serial interface on the PC motherboard, and also allocations of possibility for further teaching of principles of operations and devices interactions on USB bus.

Application module consists of:

- Microcontroller of HCS12 family by Freescale corporation (U1)
- Various peripheral components (buttons, switches, LEDs, contacts etc.)
- Serial interface for connection to a PC (COM)
- Debug unit, equipped with USB interface
Turbo BDM Light (TBDML) debug unit provides possibility of in-circuit debugging in real time by means of BDM (Background Debug Mode) interface installed on microcontrollers of HCS12 family. This mode allows you to perform basic procedures of debugging – to view and modify the contents of registers and memory cells without stopping the debugged application (Barrett, 2007). Debug unit has been implemented on the basis of the microcontroller MC908JB16 (U4) (see fig. 2), operating at a frequency of 6MHz (Freescale, Inc., 2005) and provides debugging of the target microcontroller at frequencies around 30-35MHz.

For the input-output organization on the given type of the microcontroller is possible to use interface SCI (Serial communication Interface) which provides a standard asynchronous format of reception-data transmission with one start-bit and one stop bit, eight data bits and possibility of transfer of 9th (check) bit (Sharugin, 2004). Hardware module support of USB on this microcontroller is compatible with USB 2.0 standard (USB Implementers Forum, Inc., 2009).

Thus, the TBDML-compatible firmware of the microcontroller of debug unit and application programming interface library (tbdml.dll) have been developed. For realization of data exchange operations with the target microcontroller, applications use procedures read_sci() and write_sci(), that realized in debug library. In general, the interaction of hardware and software level occurs under the scheme presented in a fig. 3 (Agurov, 2006).

The firmware consists of 5 object modules (see fig. 4):

- The Main module (choice of startup mode, hardware initialization, main loop)
- USB-module (USB interrupt handler, USB-descriptors)
- The Commands processing module (the command buffer, determination of command type, command execution)
Fig. 2. Schematic diagram of TBDML debug unit

**Hardware Level**

Serial Communication Interface

**HCS12 Target Microcontroller** ↔ **MC908JB16 Debug Unit Microcontroller** ↔ **USB Host Controller**

**Universal Serial Bus**

Software Level

**Transactions** ↔ **I/O Request Packets** ↔ **Commands**

**USB Host Controller Driver** ↔ **USB System** ↔ **Universal Classless USB** ↔ **Debug Interface Library**

Packets → **Commands** → **Bytes Flow**

**USB Module of Debug Unit** ↔ **SCI Module of Debug Unit** ↔ **Client Target Microcontroller Firmware**

Fig. 3. Interaction of an application with the microcontroller
The code of the **Main module** receives control from the reset interrupt handler and determines a startup mode. In case of start conditions in ICP (In-Circuit Programming) mode are satisfied, it jumps to procedures of in-circuit programming through USB, which are located in ROM. If you’re running in normal mode, it proceeds to initialize the hardware components and BDM-connection. Then it enables interrupt handling and passes to main loop in which contains the background procedures responsible for support of power savings on USB bus.

In the **USB-module** all code, except initialization procedure, is executed in USB interrupt handler. It identifies the cause of interruption and performed the necessary steps for processing. If the reason for interrupt was receiving a SETUP packet (USB Implementers Forum, Inc., 2009), then the host controller receives an array of USB-descriptors from the device. In that case, if the interrupt was caused by a request for input-output from the host controller, then it performs the data transmission and control is transferred to the command processing module.

In the **Command processing module** there is a processing and filling the command buffer: identifying type of the incoming command; parsing parameters; execution of the command by BDM – or the SCI-module depending on type; the result is located in the command buffer and is transferred in USB-module for sending.

**SCI – and BDM-modules** are responsible for setup of connection and transfer the data on appropriate interfaces. The BDM-module contains a set of
the appropriate procedures that called from the commands processing module as required. The SCI-module contains the interrupt handler of an appropriate hardware component in which operations with the reception-transfer buffer are carried out.

Thus, it was possible to expand functionality of the debug unit of CSMB12 module without application of additional components and changes in its circuit. Dependence on COM-port presence on the motherboard of the computer for data exchange with the applied software is eliminated. The developed method is possible to apply at teaching of students and at designing of devices with usage of the given application module.

References:


COMPLEX SHAPE NANOTUBE STRENGTH ON BENDING

O. Glukhova, A. Kolesnikova
Saratov State University

Bamboo nanotube, peapod, strength, bending, strength factor, crosspieces, fullerene

Structures with topological cage defects are formed under the certain conditions of synthesis: five-, seven- or eight polyhedra in the structures [1-3]; joining heteroatoms and introducing internal crosspieces are possible. The cage defects led to the change of structural properties. For example, energetics of the nanotube is obviously changed at the introduction of nitrogen atoms into the nanotube and at the increase of their concentration: when emissivity decreases conductivity becomes semiconducting [4].

In the present paper the empirical method was used for the investigation of single-wall bamboo carbon nanotubes and peapods consisting of the $C_{60}$ and amchair (10,10) nanotubes.
The aim of this paper is a theoretical investigation of complex shape carbon nanostructure strength on bending.

A peapod (fig. 1a) is seen as a model of the (10,10) nanotube filled with 27 C$_{60}$ fullerenes (fig. 1b). The C$_{60}$ molecules are situated at the distance of 0.339 nm from the tube wall and are centered on the tube axis in step 0.3 nm.

Fig. 1. Carbon nanotube: a) ideal hollow nanotubes; b) the bamboo nanotube; c) the peapod consisting of the C$_{60}$ and armchair (10,10) nanotubes

Simulations of the bamboo nanotube were performed in the following manner: a crosspiece is “introduced” into the carbon nanotube (10,10) and connected by a chemical bond with the inner wall of the nanotube (fig. 1c). The crosspiece is considered to be a fragment of the C$_{240}$ fullerenes. The crosspieces of the bamboo nanotube are situated at the distance of 0.679 nm. In the bamboo nanotube the length of which is 24,327 nm there are 24 crosspieces.

Constructing elements of electronic unit on the basis of carbon nanotubes, high mechanical strength is one of the important characteristics. The strength of nanotubes is measured experimentally as follows: mechanical loading is applied to the tight nanotube plaits, suspended between two poles, with the help of an indenter on atomic–powered microscope. Consequently the bond between loading F and deflection δ [5] is established: this bond is linear to some value of the applied force for the tight plaits mode of hollow single–wall nanotubes. The strengthening process of the single-wall nanotubes was simulated, and the δ–F dependence on a molecular mechanical model was calculated.

The carbon nanostructure bending was changed from 5 up to 20 degrees. This bending is shown in fig. 2. The ends of the nanotube cage were fixed with every bending. The carbon nanotube bending is optimized by energy minimization.

The total energy of carbon tubular nanostructure is defined by an empirical, molecular–mechanical model as a polynomial, whose components have their weight coefficient being resulted in the processing of experimental data. Taking into account of Van der Waals interaction of unbound atoms the model of the valence force field was taken by us as the basis.
The nanotube bending, anchored on two poles, under $F$ (shift from equilibrium position)

$$E_{tot} = \sum k_r (r - r_0)^2 + \sum k_\theta (\theta - \theta_0)^2 + \sum \left( \frac{k_a}{r_{12}^6} - \frac{k_b}{r_6^6} \right).$$ \hspace{1cm} (1)

Here the first term takes into account the change of the binding length in the nanostructure in relation to the binding length in the graphite ($r_0=1.42\text{Å}$), the second term – the change of angles between the bindings in relation to the angle between the bindings in the graphite ($\theta=120^\circ$), and the third term – Van der Waals interaction (Lennard-Jones potential), $K_r, K_\theta, K_a, K_b.$ – weight coefficients.

Such a method of representing the total energy of carbon tubular nanostructures was chosen as one of the most optimal. The weight coefficients were found as the solution of the minimax problem with the limitations in the following manner:

$$\text{min max } S(A), \quad \text{где } S(A) = \sum_{i=1}^{3} \left| r_i - r_i^0 \right|. \hspace{1cm} (2)$$

Here $\{r_i\}$ – a set of C-C binding length, $\{r_i^0\}$ – a set of known (calculated and experimental) values, $A=(K_r, K_\theta, K_a, K_b)$ – a vector of varied parameters.

The surface of the goal function was created to find the global minimum for every set $(K_r, K_\theta, K_a, K_b)$. The basis point was shifted corresponding to its surface contour.

Set $\{r_i\}$ was found with the help of nanotube total energy on the coordinates of all atoms.

The values of weight coefficients were obtained in the result of the solution of the minimax problem (2) as follows:

$$K_r = 3.25 \cdot 10^2 \frac{\text{Дж}}{\text{м}^2},$$

$$K_\theta = 4.4 \cdot 10^{-19} \frac{\text{Дж}}{\text{рад}^2},$$

$$K_a = 4.0 \cdot 10^{-19} \frac{\text{Дж}}{\text{м}^{12}},$$

$$K_b = 1.5 \cdot 10^{-80} \frac{\text{Дж}}{\text{м}^6}. \hspace{1cm} (3)$$
The measured and calculated diameters of some nanotubes are represented in the table. The diameter values calculated by the known formula of a nanotube model radius \( R = a\sqrt{3(n^2 + m^2 + nm)} / \pi \) (a = 1.42 Å) [6] are shown for the comparison. The nanotube model is obtained by folding graphene and calculated on the molecular mechanical model by Ring–MD package with force factors (3).

It is known that mechanical properties of polyatomic (some thousand atoms) tubular nanostructures, among them irregular, can be investigated on the empirical model.

The tube length decreases with the increase of the bending angle. The force required for bending is calculated according to deformation energy \( \Delta E = F \cdot \Delta L / 2 \). The graph demonstrating the linear force increase \( F \) with the increase of a core tube shift \( \delta \) relative to the initial state is represented in fig. 3.

![Fig. 3. Force change, necessary for bending of nanotube, with the increase of bending shift](image)

<table>
<thead>
<tr>
<th>Nanotube</th>
<th>Calculation for the model graphene</th>
<th>Experimental data</th>
<th>Calculation by RING-MD</th>
<th>Theoretical calculation (a semiempirical model, \textit{ab initio})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4,0)</td>
<td>0.313 нм</td>
<td>0.33 нм [8]</td>
<td>0.336 нм</td>
<td>0.317 [12]</td>
</tr>
<tr>
<td>(5,5)</td>
<td>0.678</td>
<td>–</td>
<td>0.685</td>
<td>0.69 [10], 0.686 [12]</td>
</tr>
<tr>
<td>(8,8)</td>
<td>1.085</td>
<td>–</td>
<td>1.092</td>
<td>1.098 [12]</td>
</tr>
<tr>
<td>(10,10)</td>
<td>1.356</td>
<td>1.36 [9]</td>
<td>1.360</td>
<td>1.37 [12]</td>
</tr>
<tr>
<td>(17,0)</td>
<td>1.331</td>
<td>1.35 [11]</td>
<td>1.337</td>
<td>1.374 [12]</td>
</tr>
<tr>
<td>(18,0)</td>
<td>1.409</td>
<td>1.43 [11]</td>
<td>1.422</td>
<td>1.427 [12]</td>
</tr>
</tbody>
</table>
The strength of nanotubes is easy to characterize by coefficient $k = \frac{F}{\delta}$, having dimension $\frac{N}{m}$ of stiffness ratio according to Hook law.

For the hollow (10,10) nanotube as is seen from the diagram in fig.3, $k = 0.19 \frac{N}{m}$; for the peapod $k = 0.23 \frac{N}{m}$; for bamboo carbon nanotubes $k = 0.008 \frac{N}{m}$.

The coefficient having the meaning of strength parameter also can be a form factor of nanostructures. Really, if the analogy is taken from classical mechanics, then the coefficient of proportionality between the force and the bending shift is defined as Young model, the length and inertia momentum of tube cross section [7]. However, all the enumerated nanotube parameters for nanostructures are either unknown at all, as inertia momentum of tube cross section, or measured with errors, or calculated on these or other simplified models. Therefore the introduced strength factor has great advantage, as long as only the results of the physical and numerical experiment are required for its calculation, even without the structure specification of the nanotube case and chirality or a method of filling the cavity.

Complex shape carbon nanostructures possess an increased strength. The peapod strength factor exceeds the ideal (5,5) nanotube strength factor by 21%, but the strength factor of the ideal (10,10) nanotube exceeds the simple bamboo nanotube strength factor by 96%. Then it can be deduced, that the peapods are more strengthened materials, than the ideal and simple bamboo structures.

References:

Implementation of a complex software system is required to solve a large number of scientific problems. The use of a high-level programming language Python can simplify this task greatly. This paper presents a research on Python as a tool for science work.

Python is an interpreted, object-oriented, high-level general-purpose programming language. Python's simple, easy to learn syntax emphasize readability and therefore reduce cost of program development and maintenance. Python is open source and completely free, even for commercial use and distribution. It also runs natively on Linux, Mac OS, Windows and others platform. [1]

Python has huge standard library with very useful modules («batteries included»). A standard Python distribution includes mathematical functions, routines for interfacing with operating system, email and networking tools, regular expressions, cryptography, unit testing and more [2]. Also numerous scientific libraries and extensions are available for Python: NumPy/SciPy, Cython, matplotlib, IPython.

Useful data structures is required to implement the most algorithms. Python has tuples, lists, sets, dictionaries, strings, files and more built-in types. An n-dimensional arrays are available from third-party library NumPy. Tuples, lists and strings are sequence types that can be sliced, indexed, joined and split. Lists also is mutable sequence data type, that supports additional operations that allow in-place modification of the object, which allow to use lists as stack data structure. Strings and tuples are immutable sequence type, and therefore more effective performance and memory using. Lists and tuples hold arbitrary data objects. Sets hold unordered, unique elements and support
mathematical operations like union, insertion, difference, and symmetric difference. Dictionaries map unique key to objects. In other languages founds as «associative arrays», «associative memory» [3].

Another feature of Python is the support different programming paradigms: functional, procedural, and object-oriented. Some paradigms are much better suited to one task than to another. Python development is 5-10 times faster than C/C++ and 3-5 times faster than Java.

Numpy is a library that provides array manipulation and computation capabilities similar to those found in IDL, MATLAB. Numpy can be extended with C-code for functions where performance is highly time critical. Also the library provides tools for integrating existing FORTRAN code to Python.

SciPy is library of scientific packages for Python. It gathers a variety of high level scientific and engineering modules together as a single package. SciPy provides tools for statistics, graphics and plotting, optimization, numerical integration, linear algebra, genetic algorithms, signal and image processing and others.

One of Python’s most useful features is interactive interpreter. This system allows very fast testing ideas, learning new library interfaces and more without the overhead of creating test source files as in typical in most programming languages. IPython is another interactive shell designed to perform interactive and exploratory computing [4].

Python is interpreted and dynamically typed language. This means, those types of variables discovered at execution time. Python doesn’t use explicit datatype declaration and figure out what type a variable is when we first assign it a value. On the one hand this allows very flexible coding, on the other reduce performance because Python code can’t be easily compiled into machine code and optimized. Therefore, Python is slower than compiled, statically typed languages such as C, FORTRAN.

There are several approaches to increase performance. The first approach is to use high-level objects, optimized operations on this objects and routines in Python written in low-level languages. This is approach of MATLAB, NumPy and many SciPy modules. For example, NumPy arrays are implemented in C, and SciPy linear algebra package uses routines from BLAS library written in low-level language. Thus the high-level Python code, which uses NumPy arrays and linear algebra from SciPy, as fast as code in C/C++ or FORTRAN.

In many cases, algorithms need loops and other coding structures that can’t be optimized by previous approach. To write high-performance mathematical code in Python can be used Cython. Cython is a programming language based on Python with extra syntax allowing optional static type declarations. Cython allows translating Python module to equivalent into optimized C/C++ code and compiled as Python extension. By itself, it doesn’t give much of speedup because it runs the python interpreter through the Python-C interface, but it allows call external C libraries from extension. Dynamic typing is what forces the code to be run through an interpreter. However, declaring variables as
being statically typed using Cython extra syntax allows compiling those parts directly in machine code, which gives much of speedup [5].

Aside from Cython, there are several other ways to effectively bind python code to other languages: ctypes, swig, f2py, weave and other. Performance comparison of various methods available from [6].

A large amount of computations is required to solve many scientific problems. Such problems can’t be solved in single machine. To solve these problems we need to parallelize a sequential algorithm and run it on parallel computers.

In case of a simple parallelization a job is divided into several smaller jobs, which can be executed parallel. Each small job runs in separate thread or process on multicore machine. The standard Python library includes modules for multithreading and multiprocessing. Threads are generally ‘lighter’ than processes, and can be created, destroyed and switched between faster than processes. But multithreading in Python has a key limitation; Global Interpreted Lock (GIL). Python designed in such a way that only on thread can be accessing the interpreter at a time. This almost means that we don’t take any advantage of multithreading processing at all. The exceptions are few but important: while the thread waiting for IO (for example, for something to come from the disk) Python release the GIL so other threads can run. One way to overcome the limitations of the GIL is to use multiple full processes (multiprocessing module) instead of threads. Each process has it’s own GIL, so they don’t block each other in the same way that threads do.

In case of a sophisticated parallelization we run jobs on computer cluster, which need to communicate with each other frequently. This is subject for graduate courses in computer science. But there are some Python tools to implement the parallel programs. MPI for Python (mpi4py) provides bindings of the Message Passing Interface (MPI) standard. This package provides object oriented interface, which closely followed MPI-2 C++ bindings. It support point-to-point and collective communications of any picklable Python objects as well as optimized communication of Python object exposing the single-segment buffer interface (NumPy arrays, built-in bytes, string, array objects) [7].

Python is real programming language that allows develop a large programs. Modular programming, simple «pseudo-code»-like syntax allows organize code into readable, easy to understand structure. A huge number of useful science, visualization, network and other libraries, language extensions, bindings to other languages nominate Python as key component in building science computing.

References:

QUALITY CONTROL OF MULTIVITAMIN DRUGS.
CHEMOMETRIC APPROACH

S. Kolesnikova, S. Mushtakova, Y. Monakhova
Saratov State University

Independent component analysis, Multivariate curve resolution, Vitamins, Microelements, Multivitamin drugs

There are many different accurate qualitative and quantitative analytical methods (physical, chemical and biological) [1,2]. But only few of them could be used for simultaneous determination of different components, thought such problem is one of the most important [3]. Besides the principal obstacles for using some methods are the absence of standards and complexity of objects under study (i.e. microelements and vitamins in multivitamin drugs), and also the presence of preventive ions. So the special sample preparation is needed.

UV-Vis spectroscopy is one of the methods used for multicomponent analysis of mixtures of vitamins and microelements [1,2,4]. In case of metals determination is based on formation of stable complexes of metal cations with organic reagents. To cope with extensive spectral similarities and overlaps shown by substances in the UV region, pre-processing by taking derivatives of spectral signals in the visible light region [5] and the use of derivative spectrophotometry [6,7] for isolation of some components and their consequent quantitative determination have been proposed. Unfortunately, these methods also have essential drawbacks [6]. For example, in that case only three analytes can be determined simultaneously.

Thus it is important to develop reliable, accurate and available tool for determination of vitamins and metals in multicomponent mixtures. Such possibility can be found in application of modern chemometrics approaches to resolution of overlapping (UV–VIS) spectra of complex mixtures.
Self-modeling curve resolution (SMCR) is a set of complex mathematical algorithms for estimation of individual components spectra and it’s concentrations when one have only experimental spectra of mixtures at hand. The goal of SMCR is to resolve spectral signals of each component and find it’s concentration from experimental information about multicomponent system without using any model or prior knowledge about the system under study [8].

In this article the method for simultaneous spectro-chemometrical determination of vitamins and metal cations (calcium, magnesium, manganese, cobalt, copper and zinc), which are the most important microelements, based on the decomposition of spectra of complex objects (i.e., food stuff, pharmaceutical preparations) in the UV region, is shown.

In this investigation such algorithms as MILCA (Mutual Information Least Dependent Component Analysis) and MCR-ALS (Multivariate curve Resolution – Alternating Least Squares) were used.

Theoretical foundations of these methods were described in [9-13]. The key features of the MILCA are simplicity, accuracy and reliability. Comparisons between the new algorithm and other established methods (MCR-ALS, and other ICA techniques) were made. Results indicate that in most cases MILCA is comparable or even outperforms other chemometrics methods taken for comparisons [11,12]. It is interesting to examine the applicability of the new MILCA algorithm to determination of vitamins and microelements and, thereby, present an analytical method to quantify them in complex mixtures. This research is really up-to-date because only low number of works deals with this problem [11]. Besides self-modeling curve resolution methods (including the MILCA method) for multicomponent analysis of mixtures have not been used.

MILCA and MCR-ALS used have MATLAB interfaces and are available for free at the websites: http://www.klab.caltech.edu/~kraskov/MILCA/, http://www.cid.csic.es/homes/rtaqam/. Decomposition of spectra in all trials was no more then 3 minutes.

Equipment and reagents. The UV-VIS spectra (200-450 nm) were recorded at 1 nm resolution on SHIMADZU-1800 spectrometers with the cells having path-lengths of 1 cm.

A liquid chromatographic system (Aquilon, Moscow, Russia), equipped with a binary pump and a UV-Vis diode array detector working at 190-600 nm, and a reversed-phase chromatographic column Phenomenex Luna 5u C18(2) (150 mm × 4.6 mm, 5 µm particle size, Torrance, CA, USA) were used in our experiments. It was controlled by MultiChrom 2.4 Rus for Windows software. All chromatograms were registered at 270 nm. The flow rate was 1 ml min⁻¹. Gradient and isocratic elution profiles were used for the separation. The mobile phase consisted of potassium PBS pH 6.72 and acetonitrile. The process started from the 99:1 ratio, which was constant in the first 7 min, then the ratio was decreased to 40:60 during the next 1 min, and kept constant for the next 6 min, and then the ratio was further decreased to 1:99 during the next 1 min, and kept constant for the last 20 min.
All materials and solvents used were of analytical-reagent grade. We used certified samples of vitamins E, A (BASF, Dresden, Germany) and vitamins B6, PP (Nita-Pharm, Saratov, Russia). Solutions of vitamins should be kept in dark glass flasks. In these conditions vitamins are stable for at least one month. All solutions were prepared on methods, suggested in [3,14].

We used EDTA because it forms stable complexes in ratio 1:1 with wide range of elements with large values of molar coefficient and because it is rather available reagent.

Multivitamin drugs “Sana-Sol” (Kruger GmbH & Co. KG, Bergisch Gladbach, Germany), “Complivit” (UfaVita, Ufa, Russia), “Pikovit Forte” and “Duovit” (KRKA, Novo, Slovenia), “Elevit Pronatal” (Roche, Basel, Switzerland), “Multi-tabs Junior” (Ferrosan/Pharmacia&Upjohn, Copenhagen Denmark) and “Alphavit” (Akvion, Moskow, Russia) were used as real objects.

All spectra were registered for three times. Means with confidence interval are shown in the tables (p=0.95).

Model mixtures of vitamins. We tested the applicability of the MILCA algorithm for qualitative and quantitative analysis of binary and ternary model mixtures of vitamins C-E-PP. As an example, experimental spectra and the results of qualitative analysis of this system by MILCA, are shown on fig. 1. It can be observed that calculated and experimental spectra are rather similar; the relative error in absorption peak locations is about 1 nm that is comparable with instrumental uncertainties. Values of correlation coefficient indicate that identification of components is performed with high level of confidence.

The results of quantitative analysis of the systems under study MILCA are reported in table 1. We observe that the performance of MILCA is comparable with MCR-ALS – well-known chemometrics tool for spectra decomposition.

Thus, our results indicate that MILCA algorithm is suitable for simultaneous analysis of vitamins in complex mixtures.

<table>
<thead>
<tr>
<th>System</th>
<th>Mixture</th>
<th>C</th>
<th>E</th>
<th>PP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Declared</td>
<td>Found</td>
<td>Declared</td>
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<tr>
<td>C-E-PP</td>
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<td>3.5±1.5</td>
<td>5.0</td>
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<td></td>
<td>2</td>
<td>10</td>
<td>11±1</td>
<td>3.0</td>
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<tr>
<td></td>
<td>3</td>
<td>7.5</td>
<td>7.3±0.3</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Table 1

Decomposition of model mixtures of vitamins by MCR and ICA algorithms (n=3, p=0.95)
Model mixtures of metals. Complexonates of metals have low molar coefficients of absorption of spectral curves in visible region. So for estimation of the applicability of the MILCA algorithm for qualitative and quantitative analysis of multicomponent mixtures of metal cations we decomposed spectra of binary mixtures with different ratio of complexonates of calcium and magnesium in UV region (200-400 nm). Correlation coefficients of calculated and experimental
spectra are rather similar; the relative error in absorption peak locations is about 1 nm that is comparable with instrumental uncertainties. Values of correlation coefficient indicate that identification of components is performed with high level of confidence. The relative error is found to be no more than 5 %.

It should be noted that one can use not only the EDTA. Also, any organic compound, which forms stable complexes with metals with high molar coefficients, may be suitable.

Analysis of real objects. Approbation of ICA decomposition algorithms on real objects is of great practical interest, especially where mixture composition is not known exactly.

SMCR methods were used for analysis of multivitamin drugs which contain mineral substances and vitamins. The analysis of such type of objects is interesting now because they have complex matrix (extenders and so on).

We registered spectra of solutions prepared by mixing the appropriate aliquot of the medicine with EDTA (pH 10) with and without standard addition of all metals (Fig. 2a). Then spectra decomposition is performed and identification of calculated spectra of individual components were made by comparison spectra curves and by an increase of relative concentration of this metal in the mixture with it’s addition. As an example there are experimental absorption spectra of drug “Elevit Pronatal” with and without the addition of standard metal solutions, and resolved spectra of complexonates on Fig 2.

The results of quantitative analysis of metals in these drugs are shown in table 2.

Table 2

<table>
<thead>
<tr>
<th>Object</th>
<th>Metal</th>
<th>Ca</th>
<th>Mg</th>
<th>Zn</th>
<th>Mn</th>
<th>Cu</th>
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<td>100</td>
<td>50</td>
<td>---</td>
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</tr>
<tr>
<td></td>
<td>MILCA</td>
<td>108±10</td>
<td>46±5</td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td>MCR-ALS</td>
<td>105±8</td>
<td>48±3</td>
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<td></td>
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<tr>
<td>“Complivit”</td>
<td>Declared</td>
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<td>16</td>
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<tr>
<td></td>
<td>MILCA</td>
<td>62±7</td>
<td>18±2</td>
<td>2,5±0,3</td>
<td>1,9±0,3</td>
<td>0,72±0,05</td>
</tr>
<tr>
<td></td>
<td>MCR-ALS</td>
<td>50±4</td>
<td>15±1</td>
<td>2,3±0,2</td>
<td>2,8±0,3</td>
<td>0,70±0,6</td>
</tr>
<tr>
<td>“Elevit Pronatal”</td>
<td>Declared</td>
<td>125</td>
<td>100</td>
<td>0,75</td>
<td>0,10</td>
<td>0,10</td>
</tr>
<tr>
<td></td>
<td>MILCA</td>
<td>127±7</td>
<td>108±10</td>
<td>0,78±0,05</td>
<td>0,10±0,03</td>
<td>0,09±0,01</td>
</tr>
<tr>
<td></td>
<td>MCR-ALS</td>
<td>120±8</td>
<td>95±8</td>
<td>0,73±0,05</td>
<td>0,09±0,01</td>
<td>0,11±0,01</td>
</tr>
<tr>
<td>«Alphavit»</td>
<td>Declared</td>
<td>---</td>
<td>40</td>
<td>12</td>
<td>2,0</td>
<td>---</td>
</tr>
<tr>
<td></td>
<td>MILCA</td>
<td>44±5</td>
<td>10±2</td>
<td>1,7±0,3</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCR-ALS</td>
<td>42±4</td>
<td>14±1</td>
<td>1,8±0,1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The qualitative analysis of vitamins in such case was carried out without using standard samples. It was simultaneous identification of 5 water- and fat-soluble vitamins. Only the spectra of multivitamin drugs were used for the analysis. After that we get the data of relative concentration of mixture components, which are shown in table 3.

As we can see in both cases mixtures are decomposed in independent components and correlations between different substances in these mixtures agreed with indices, declared by producers, and results of HPLC. Analytical error of MILCA and ALS is compatible and in most of cases it is no more then 8-10 % rel.
Fig. 3. Absorption spectra of drugs “Sana-Sol” (1), “Complevit” (2), “Duovit” (3), “Pikovit Forte” (4), “Multi-tabs Junior” (5) (a); b – resolved spectra of all vitamins (MILCA) (correlation coefficients were found to be in 0.87-0.95 interval)

Table 3

Determination of vitamins in multivitamin drugs (weight percent)

<table>
<thead>
<tr>
<th>Drug</th>
<th>Vitamin</th>
<th>Vitamin C</th>
<th>Vitamin PP</th>
<th>Vitamin B6</th>
<th>Vitamin A</th>
<th>Vitamin E</th>
</tr>
</thead>
<tbody>
<tr>
<td>“Duovit”</td>
<td>Declared</td>
<td>4.8</td>
<td>0.16</td>
<td>1.0</td>
<td>1.13</td>
<td>0.8</td>
</tr>
<tr>
<td>MILCA</td>
<td>5.0±0.3</td>
<td>0.12±0.01</td>
<td>0.80±0.09</td>
<td>1.2±0.1</td>
<td>0.73±0.06</td>
<td></td>
</tr>
<tr>
<td>MCR-ALS</td>
<td>5.1±0.3</td>
<td>0.14±0.01</td>
<td>1.1±0.1</td>
<td>1.1±0.1</td>
<td>0.81±0.05</td>
<td></td>
</tr>
</tbody>
</table>
Thus, SMCR-methods (MILCA, MCR-ALS) were used for multi-component analysis of metal cations and vitamins in model systems and real objects. In such cases ICA is a fast, accurate and reliable method to provide qualitative and quantitative analysis of a bundle of substances in a single analytical run. The proposed method is a promising analytical tool to improve the productivity and reliability of determination of fat- and water-soluble vitamins and microelements in food control and analytical laboratories.

References:

THE LABORATORY COMPLEX FOR RESEARCHING PROCESSES IN BRUSHLESS DC AND STEPPER MOTORS MICROPROCESSOR CONTROL SYSTEMS

E.V. Komarov, A.V. Polyakov

AVR Microcontroller, ELVIS II, LabVIEW, Multisim

Today, in the modern industry, the more widespread occurrence receives transmission devices, precise positioning and measuring devices are based on brushless direct current (BLDC) and stepper motors. The reasons of using this types of motors are caused by higher efficiency in comparison with other types of DC motors and the ability to quick start, stop and reverse direction. The use of this type of DC motors requires microprocessor control systems.

The typical system uses BLDC motor is shown on fig. 1.

![BLDC Motor Control System Block Diagram](image)

Fig. 1. The BLCD motor control system block diagram

Elements of the motor control system are:
• the control unit consists of a microprocessor or microcontroller (MCU) that generates sequences of control pulses;
  • a PC communication interface;
  • the driver unit converts low power digital pulses from control unit into high power outputs are connected to the motor windings;
  • BLDC or Stepper motor;
  • feedback chains.

The purpose of the work was to develop hardware and software complex for designing and researching in BLDC or Stepper motor's control systems, based on National Instruments (NI) technologies [http://www.ni.com]. The complex also will be used for teaching students of the functioning principle of stepper and BLDC motors and their control systems.

Laboratory Complex Description

The developing of control system requires an understanding of the physics of processes occurring in it and a availability monitoring devices. Thus, there is a need to a stand, which contains a set of software and hardware management and can monitoring system in various locations. Therefore the laboratory stand was offered to do on NI ELVIS II (Educational Laboratory Virtual Instrumentation Suite) platform [2]. This platform allows you to manage and measure the different variables are used in a system (fig. 2).

Fig. 2. NI ELVIS II platform

NI ELVIS II platform used for data collection, generation and coordination of signals are fed to the scheme developed at the protoboard. It is also has USB interface for communication with a PC. ELVIS II platform includes the following devices:
  • 8/16 input ADC channels with 16 bits resolution, 1,25 MHz;
  • 2 output DAC channels with 16 bits resolution, 2,8 MHz;
  • 24 input/output digital channels, 10 MHz;
• 2 timers/counters;
• Adjustable DC voltage generator ±12 V;
• Stabilized DC Voltage generator +5 V, ±15 V;

The hardware of a designed laboratory complex is a module that directly connects to the NI ELVIS II protoboard. The module's block diagram is shown on fig. 3.

Fig. 3. Hardware block diagram

The module implements:
• the ability to connect different BLDC and stepper motors with the number of windings not exceeding four, with an operating voltage up to 12 V and winding’s current up to 8 A;
• the ability to connect both unipolar and bipolar types of motors;
• different modes of the motors are connected to (accelerating, braking, maintaining speed mode);
• controlling windings’ current overloading;
• the ability to control BLDC and stepper motors with NI ELVIS II platform or Olimex AVR-H128 ATMega128 header board [3];
• MCU connection to the PC via RS-232;
integration NI LabVIEW that is interactive, graphical programming language [4];
measurement of phase voltages and currents in real time by using ELVIS II platform’s ADC;
the ability to connect rotor position sensors to ELVIS II platform’s ADC;
the ability to connect an external power source to supply the motor windings.

The module management can be done in two ways:
The first way is using Olimex AVR-H128 header board is based on an Atmel ATMega128 microcontroller. The MCU generates sequences of control pulses. NI ELVIS II platform uses to control the system. It also has RS-232 interface for communication with a PC.
The second way is using software has written in LabVIEW. In this case, reached the maximum flexibility and efficiency of using the complex. In the first place, the developed software has an intuitive user interface for specifying sequences of control pulses and switching motor’s mode; secondly, you can make digitizing of measured windings’ voltages and information from the position sensors for future researching of processes occurring in the motor’s windings; third, it implements a graphical representation of measured values. Other advantages of this method are:
the ability to save received data from the control system on any type of storage device;
the ability to change control system variables in real time;
In general, this range is equally suitable for educational, research and applicational tasks:
implemented schematic design and modeling processes occurring in it in the NI Multisim environment [5];
developed software in NI LabVIEW implements the various modes of BLDC and stepper motors, and allows you to monitor the currents and voltages in the windings.

References:
AN IMMUNOCHEMICAL TEST FOR RAPID SCREENING OF T-2 TOXIN

A. Koptel, E. Basova

Saratov State University

Non-instrumental test, visual detection, Fusarium toxin, T-2 toxin, mycotoxin, feed

Mycotoxins are natural toxic secondary metabolites produced by several fungal species on agricultural commodities in the field or during storage, which cause food- and feed-borne intoxication, and many are cytotoxic, carcinogenic, mutagenic, or immunosuppressive [1].

The *Fusarium* is the most prevalent toxin-producing soil fungi, which contaminate food grains in the temperate regions of America, Europe, and Asia. They produce mycotoxins of the class trichothecene, which are highly toxic to animals and humans. The trichothecene of interest in this study is T-2 toxin, well-known for causing alimentary toxicity. Estimation of trace amounts of T-2 toxin present in food sample due to fungal contamination is a difficult task, as it requires laborious and extensive cleanup treatments to remove interfering substances from the sample matrix before analysis. Therefore, there is a demand for rapid and reliable methods for the detection of T-2 toxin in food samples [2].

Immunochromic methods, especially microtiter plate ELISA, offer the required sensitivity and are widely used for simultaneous analysis of a large number of samples. However, these methods are time-consuming and require sophisticated equipment and complicated sample cleanup (generally, solid-phase extraction or immunoaffinity column). Most of the developed analytical tools for mycotoxin screening are analytical methods based on chromatographic principles. But an application of these methods needs dearly equipment, long and difficult sample pretreatment.

Non-instrumental immunochromic methods for mycotoxin detection are quick and do not require long and difficult preparing the test.

The aim of this article was to develop a non-instrumental test for detection of T-2 toxin, in feed samples. In poultry feed mixtures, this mycotoxin is the most frequently occurring among eight toxicologically significant *Fusarium* toxins. Feed is characterised by a substantial variety of interfering compounds, caused by the different ingredients and processes. To decrease matrix effect in the developed assay, sample extract was run through an additional column with clean-up sorbent. The assay column design is presented in Fig. 1.

The gel-based immunoassay was developed as a visual qualitative test, giving a yes/no response to the level of the target analyte/analytes. Negative tests gave coloured test line/lines because of the inverse relationship between analyte concentration and intensity of the colour development. Construction of the test
inside a cylindrical cartridge allowed the test to be combined with another cylindrical cartridge with clean-up layer and to use high volume of washing buffers. Therefore, gel-based immunoassay columns were used before to analyse intense-coloured samples and samples with substantial matrix influence such as coffee, cocoa and spices.

Rabbit anti-mouse immunoglobulin coupled gel which was used for coupling of anti-T2 antibodies was prepared as follows. Sepharose (0.5 g, which gives about 1.8 mL final gel volume) was washed on a sintered glass filter using 1 mM HCl (200 mL/g gel). Rabbit anti-mouse immunoglobulins (250 μL) and 100 μL of coupling buffer (NaHCO3 buffer, 0.1 M, pH 8.3 containing NaCl 0.5 M) were mixed with the gel using an orbital shaker for 2 h at room temperature. Afterwards, the gel was washed with 5 mL coupling buffer to remove excess of rabbit anti-mouse antibody. The remaining active groups were blocked by adding of blocking buffer (7 mL, 0.2 M glycine, 0.1 M NaHCO3, 0.5 M NaCl, pH 8.0) to the coupled gel for 2 h at room temperature. The gel was then washed with at least three cycles of alternating pH and at least five gel volumes of each buffer. Each cycle consisted of a wash with 0.1 M acetate buffer pH 4.0 containing 0.5 M NaCl followed by a wash with coupling buffer pH 8.3 containing 0.5 M NaCl. The prepared gel was suspended in PBS (1:3, v/v) and stored at 4–8°C.

Blocked gel was used for dilution of the antibody coupled gels. It was prepared as follows: 2 g of sepharose was washed on a sintered glass filter using 400 mL of 1 mM HCl. Then, the active groups were immediately blocked by adding 35 ml of blocking buffer for 2 h at room temperature. Washing and suspending procedures were the same as for the coupled gels.

The T2 test layer was prepared as a mixture (1:500) of the anti-T2 gel and the blocked gel, both diluted 1:3 with PBS.

The test column consisted 150 μL of the mixture of anti-HRP gel and blocked gel were added on the bottom polyethylene frit in an empty 1-mL Bond Elut cartridge and then covered with a second frit. The test columns were not reusable.

The clean-up sorbent (50 mg of Bondesil NH2) was placed on the bottom of a 1-mL Bond Elut cartridge above a polyethylene frit. A second frit was put on the top of this clean-up layer. The concentrations of immunoreagents were optimised according to the following criteria:

1. the appearance of a clear blue colour on the test layer for negative samples within a reasonably short time;
2. no blue colour development at the test layer for samples containing mycotoxins above a predetermined cut-off level within the detection time.
To control the sensitivity of the test layers for each experiment, two columns with identical test layers were prepared. Blank solution was applied for the first one, while a spiked mycotoxin solution of 10 μg/L was brought onto the second column. This spiked 10 μg/L concentration was based on the targeted assay sensitivity of 100 μg of T2 per 1 kg of feed.

For the T2 test layer the dilutions of the anti-T2 gel with the blocked gel and the HT2-HRP conjugate were optimised. Anti-T2 gel dilutions of 1:10, 1:100, 1:500 and 1:1000 were tested and 1:500 was chosen as the optimal. HT2-HRP conjugate solutions were tested in the range of 1:1,000 to 1:1,000,000. Satisfactory results were obtained for the dilutions in the range of 1:10,000–1:25,000. Increasing of the dilution resulted in decreasing of colour intensity and longer development time.

The developed gel-based assay allows for the first time onsite screening for the determination of Fusarium toxin in feed samples within a few minutes. For reduction of matrix influence, an additional column with clean-up layer was used.

References:

THE MODIFICATION OF THE MODEL OF A CAUSE-EFFECT COMPLEX

R. Lapkovsky

Saratov State University

Cause-effect relation, cause-effect complex, mechatronics, man-machine system, information system, modeling

A modeling of complicated systems (factory, plane, submarine, power station), especially troubleshooting in same ones, is very difficult and actual task now. The same systems, as a rule, consist of a lot of heterogeneous components. You have to use a special model and a special list of properties to describe each of them. All components of complicated systems interact closely on each other; therefore the authors of (1) presented using the general cause-effect approach to describe the interaction. It allows developers to format the
interaction between all components, even between heterogeneous ones, in a general view. Also the authors of (1) presented a formalized cause-effect model – the cause-effect complex. This article describes a modification of this model. The modification extends the possibilities of cause-effect complexes and orients it for realization on multiprocessor computers.

The most general form of describing interconnections and interactions between heterogeneous components of complicated system is a cause-effect relation. But, modern tasks cannot be efficiently solved using an ancient conception of the case-effect relation (fig. 1). Therefore, the authors of (1, 2) presented the conception of cause-effect complexes, which includes a cause group and an effect group (not only a cause and an effect). Also, complex includes a core, which implements the cause-effect relation (fig. 2). The core may be implemented by different ways; it may be a formula, a table, an algorithm and any other way to get some effects if the core has some causes. It allows you to create cores very flexible.

Also, it was developed algebra of the cause-effect complexes. The algebra describes how complexes can connect with each other to create more complicated ones (fig. 3). Elements of the case group and the effect group are a subset of a set of all system states, which describe the complex.
The shortcomings of the classical cause-effect complexes model

The classical model of cause-effect complex is general model. This generality allows model to accentuate a main idea of using this approach. But the generality hampers applications for solving tasks. When you will implement the model on a computer, you will have some problems. And you can not use this model efficiently.

The first problem or shortcoming is that the complexes structure describes occurrence instantly (without using steps in runtime). An event tree (without any cycles) defines different trains of events, which describes different ways of phenomena progress. It disallow using cycles in a complexes composition, by-turn, it limits the range of tasks, which can be solved by one cause-effect complex.

The second problem is a large set of system states. In big systems the number of elements of a cause group and an effect group is very large. And they are heterogeneous. The idea of consolidation such variety of different properties and states just using a basic subset of global set is very bulky solve. You have to create the set of all system states and combinations of them. It is practically impossible for complicated systems; also the cores developing will be very hard.

Notice, the problems appear in small systems too, if you use a lot of different input values (3).

The modification of cause-effect complexes model

For practically using and computer realization the author offers the modification of classical cause-effect complexes. The modification saves the main idea and the conception of developed approach: the structure of a cause-effect complex consists of cause-effect links, connected with each other. A cause-effect link can be a cause-effect complex too.

As opposed to the classical model, the modification defines elements of cause and effect groups as blocks of data, which has own type and structure. This data blocks are called packets. When a complex gets necessary “cause” and “condition 1”, the core takes it and creates appropriate “effect” and “condition 2” in form of packets. A structure and contents of the packets completely describes the derived effect. After that the packets are moving along links. When the packets get to a next complex the core derives a next reaction. The complex is functioning step by step, not instantly as compared with the classical version. It supplies by a special mechanism of core functioning, when it gets a regular packet. When the packet gets to a complex, the analysis block decides the complex is ready or not (figure 4: analysis). The complex is ready, when it has some packets in his cause group, needed for creating packets of his effect group. The ready condition defines by a global task and a functional role of the complex.

The ready complexes have all heeded information to form effect packets. Then the second stage starts, the core get some packets form cause group, processes them, and forms effect packets (fig. 4: core).

These effect packets are passed to cause group of another complex, etc.
On the figure 5 you can see the example part of a cause-effect complex, consists of 3 complexes: H1, H2, H3. The complex H1 is ready, when it gets a cause, described by the packet P1, the complex H3 is ready, when it gets the packets P1 and P2.

For example, you have packet P1 in the entry. Using links it gets to complex H1, and to complex H3. Complex H1 process the packet and form effect P2 and effect condition P3. P2 get to complex H2, and add to a list of causes of complex H3. Note, that complex H3 form an effect packet only when it has a list of two cause packets P1 and P2.

The presented conception of packets, which describes elements of a cause group and an effect group, allows creating complicated structures of causes, effects and conditions. You can update and change the structure of same classes of packets, if you know nothing about structure or existents of other ones. Note, that it is very useful using the principles of object-oriented programming for describing classes of cause and effect packets.

The presented mechanism of core functioning allows using cycles in a complexes composition. It extends a range of tasks, which can be solved, using the modification of the cause-effect complexes model.

The modified model implements by using a multiprocessor computer easily than by the classical model. In the first place, it is because of using developed approach of links organization between information systems and because of using advantages of object-oriented programming.
The presented modification of the cause-effect complexes model gives an opportunity to overcome some difficulties and shortcomings of the classical model.

Developers can create complexes, using cycles. It extends a range of tasks, which can be solved, using one cause-effect complex. The presented mechanism can be easy realized on a computer, especially on multiprocessor one.

The conception of cause and effect packets allows developer to order and structure the space of his system states and events. Thus, complexes interaction is more clear and efficient.

References:


MODE COUPLING IN FOUR-CORE FIBER LASER

A. Melnikov, L. Melnikov

Saratov State University

The mathematical model of mode coupling in multi-core fiber via cladding mode excitation is presented. The model includes the coupled equations for mode amplitudes evolution during beams propagation along the fiber ring laser. This model has been applied to the description of 4-core Yb-doped fiber laser.

Recently more and more steadfast attention involves possibility of making lasers based on fiber-optics systems. Fiber lasers are one of arrivals of a fiber-optics and the laser physics. The main advantages of fiber lasers are: an effective heat-conducting path, compactness and small weight, high quality of output beam, high stability, and high efficiency of use of a pumping and at all it rather low cost.

It is known [1], [2], that in a fiber laser with the several single-mode cores which are separated enough to prevent mode coupling through overlap of fields, there are regimes at which phase locking between fields in various cores is observed. Influence of cladding mode [1] can be the parent of it.

Special interest has build-up of mathematical model of operation multi-core laser. In this article derivation of the equation of generation, its
solution and application of the gained results for the description of mode of operations four-core variant of its execution featured in [1] and [2] is presented.

For calculation of fiber eigenmodes the equation for magnetic field is to be solved:

$$\nabla_\perp^2 \begin{pmatrix} H_x \\ H_y \end{pmatrix} + k^2 \varepsilon(x, y) \begin{pmatrix} H_x \\ H_y \end{pmatrix} + \begin{pmatrix} \frac{\partial \ln \varepsilon}{\partial y} \\ -\frac{\partial \ln \varepsilon}{\partial x} \end{pmatrix} \begin{pmatrix} \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} \end{pmatrix} = \beta^2 \begin{pmatrix} H_x \\ H_y \end{pmatrix}, \quad (1)$$

where $H_x$, $H_y$ are the transverse components of magnetic field, $k$ is wave number, is the distribution of dielectric constant. This equation was solved using finite element method for parameter set corresponding to Fig.1 at the wavelength 1030 nm.

From a set of solutions, the configuration supporting cladding mode is sampled in Fig.2. For a mode with effective mode index, equal to 1.499448, field distribution well matched with experiment data from Ref. 1.

Using a method of the balance equations [3] the equation featuring variation of amplitude of a field at propagation in the active fiber was written as:

$$2i\beta \frac{dA(z)}{dz} + k^2 \frac{\int d\vec{r} \chi(\vec{r})|\psi(\vec{r})|^2}{\int d\vec{r} |\psi(\vec{r})|^2} A(z) = 0, \quad (2)$$

![Fig. 1. Model of four-core optic fiber. $d_{\text{core}} = 6.5 \, \mu$, $d_{\text{dist}} = 28 \, \mu$ and $d_{\text{cladding}} = 200 \, \mu$. $n=1.5$](image-url)
where $G = g/k$, where $g$ is the gain, $J$ is dimensionless intensity, $\Im(x) = 1 / (1 + x^2)$ is the dispersion function, $\chi(\bar{r}) = G \frac{(\omega_0 - \omega)}{\gamma} \frac{\Im}{1 + J(\bar{r})^3} - iG \frac{\Im}{1 + J(\bar{r})^3}$, $\beta$ is the propagation constant of a fiber mode, $\beta = kn_{\text{eff}}$, where $n_{\text{eff}}$ is effective refractive index of the mode.

For $|\psi(\bar{r})|^2$ the Gaussian approximation [4] was used:

$$
\psi(\bar{r}) = a \exp \left( -\frac{1}{2} \frac{r^2}{R_0^2} \right), \quad R_0 = \frac{a}{\sqrt{2\ln V}},
$$

where $a$ is diameter of fiber core, $V$ is the characteristic frequency.

The system of equations for four-core fiber including mode coupling, using the expressions featuring cross-talk between pairs and arrays of symmetrical cylindrically fibers [4], is as follows:

$$
\frac{dA_j(z)}{dz} - i d_j A_j(z) - \frac{g}{2n_{\phi}} \frac{3\ln \left( 1 + |A_j(z)|^2 \right) \exp(-2a / R_0^2)}{4|A_j(z)|^2} A_j(z) + iC_j B(z) = 0,
$$

Fig. 2. Transverse distribution of field in four-core fiber. Numerical experiment, cladding mode $n_{\text{eff}} = 1.499448$
here $C_j$ are coupling coefficients of modes for separate cores to cladding mode, $d_j$ and $\phi$ describe the losses and phase delay for modes.

Coupling coefficients were estimated using the expressions from Ref. 2. For calculation the value 0.12 was used for all coefficients.

The system (4) represents the equations of mode propagation for the four-core fiber laser in which binding of modes through cladding mode is considered.

Model of unidirectional fiber ring laser is shown in Fig. 3. Field transformation from fiber input end to output end is given by the solution of the system (4). After passing through output coupler the modal amplitude should be multiplied by $t$. Due to fiber bend the phases delay for core and cladding modes may be different. Transmission coefficient $t$ (Fig. 3) which features losses in the cavity.

By means of the solution of this system, it is possible to observe spatio-temporal dynamics of modes in cores and in a cladding.

In the numerical results shown below time unit is cavity round trip time, coordinate unit is fiber length.

Changing the parameters of the active fiber from the system (4) it is possible to simulate various regimes of operations of the laser, such as a regime of beats (Fig. 4) and a regime of synchronization of modes of cores, means cladding mode (Fig. 5).

In these Figs the temporal and spatial dynamics are shown for intensities of core and cladding modes. The total intensity is shown also. Their oscillations allow to estimate whether the synchronization exists. It is obvious, that presence of phase differences in the fields of separate modes will lead to beating of their intensity from one round trip to another. The spatial dynamics dem-

\[
\frac{dB(z)}{dz} - i\phi B(z) - i \sum_j C_j A_j(z) = 0, \quad j = 1\ldots4
\]
onstrate intensity variation along the fiber and «jumps» due to passing through output coupler. High-frequency pulsations in spatial dynamics are characterized by value $\phi$.

Summarizing the mathematical model of the four-core ring fiber laser with mode locking via cladding mode has been proposed. Using the model spatio-temporal dynamics of modal fields are simulated numerically showing good agreement with experiments [1, 2].
Fig. 5. Temporal (a) and spatial (b) dynamics of total intensity of laser (1), field’s intensity in one core (2) and intensity of cladding mode (3). A locking regime

References:

MULTIPLE SCATTERING OF FIBRILLAR MEDIA
WITH MACROSCOPIC BIREFRINGENCE: THEORETICAL MODELING
AND DIAGNOSTICAL ASPECTS IN BIOMEDICINE

A. Mikhaylova
Saratov State University

Scattering, anisotropic medium, energy density approach, fibrous tissue

A number of media such as composite structures or fibrous tissues (for example, bone, muscle fibers, derma, cartilage) possess birefringence properties which are due to their structure. Optical properties of tissues such as the value of effective refractive index, scattering coefficient, anisotropy, etc. are closely related to their biochemical and morphological structure and can be considered as one of the fingerprints of tissue functional state.

Fibrous tissues constitute approximately 50% of body weight and have similar construction and physical properties [1]. The fibrillar structure (or fibrous tissue) can be described as a multicomponent structure consisting of collagen fibers in carbohydrate matrix. The fibrils are actually composed of collagens of several types. There are 14 types of collagen depending on the arrangement order of amino acids in polypeptide chain, on their hydroxylation degree and quantity of a carbohydrate component [2-9]. Only five types of collagen are well investigated. Various types of collagen are contained not only in fibers, but also in structure of basal membranes of epithelial tissue, vitreous body and other structures [1]. The surrounding medium is a composition of glycosaminoglycans and proteoglycans.

For the fibrous tissues with partially oriented fibrillar structure the transport parameters, which characterize propagation of probe light through a probed tissue, become polarization-dependent. That is why the optical probing of fibrous tissues with polarized light in visible and near infrared region can be used for rapid monitoring and visualization of pathological changes in tissue [10,11], especially some deviations in fiber orientation and packing from the normal state. The analysis of tissue morphology is based on illumination of interesting object by polarized light and registration of two linear polarized parts of scattered light. The value of optical anisotropy is the difference between two refractive indices. Here and are the refractive indices for two polarization states of propagating light wave: with the electric vector parallel or orthogonal to the direction of fiber axes.

The energy density approach is used as a modification of the coherent potential approximation [12] for the theoretical determination of optical anisotropy. The latter one takes into account the existence of multiple scattering effects (the volume fraction of scatterers is in the range 0.2-0.6 for most of the biological tissues, in this case we must take into account multiple scattering effects).
We have considered the homogenous anisotropic medium consisting of coated cylinders as a model of fibrous tissue. In these coated cylinders the core is equivalent to real fiber, and the coating is a basic substance. For these cylinders four parameters are introduced: the refractive indices of coating \( n_1 \) and core \( n_2 \), the radius of cylinders \( R \) and their volume fraction \( \varphi \), where \( n_1 \) is the radius of coating. Such modeling was used previously to compare theoretical data with experimental ones [13] for the rat derma (see Fig.1).

![Fig.1](image1.png)

Fig.1. The theoretical curve corresponds to typical structure of human and rat derma. Experimental value of optical anisotropy was equal to \( |\Delta n| = (2.3 \pm 0.2) \cdot 10^{-4} \).

Let us consider some examples of possible applications of the energy density approach for modeling of influence of biochemical properties change on the optical anisotropy spectrum of collagenous tissue. In previous study we revealed that there is a strong relation between changes in physical and chemical state of tendon in the course of aging and variations in optical anisotropy (see the Fig.2). The process of aging is considered in detail in [1-3,14,15].

![Fig.2](image2.png)

Fig.2. Influence of aging. The data correspond to *supraspinatus* tendon.
As we noticed before, the birefringence of a normal tissue and a burned one will be different because in this case the change in refractive index and decrease of optical anisotropy value are caused by close values of refractive indices of basic substance and fibers (this is valid if deviations of other parameters do not exceed 2-3 %).

The discussed approach can also be useful for interpretation of polarization data obtained for optically cleared tissues at various stages of clearing (exchange of water and clearing agent in a basic substance, partial penetration of clearing agent into the fibers, etc.).

But energy density approach does not take into account the presence of various directions of fibers in tissue. The method is offered for correction of obtained theoretical data for real tissue with partially oriented fibers in work[10]. Taking into account this partial orientation, we obtain the values of birefringence smaller than the similar ones for model medium with parallel fibers (in 1.6 times for derma, and 1.1 times for tendon) in this case. Fig. 3 shows various fragments of microscopic images for derma and tendon, which illustrate the effect of partial orientation of collagen fibers.

Fig. 3. (a,b,c,d) Microphotographs of derma (e) Section of the achilles tendon

The theory and experiment have shown a good agreement for the rat derma [10]. So we can conclude that the value of optical anisotropy characterizes the state of fibrous tissues and polarization-sensitive optical technologies are appropriate tools among other diagnostical methods for screening of the morphological and functional state of connective tissues.

Also considered method can be useful for interpretation of experimental data for various biochemical processes (for example, pathological changes) and prediction of anisotropy spectrum behavior for various morphology changes (as an example, aging).

In conclusion it is necessary to note that the polarization measurements as an experimental technique combined with the energy density approach as a theoretical method can be applied as an instrument for monitoring of morphological and functional state of in-vivo tissue.

References:


**METHODS OF GEOECOLOGICAL RISKS’ GEOINFORMATIONAL MAPPING OF OILFIELD EXPLOITATION**
(Saratov Region as an example)

*A. Molochko, D. Khvorostukhin*

*Saratov State University*

Risk, geoeconomic risk, geoeconomic risk factors, risk-analysis, oil industry, oil sector’s stages, cartographic method of risk-analysis, GIS, risk mapping

“Risk” as a concept became customary for modern society. We can find the “risk” term and its derivatives (“hazard”, “damage”, “risk situation”, etc.)
in any area of human activity. But still there is no general point of view on what we can interpret as a “risk” term. For some scientists, risk is the uncertainty of supposed events which lead to negative consequences. For State Standard, risk is a probability of event and its consequences. For guidance documents, risk is a combination of frequency and consequences of a certain hazardous occurrence (1, 2, 3, 4). Interpretation of term “geoecological risk” is more intricate. For geographers, geoecological risk is a risk of human environment’s unbalancing, all the factors that influence its structure, safety, mobility and perceptiveness. Geoecological risk is not only the demonstration of danger for human beings following from geological component of natural environment; this is a complex demonstration of negative influence of all natural environment’s components. Ecological, geoecological and other natural risks are capable to lead to pecuniary, engineering and human loss. That is why it is important to use all risk-analysis tools for lowering of probable negative natural processes and phenomenons’ impact and their monitoring.

Risk-analysis is the whole set of methods, that make possible to show probable hazards, estimate risk, work out the system of recommendations and methodology for management and reduction of aftereffects (5).

The general chart of geoecological risks analysis can be represented in the following segments (fig. 1):
1. Identification of geoecological risk factors
2. Identification of risk sources and recipients
3. Choosing risk estimation methods
4. Creating of subsequent processes development prognosis and making adaptation of processes

In general geoecological risk factors can be divided into 3 groups: natural, social and anthropogenic. Usually for industrial productions all these risk factors work in complex and it becomes hard to appraise the individual value of each factor.

General risk-analysis methods are schemed by “quantative – qualitative” and are further divided into engineering, modeling, expert, sociological etc (6). A separate group of risk analysis methods is a cartographic method, witch allows of organizing cartographic data visualization. This cartographic visualization makes it possible to change and speed up the process of making decision because of visual representation of existing, already established, and probable geoecological situation within the particular area.

Oil sector cartographic risk-analysis
Oil sector as a complex multifunctional system consists of successive steps (fig. 2):
1. Preoperational stage (geological-prospecting work, oil-field construction etc.).
2. Operational stage (oil extraction, oil processing, oil transportation and oil storage).
Fig. 1. Geocological risk estimation
Fig. 2. Geocological risk-analysis of oil-fields exploitation with application of GIS
3. Afteroperational stage (conservation of oil well, land reclamation etc.).

Oil sector is a very opportune environment for existence, development and transformation of various risks. Natural risks are a separate group of oil sector risks. These risks exist beyond the human activity and industrial project, but may increase and transform into natural-anthropogenic in the process of human activity. Oil sector risk-analysis is developing very fast in the last decades.

Various methods of quantitative estimation and analysis of industrial accidents and risks of pipeline, oil storage and processing objects found their application at the biggest Russian oil enterprises. But cartographic risk-analysis of oil fields and service objects is not widespread popularized.

Objective reason of cartographic risk-analysis importance is that data variety of pollutants and risk recipients usually look like pile of tables, texts and circuitries. This form of geocological environment data representation is not practical for perception and usually many processes remain unanalyzed and do not cover of monitoring network or regulating documents.

Also, cartographic risk-analysis means risk differentiation:
1. Anthropogenic risks, for example, probable accidents on the oil-field construction objects, equipment failures as a result of spoilage in production or human factor.
2. Natural risks, for example, stability of the territory to oil pollution.

In terms of natural features of Saratov region, we can pick out following expected and real risks for oil fields exploitation:
- The risk of oil field impoundment in the issue of seasonal river water level fluctuations;
- The risk of oil field area flooding in the issue of Volgograd storage pound water level increasing;
- gravitational processes risks;
- abrasion activity risks;
- soil environment risks;
- dangerous atmospheric agents and processes;
- landscape features of the territory;
- risk of the territory pollution because of oil inrush;
- risk of fire-hazardous situation;
- fire or explosion risk because of the neighboring objects;
- accident risk because of staff carelessness or incompetence;
- subversive act risk etc.

Many-sided cartographical risk-analysis is able to influence making decision process during risk situation on any stage of the oil sector’s functioning.

GIS using in risk mapping process

Geoinformation mapping as a one of the GIS tools, is a long-range trend to achieve aims of rational nature management and security policy.

Geographical information systems (GIS) make it possible do following things:
– simplify and sort out information gathering and storage;
– carry out information editing with the help of data base and distributed database management system implementation;
– actualize information with the help of remote sensing data;
– organize the whole spatial data analysis for general and applied problem solving;
– carry out geoecological monitoring;
– model development and ways of prevention of dangerous geoecological phenomena;
– make cartographical visualization in a traditional paper-maps style and digitally (electronic maps, cartographical animations, anamorphoses, etc.).

Fig. 3. Geoecological risk management subunit structure
Most of the projects that use GIS facilities, take inventory or management aims. But GIS facilities found their application in nature conservation activity on the oil sector objects. Monitoring aims that are being solved with the GIS hardware and software complex, are capable of reducing negative influence of oil industry on natural environment and people. That is why the development of the integrated geoecological risk management module was suggested (fig.3).

The principal features of this integrated GIS module are:

1. Spatial and attributive geoecological data bases. Those bases contain remote sensing data (aero- and spacephotos of high and ultrahigh resolution), Global Positioning System (GPS) data (position data of model areas), photo and video information showing the present geoecological condition of the territory.

2. Risk modeling subunit with cartographic information, that shows natural and anthropogenic risks within the research area.


4. Estimated and expected risk maps.

The other feature of this system is that it can be used both as separately based on MapInfo 8.5. platform, and integrated to other oil field GIS of Saratov region.

References:


The applications for collection and visualization of data received from the wireless sensor network were developed during this study. It was designed to make it easier for scientists, researchers and other, who have may little or no computer programming practice, to modify and extend applications that collect sensor data over long period of time. In research Sun Small Programmable Object Technology (SPOT) hardware platform was used.

Sun SPOTs are small, Java-based, wireless devices developed at Sun Labs. Standard Sun SPOT development kit consists of one basestation unit and two free-range SPOT units. Basestation has an eSpot main board without a battery or an application board. The eSPOT main board contains the main processor – 180MHz 32 bit AT91RM9200, 512K RAM, 4M Flash, 2.4GHz IEEE 802.15.4 radio with integrated antenna and AT91 timer chip. Power is supplied by a USB connection to a host workstation. The basestation serves as a radio gateway between other Sun SPOTs (and theoretically other 802.15.4 devices) and the host workstation. The structure of eSPOT main board shown on Fig. 1.

![Fig. 1. Structure of eSPOT main board.](image-url)
The free-range SPOT contains the main board with a rechargeable LI-ON prismatic battery and an example of the eDEMO board. On Fig. 2 there is a structure of eDEMO board. It contains a 2G/6G three-axis accelerometer, temperature sensor, light sensor, 8 tri-color LEDs, 6 analog inputs, 2 momentary switches, 5 general purpose I/O pins and 4 high current output pins.

The Software of SPOTs consists of Squawk VM – Java Virtual Machine for Sun SPOTs that enables to run Java applications on Sun SPOTs and SPOT device library which used by SPOT applications. The library contains drivers for:
- the on-board LED;
- the PIO, AIC, USART and Timer-Counter devices in the AT91 package;
- the CC2420 radio chip, in the form of an IEEE 802.15.4 physical interface;
- an IEEE 802.15.4 MAC layer;
- an SPI interface, used for communication with the CC2420 and off-board SPI devices;
- an interface to the Sun SPOT’s flash memory (Sun Labs, 2009, p. 33).

Besides described above hardware and software in work was used the ant utility, integrated development environment NetBeans 6.7 and Solarium java application. The ant used for building, deploying and running applications in Sun SPOTs. Solarium used to remotely manage a network of Sun SPOTs: it discovers and displays SPOTs that are connected to the desktop via USB or can be reached via radio communication, interacts with SPOTs and provides a special deployment view to manage network of Sun SPOTs (Sun Labs, 2009, p. 14).

Fig. 2. Structure of the eDEMO board
The idea of developing the applications for collection of data from wireless sensors was implemented by using base Sun SPOT library. There are two logic parts of developed applications: the first part represents the application for free-range SPOT unit for gathering data from sensors and sending it to another Sun SPOT or basestation SPOT over the «radiogram» protocol. The second part represents a number of running on host computer applications, that receives data from remote Sun SPOTs over basestation unit. As a result obtained the system of monitoring, collection and visualization of data from wireless sensors.

The algorithm of working of free-range SPOT application is this. At first the program starts and opens a connection with another free-range SPOT or basestation SPOT. To establish a point-to-point connection both ends must open connections specifying the same port number (value of DATAPORT in the text of program) and corresponding IEEE addresses (value of IEEEAddress).

Port numbers between 0 and 31 are reserved for system services (Sun Labs, 2009, p. 38). By default these ports are not using by applications, because their using may lead to conflicts. It is also possible to configure application in broadcast mode, where radiograms are delivered to all listeners on the given port. Making different combinations of IEEE addresses in the text of program (after that the program must be rebuild) it is possible to realize such wireless sensor network topologies as star and cellular topology.

![Diagram of wireless sensor network](image)

**Fig. 3. Possible location of wireless sensors**

On Fig. 3 shown an example of configured sensor wireless network. The circles are free-range SPOTs and red circles are free-range SPOTs in broadcast mode. Black lines mean that the data is transmitting or receiving, otherwise the lines are red.
The key moment in configuring the topology of wireless network is preventing data leakage. On the level executing program this situation is excluded and the data leakage occurs only if Sun SPOT was placed too remotely from another destination SPOTs or basestation unit.

After configuring sensor network free-range SPOT’s application initializes temperature sensor, light sensor and accelerometer. Then followed the main loop of program, during which all values of from sensors transmit every intervals of time that are specified in the program. The minimum value of that interval for correct working is $10^{-3}$ seconds. The temperature sensor works correct in the temperature range -40 to +125 degrees Celsius with an accuracy of 0.25 degrees Celsius. The light sensor returns an integer that ranges from 0 to 750. The one of this value corresponds the 2 lx. Zero represents complete darkness. Peak sensitivity of light sensor is at 600 nm wavelength (Sun Labs, 2009, p 24).

Not only values of luminance, temperature and acceleration sent, there is also sent the value of SPOT’s speed, despite the fact that there is no speedometer in device. Because the definite integral of acceleration at a given time interval is the value of average speed on that time interval it is possible to calculate speed of device in 3 planes knowing the acceleration in this planes. By default the value of that time interval is $10^{-2}$ seconds.

The algorithms of working on host computer desktop applications are alike each other with some differences. In all developed desktop applications the first step is configuring the basestation in server mode (by default), where any radiogram sent on the given port will be received. After receiving data there are several options in different applications.

In the first program all received data displays on terminal. The second realized application has graphic user interface for visualization of data. It creates one window with graph for each instance of transmitting wireless sensor, not free-range device. For example, if one Sun SPOT transmits values of the light sensor and the temperature sensor, and another SPOT transmits values only of the temperature sensor, in total will be created 3 windows with graphs. The last developed application collects receiving from sensors values in database. In this work used a bundle of MySQL database and Glassfish with JDBC driver. All data saves in tables and after that enable to get text and graphic information about any period of receiving of data.

As a result of done work obtained the applications, that are easy to use, modify and extend. But there is another aspect to which attention should be paid. Sun SPOTs are also the objects of academic interest in the sense, that all programs for SPOTs execute on Java Virtual Machine, that runs on the bare metal. The Squawk VM is the result of an effort to write a J2ME CLDC compliant JVM in Java that provides OS level mechanisms for small devices, easing porting and debugging of the VM. The Squawk Virtual Machine has been open sourced and is hosted at http://squawk.dev.java.net, where everyone can get access to all of the source code.
The architecture of the Squawk VM was inspired in part by the Squeak and Klein VM architectures. In particular, it is mostly implemented in the language that it executes. The Squawk Java VM mostly written in Java (most virtual machines are written in low level languages such as C and assembler) and that is why it has a high portability. The Squawk bytecodes are a compact version of Java bytecodes and were optimized for space, in-place execution and to simplify garbage collection (Doug Simon, 2002, p. 2). Squawk supports interrupts written in Java. Also Squawk implements an isolation mechanism, can run multiple applications in the one VM, and can migrate applications to another machine that runs the same VM (Doug Simon, 2006, p. 3).

Of course, availability of listed up features increases performance of Sun SPOT device. But there are some ambivalent moments. First the Squawk's approach to supporting interrupts and doing garbage collection, which while making programming easier and less error prone in Java, play havoc with the ability to perform deterministic control operations. Second, Squawk is based on the J2ME virtual platform, which is neither real time nor deterministic and more appropriate for cell phones. For these reasons it is impossible to say, that Sun SPOTs work in real time mode.

So, during this research were developed easy-to-use and high performance applications on the basis of modern and available Java-technologies, that may be successfully used in problems of gathering and analysis large volumes of data from remote sensors.

References:

Surface acoustic wave, phase velocity, rotation, Coriolis force, high accuracy

Surface acoustic wave (SAW) devices are widely applied in moving objects for carrying out of coordinates, velocities, accelerations and electromagnetic signal parameters accurate measurements. It’s known that the rotation influences upon a phase of resonance structure mechanical oscillations and on ultrasonic wave velocity [1]. SAW device rotation leads to SAW phase velocity deviation. In order to meet the demand of phase velocity stability in high accuracy modern SAW devices it’s required to carry out exact numerical analysis of phase velocity deviation arising in SAW devices under rotation.

In order to calculate phase velocity change in SAW device under rotation it’s necessary to introduce Coriolis force into the piezoelectric medium movement equations and into the boundary conditions on surface of piezoelectric crystal.

The piezoelectric medium movement equations can be expressed as [2]:

$$\rho \ddot{u}_i = c_{ijlm} \partial_j \partial_l u_m + e_{lij} \partial_j \partial_l \varphi,$$

where $\rho$ is the crystal density, $u_i$ are the elastic displacement components, $c_{ijlm}$ are the elastic constants, $e_{lij}$ are the piezoelectric constants, $\varphi$ is the scalar electric potential, $\partial_i$ is the differentiation operator. In these equations, the summation convention for repeated indices is employed and the tensors are expressed by Einstein’s expression.

The Coriolis force is [3]:

$$\ddot{K} = 2\rho \dot{v} \ddot{\Omega},$$

and it’s components take the form:

$$K_m = 2\rho \epsilon_{mjk} \dot{u}_j \Omega_k,$$

where $K_m$ are the Coriolis force components, $\epsilon_{mjk}$ are the Levi-civita tensor components, $\Omega_k$ are the angular velocity vector components.

Then, the modified piezoelectric medium movement equations under rotation can be written as:
\[ \rho \ddot{u}_i = c_{ijklm} \partial_j \partial_l u_m + e_{ijk} \partial_j \phi + 2 \rho \partial_j \dot{u}_j \Omega_k. \]  

(3)

For the plane harmonic wave the elastic displacement components and the scalar electric potential can be expressed in the forms:

\[ \{\ii, \phi\} = \{-i, \bar{\phi}\} \exp \left( \omega \cdot \begin{pmatrix} m \\ m \end{pmatrix} \right). \]  

(4)

Substituting (4) into (3), we obtain the following four linear equations for the four undetermined constants \( \vec{u}_i \) and \( \bar{\phi} \):

\[ \left( \rho \omega^2 \delta_{im} - c_{ijklm} k_j k_i + 2i \rho \omega e_{ijm} \Omega_j \right) \vec{u}_m - e_{i\ell} k_j k_i \bar{\phi} = 0. \]  

(5)

The mechanic boundary conditions on surface of piezoelectric crystal can be expressed as [2]:

\[ \sigma_{i3} = 0, \]  

(6)

where \( \sigma_{ij} \) is the Cauchy stress tensor components.

As Coriolis force acts upon the moving medium particles located on crystal surface \( (x_3 = 0) \) on the part of all the moving medium particles under crystal surface \( (x_3 < 0) \) the conditions of free surface equilibrium can be written as:

\[ \sigma_{i3} + \int_{-\infty}^{0} F_{\text{Cor},i} (x_3) dx_3 = 0. \]  

(7)

The four-component SAW elastic displacement components can be expressed as

\[ U_j = \sum_{\nu=1}^{4} u_j^{(\nu)} = \sum_{\nu=1}^{4} P_{j\nu} \phi_{\nu}, \]

where \( U_j \) are the SAW elastic displacement components, \( u_j^{(\nu)} \) are the SAW partial mode elastic displacement components, \( P_{j\nu} \) are the polarization coefficients, \( \phi_{\nu} \) are the partial scalar electric potentials.

The mechanic boundary conditions on surface of piezoelectric crystal under rotation can be expressed as:

\[ \sum_{\nu=1}^{4} \left( e_{i3lm} P_{mv} + e_{i\nu3} \right) (-ik_1^{(\nu)}) \phi_{\nu} + \int_{-\infty}^{0} F_{\text{Cor},i} (x_3) dx_3 = 0. \]  

(8)

Coriolis force acting on particles which participate in the four-component SAW movement can be expressed as:

\[ F_{\text{Cor},i} = 2 \rho \varepsilon_{ijk} \dot{U}_j \Omega_k = i2 \rho \omega \varepsilon_{ijk} \Omega_k \sum_{\nu=1}^{4} u_j^{(\nu)} = i2 \rho \omega \varepsilon_{ijk} \Omega_k \sum_{\nu=1}^{4} P_{j\nu} \phi_{\nu}, \]

then
\[ \int_{-\infty}^{0} F \cos(x_3) dx_3 = -2 \rho \omega e_{ijk} \Omega_k \sum_{v=1}^{4} \frac{P_{j\nu}^{(v)}}{k_3^{(v)}} \phi_v, \]

and on the basis of (8) we can write:

\[ \sigma_{i3} = -i \sum_{v=1}^{4} \left( c_{i3h} P_{mv} + e_{l3} \right) k_j^{(v)} \phi_v - 2 \rho \omega e_{ijk} \Omega_k \sum_{v=1}^{4} \frac{P_{j\nu}^{(v)}}{k_3^{(v)}} \phi_v = 0, \quad (9) \]

Then, the mechanic boundary conditions on surface of piezoelectric crystal under rotation (8) can be written in the form:

\[ \sum_{v=1}^{4} \left( c_{i3h} P_{mv} + e_{l3} \right) k_j^{(v)} \phi_v - i2 \rho \omega e_{ijk} \Omega_k \frac{P_{j\nu}^{(v)}}{k_3^{(v)}} \phi_v = 0. \quad (10) \]

The strict decision of a boundary problem for the Maxwell equation \( \text{div} \mathbf{D} = 0 \) and the piezoelectric medium movement equations (3) with boundary conditions for the electric field and the elastic stress is obtained based on invariant algorithm [4], including Coriolis force effect.

Calculations have been carried out for phase velocity deviation in ST-cut quartz-based SAW device operating at 30 MHz under rotation with angular velocity 360º/s. We chose the frequency 30 MHz because it’s the lowest operating frequency on SAW devices. Phase velocity change effect is inversely proportional to operation frequency and it’s essentially proportional to angular velocity. Figure show the results of the calculation for the angular velocity vector orientation across the device base planes.

![Diagram](image)

Phase velocity deviation in ST-cut quartz-based SAW device operating at 30 MHz under rotation with angular velocity 360º/s for the angular velocity vector orientation across the device base planes.

We can conclude, that phase velocity relative deviation arising in SAW devices under rotation with angular velocity 360º/s can achieve the value of
10^{-8}. Whereas a phase velocity stability requirement of a SAW device is 10^{-11}. Therefore in order to prevent such phase velocity deviation in high-accuracy modern SAW devices it’s necessary to use high frequencies and to choose the spatial orientation of SAW device in moving object.

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**PARTIAL GENERALIZED SYNCHRONIZATION IN GINZBURG-LANDAU EQUATIONS**

*N. Phrolov*

*Saratov State University*

Generalized synchronization, chaos, self-oscillated systems, Ginsburg-Landau equations

Synchronization of chaotic oscillations is one of the most important fundamental nonlinear phenomena. On the one hand, extensive studies in this area improve theoretical understanding of the general laws governing the interactions between complex nonlinear systems of different (chemical, physical, biological etc.) nature. On the other hand, the practical applications of these studies include information transmission technologies using deterministic chaotic oscillations, dynamics of neural ensembles, disease diagnostics, etc.

One of the most important examples of chaotic synchronization is generalized synchronization of chaotic oscillators, which is defined as appearance of functional relation between the states of coupled systems with increase of relation between systems [2]. Generalized synchronization is traditionally applied for systems with a low number of degrees of freedom and unidirectional relation [2], when one of subsystems appears as drive, interacts with response generator and suffers no feedback. The research of generalized synchronization of coupled distributed self-oscillating systems demonstrating space-time chaos took place in the number of works [2, 4]. Coupled unidirectional Ginsburg-Landau equations were selected as the object of these researches [3]:
\[ \begin{align*}
\frac{\partial u}{\partial t} &= u - (1 - i\alpha_d)\|u\|^2 u + (1 + i\beta_d) \frac{\partial^2 u}{\partial t^2}, \\
\frac{\partial v}{\partial t} &= v - (1 - i\alpha_r)\|v\|^2 v + (1 + i\beta_r) \frac{\partial^2 v}{\partial t^2} + \varepsilon H(t - \tau) F[u, v],
\end{align*} \tag{1} \]

\[ \begin{align*}
\frac{\partial v_a}{\partial t} &= v_a - (1 - i\alpha_r)\|v_a\|^2 v_a + (1 + i\beta_r) \frac{\partial^2 v_a}{\partial t^2} + \varepsilon H(t - \tau) F[u, v_a].
\end{align*} \tag{3} \]

\(u\) – drive system, \(v\) – response system, \(\alpha_d, \alpha_r, \beta_d, \beta_r\) - system parameters, \(F[u, v]\) – coupling function.

In similar case the increasing of coefficient \(\varepsilon\) involves the establishing of functional relation between space-time states of systems \(v(x,t) = G(u(x,t))\).

To detect generalized synchronization in distributed systems, we apply the auxiliary system method. In this method, an auxiliary system identical to the response system is considered.

The initial state of the auxiliary system is different from the initial state of the response system, but lies in the same basin of attraction. When the coupled systems are not synchronized, \(x_r\) and \(x_a\) are different state vectors belonging to the same chaotic attractor. In a generalized synchronization regime, since the relation \(x_r = F(x_d)\) entails \(x_a = F(x_d)\) the states of the response and auxiliary systems must become identical \((x_r \equiv x_a)\) after the initial transients have died out.

In connection with observing of distributed self-oscillating systems demonstrating space-time chaos, there appears possibility of observing of generalized chaotic synchronization between different parts of active medium.

Let us consider Ginsburg-Landau equation with periodic boundary conditions \(u(0,t) = u(L,t)\) in the capacity of active medium. We can divide this medium in two parts \(u_1\) and \(u_2\) with lengths \(L_1\) and \(L_2\) properly \((L = L_1 + L_2)\) and suggest that functional relations can be reached between the whole system and on of its parts, for example between \(u\) and \(u_1\). It is possible to diagnose generalized synchronization between these two parts (the regime of partial generalized synchronization), applying the auxiliary system method and comparing behavior of auxiliary and drive systems in \(L_2\) area. In this case the criterion of partial generalized synchronization becomes the expression:

\[ u(x,t)\big|_{x \in L_2} = u_a(x,t)\big|_{x \in L_2}. \tag{4} \]

To observe the regime of generalized synchronization, it is necessary to consider auxiliary system with boundary conditions:
\[ \frac{\partial u_a}{\partial x} \bigg|_{x=0} = \frac{\partial u}{\partial x} \bigg|_{x=0}, \quad \frac{\partial u_b}{\partial x} \bigg|_{x=L_2} = \frac{\partial u}{\partial x} \bigg|_{x=L_2}. \] (5)

It is necessary to solve the equation (3) with conditions (5) to model this system. Modeling shows the balance between \( L \) and \( L_1 \) in which partial generalized synchronization is reached. Results of modeling are presented on the picture 1 (a,b).

There are two modes on these graphics: behavior of system parts is equal to each other in \( L_1 \) area \((0<x<L_1)\) and further behavior in \( L_2 \) area \((L_1<x<L)\).

As it was ascertain during the research, appearance of synchronization regime depends on values \( L \) and \( L_1 \). If \( L_1 \) is selected so that there is no synchronization between systems than gradual increasing of \( L_1 \) allows us to come to partial synchronization (in this case \( L_1 = R_i \) is the border of length of synchronization). This research shows that increasing of \( L \) involves increasing of \( R_i \).

![Fig. 1. Space-time distribution of states difference: a) Deficiency of synchronization, b) Appearance of synchronization](image1)

![Fig. 2. Dependence Ri on L](image2)
Given research shows that there is a possibility of considering generalized synchronization between different parts of active medium in systems demonstrating space-time chaos.

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WAVEGUIDING PROPERTIES OF PHOTONIC CRYSTALS

A. Plastun, A. Konyukhov
Saratov State University

It is generally assumed that photonic crystals are attractive optical materials for controlling and manipulating the flow of light. One-dimensional photonic crystals are already in widespread use in the form of thin-film optics with applications ranging from low and high reflection coatings on lenses and mirrors to colour changing paints and inks. Higher dimensional photonic crystals are of great interest for both fundamental and applied research. The first commercial products involving two-dimensionally periodic photonic crystals are already available in the form of photonic-crystal fibers, which use a micro scale structure to confine light with radically different characteristics compared to conventional optical fiber for applications in nonlinear devices and guiding exotic wavelengths. The three-dimensional photonic crystals offer additional features which may lead to new device concepts (for example optical computers), when some technological aspects such as manufacturability and principal difficulties such as disorder are under control.

So, here the question arises: What are the main principles of this technology? The base of the photonic crystal is Bragg reflection, or reflection from multilayer structure (Fig.1). In other words, when light strikes on the single layer, there is only one reflected ray. When light strikes on the multilayer structure there is a load of rays. The number of them depends on the number of layers (actually, number of boundaries between them). Figure 1a shows reflection from glass plate (single layer). Figure 1b shows Bragg reflection from stack of glass plates (multilayer structure).
Two multilayer structures form photonic crystal waveguide (Fig. 2). Electromagnetic wave propagates inside the core of this object due to the Bragg reflection from cladding.

This structure may be 1-dimensional, 2-dimensional and 3-dimensional. 1-dimensional structure can be used as a multilayered mirror (fig. 1b). Figure 3a shows dielectric mirror for He-Ne laser. In order to produce multilayered mirror the film deposition on the glass substrate is used. The SiO$_2$ film has the refractive index 1.45 and TiO$_2$ film has refractive index 2.5. Alternated SiO$_2$ and TiO$_2$ layers form the high-reflecting mirror for selected range of wavelength.

2-dimensional (2D) structure is formed by the closely packed array of thin tubes, cylinders or array of air holes in bulk glass. Figure 3b shows the array of closely packed thin cylinders. The microscopic image (fig. 3c) reveals hexagonal structure of photonic crystal. The 2D photonic crystal can be drawn into the fiber (fig. 3d). The microscopic image of the fiber cross-section is shown in the fig. 3e. The characteristic size of each element is 20 μm.

3-dimensional photonic crystals consist of an array of closely packed bubbles, rods or spheres. Each element of photonic crystal should have wavelength-compatible characteristic size.
There are two types of Photonic Crystal fibers. The first type has the solid core surrounded by air holes (fig. 4a) or low-index photonic crystal structure. The second type has the hollow core formed by defect in the periodic structure (fig. 4b).

Solid core Photonic Crystal fiber (PCF) is used in non-linear optical applications and devices. High index contrast between the glass core and air holes allows concentrating a laser beam in the micron sized area. A very high energy concentration amplifies nonlinear processes in the PCF core. Due to the high nonlinearity the optical spectrum of laser pulses can be spread into the visible spectrum – supercontinuum. We share the opinion that supercontinuum sources can be used in spectroscopy [2], optical tomography, and optical frequency metrology [3].

In Hollow core photonic crystal fibers the light beam is localized in the air core. Due to the low nonlinearity of the air hollow core photon crystal can be used for guiding pulses and beams having extremely high energy level [4]. In paper 5 sequences of picoseconds pulses of 1.06-μm Nd:YAG laser radiation with a total energy of ~2 mJ are transmitted through a hollow-core photonic crystal fiber with a core diameter of ~14 μm and they are focused onto a tooth’s surface in vitro to ablate dental tissue. Also, we consider that the hollow core PCF may be used as a gas-sensor. It’s aiming at the high sensitivity gas detection is proposed.[6]
The propagation of electromagnetic waves in photonic crystal structure (Fig. 5) is described by Maxwell equations [4]. For transverse electric field the Maxwell equations are reduced to Helmholtz-type equation:

$$\frac{d^2 E_y}{dx^2} + k^2 n^2(x) E_y = \beta^2 E_y,$$

(1)

where $k = \omega/c$ is the wavenumber of free space, $c$ is the light velocity, $n(x)$ is the refractive index.

The equation (1) was solved using Fourier transformation of $n^2(x)$ and $E_y(x)$ (plane-wave method). The results of the numerical solution are shown on the fig.6.
Fig. 6. Numerical solutions of the eigenvalue equation. Effective refractive index is $n_{\text{eff}} = \beta / k$. Structure parameters (a) $a=0.28 \ \mu\text{m}, \Lambda=1.12 \ \mu\text{m}$; (b) $a=0.2 \ \mu\text{m}, \Lambda=0.8 \ \mu\text{m}$. Dashed lines show refractive indices $n_{\text{high}}=2.8$, $n_{\text{low}}=2.7$. The material dispersion was not taken into account.

The region $n_{\text{low}} < n_{\text{eff}} < n_{\text{high}}$ corresponds to supermodes which are the superposition of fundamental modes of individual waveguides. These modes are guided by the total internal reflection. Intensity profiles of two supermodes are shown in the fig.7.

Fig. 7. Refractive index (left vertical axis) and mode profiles (right vertical axis). Field frequency is $\omega=1.216 \ \text{fs}^{-1}$ (wavelength is $\lambda=1.55 \ \mu\text{m}$).

Bottom curves in Fig.8 correspond to the modes bounded by the central low-index defect. These modes arise within the bandgap of the periodical structure. The mode is localized around structure defect (fig.8).
So, we have given a short review of optical properties of photonic crystals. The practical use of photonic crystals in light controlling devices is considered. The results of numerical simulation wave guiding properties of planar (1D) photonic crystal are presented here. We are convinced that they have a great practical use.

References:

THE DISPERSION CONTROL
OF OPTICAL MICROSTRUCTURED FIBER

A. Sadovnikov, A. Rozhnev

Saratov State University

Dispersion control, photonic crystal, microstructured fiber, Plane Wave method, Finite-Element method, supercell method

We report the control of dispersion in the optical fiber with photonic crystal cladding. The specific type of fiber is considered. The structure of fiber cladding is comprised of the hexagonal lattice of rods with finite wall thickness. We have assumed in our computations the complicated triangle-form area in the transverse section of fiber that appears during the manufacture process. We have demonstrated that dispersion slope and absolute value of dispersion coefficient of MFs can be controlled with a variation of geometrical parameters of fiber cladding. The Finite-Element method and the Plane Wave method with a supercell modification is applied to compute the dispersion.

The optical fiber with photonic crystal cladding provide new approaches for achieving single transverse mode guiding in large core fibers. Such fiber often is named [Zheltikov, A.M. “Nonlinear optics of microstructure fibers,” Phys. Usp., Vol. 147, No. 1, 2004.] microstructured fibers (MF). There are many applications of MF in fiber-optic communications, fiber lasers, nonlinear devices, high-power transmission devices, ultra-broad supercontinuum generation and broadband dispersion compensation. MF with a solid core, which has a higher average index than the microstructured cladding, can operate on the same index-guiding principle as an ordinary optical fiber. Such fiber exhibit novel dispersion properties such as ultra-flat dispersion over broad wavelength range [Saitoh, K., M. Koshiba, T. Hasegawa and E. Sasaoka, “Chromatic dispersion control in photonic crystal fibers: application to ultra-flattened dispersion,” Optics Express, Vol. 11, No 23, 843-852, 2003.]. We considered the MF with the hexagonal lattice of rods with finite wall thickness in the fiber cladding. Thereby we assumed the complicated triangle-form area in the transverse section of MF that usually appears during the manufacture of such fiber. The control of dispersion in fiber has been demonstrated by variation of geometrical parameters of fiber such as size of an air-hole defect in the fiber core and distance between holes. The effect of varying cladding parameters is estimated to find the trends of the decrease of dispersion slope and control of absolute value of dispersion coefficient and then applied to the design of an ultra-low, ultra-flattened chromatic dispersion photonic-crystal fiber.

We consider the MF that has a transverse section consisting of a hexagonal lattice of rods with finite wall thickness (fig. 1a). The number of rings of rods
is assumed to be 3. The radius of the air-holes is $r$ and the lattice pitch (the distance between air-holes) is $\Lambda$.

Fig. 1. a) The transverse section of fiber that has produced of rods with finite wall thickness. b) The intensity distribution of transverse electric field for $E_x$-mode in the core of fiber

The numerical modeling of microstructured fiber was performed using two methods, namely finite-element method (FEM) and the plane-wave method (PWM). The former assumed the explicit frequency or wavelength dependence of the refractive index. The latter was applied with the supercell modification and the material dispersion wasn’t assumed explicitly. However we summed the waveguide (geometrical) dispersion $D_w(\lambda)$ obtained by PWM and the material dispersion $D_m(\lambda)$ obtained by Sellmeier’s equation [5] and the dispersion coefficient $D(\lambda)$ is then calculated as

$$D(\lambda) = D_w(\lambda) + D_m(\lambda), \quad (1)$$

where waveguide and material dispersion are calculated with

$$D_w(\lambda) = -\frac{\lambda}{c} \frac{d^2 n_{\text{eff}}(\lambda)}{d\lambda^2} \quad \text{and} \quad D_m(\lambda) = -\frac{\lambda}{c} \frac{d^2 n_{\text{Si}}(\lambda)}{d\lambda^2}$$

respectively, $n_{\text{eff}}(\lambda)$ is the effective refractive index of the fundamental mode in MF, $n_{\text{Si}}(\lambda)$ is the refractive index of silica, $c$ is the speed of light in vacuum.

$$D = -\frac{\lambda}{c} \frac{\partial^2 n_{\text{eff}}}{\partial \lambda^2}. \quad (2)$$

For the computation with finite-element method the program for calculation of eigenmodes dispersion of the transmission line with complicated transverse section [3] was applied. The plane-wave simulation was done by MPB (MIT Photonic Bands) package [4]. Simulation was conducted by these methods to investigate the effect of varying $r$ and $\Lambda$.

The field distribution and polarization of electromagnetic field mode are shown in Figure 1b. This mode is polarized along the horizontal axis and
the results for other mode that polarized along vertical axis is omitted. The electromagnetic field energy is localized in the fiber core. It can be seen from Figure 1b, where the intensity of transverse electric field is depicted with shades of gray.

Fig. 2a shows the calculated dispersion curves for wavelength range from 0.8 to 1.7 μm for different values of distance between air-holes Λ. The dispersion curve of Λ = 1.84 μm (bold curve 3 in fig. 2a) demonstrate that there is the wavelength range 0.9 < λ < 1.1 μm with the small change in the dispersion coefficient D and the absolute value of D lies in the interval 0 < D < 7 ps/(nm·km). Figure 2b demonstrates that dispersion coefficient decreases with decrease of air-hole radius r and that there is a flat region offset in the range of shorter wavelengths.

Fig. 2. Family of dispersion curves with various a) lattice pitch: 1 – Λ = 3.68 μm; 2 – Λ = 2.76 μm; 3 – Λ = 1.84 μm and with r fixed at 0.4968 μm; b) radius 1 - r = 0.53475 μm; 2 – r = 0.4968 μm; 3 – r = 0.4485 μm and Λ fixed at 2.76 μm. Computational results obtained with plane-wave method denoted with solid lines and finite-element method – with dashed lines

However, using a MF with all of the same air-hole diameter in the fiber cladding, it is difficult to control both the absolute value of dispersion coefficient and dispersion slope in wide wavelength range. An recent publication by Saitoh et al. [2] have reported that there is a new controlling technique of chromatic dispersion in MF. It is shown from numerical results that it is possible to design MFs with both ultra-low dispersion and ultra-flattened dispersion in a wide wavelength range. We have applied this method of dispersion controlling for our system. The hole radius of each air-hole ring in the fiber cladding increases 20% from hole ring to ring relative to the first one. Figure 3a shows the result of calculation for the system with different air-hole radii of each air-hole ring: the dispersion of the system with radius
increases 20% from row to row denoted with dashed lines, for the system without air-hole radius difference the dispersion curve denoted with solid lines. The simulation was done for systems with different air-hole radius in the first ring. It was shown (curve 4 in fig. 3a) that this method can be used for control the dispersion slope of MF.

The control of chromatic dispersion in optical microstructured fiber can be done with doping the center part of the fiber with $\text{GeO}_2$ [6]. We have demonstrated that the increase of mol fraction of $\text{GeO}_2$ [7] in the silica core of our type of MF shift down the dispersion curve and it is possible therefore to design the MF with small value of dispersion coefficient in the definite wavelength range ($1.0 < \lambda < 1.05 \mu m$) as shown in fig. 3b (bold curve 2).

![Dispersion Curves](image)

**Fig. 3.** a) Family of dispersion curves with various air–hole radius $1 – r = 0.345 \mu m$; $2 – r = 0.2875 \mu m$; $3 – r = 0.2 \mu m$; $4 – r = 0.1725 \mu m$. The computational result for the system with radius increase 20% from row to row denoted with dashed lines, while solid lines denotes the system without such radius increase. $\Lambda = 2.3 \mu m$. Finite–element method. b) Family of dispersion curves with various mol fraction of $\text{GeO}_2$: $1 – x = 0$; $2 – x = 0.056$; $3 – x = 0.15$; $r = 0.4968 \mu m$. $\Lambda = 1.84 \mu m$. Plane-wave method

We have shown that the variation of geometrical parameters of optical microstructured fiber can modify the dispersion properties of such system. The Finite-Element method and Plane-Wave method have been applied. We have considered the structure of fiber cladding that is comprised of the triangular lattice of rods with finite wall thickness. We have demonstrated that dispersion slope and absolute value of dispersion coefficient of MFs can be controlled with a change of size of an air-hole defect in the fiber core, with variation of interval between holes and with a doping the center part of the fiber with $\text{GeO}_2$. Simulations and estimations shows that one can construct a system based on microstructured-fibers with minute difference of dispersion coefficient in the operating range of wavelength and dispersion control can help to improve transmission speeds and distances.
This study was supported by the Russian Foundation for Basic Research (Project No. 08-02-00621) and the Program “The Development of Science Potential of the Higher School” (Project No. 2.1.1/1738).

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DYNAMICS OF THE COUPLED NEARLY CONSERVATIVE SYSTEMS

D. Savin
Saratov State University

Henon maps, coupled systems, weak dissipation, transition to chaos, critical behavior, multistability

Systems with very small dissipation are known to demonstrate very interesting behavior (Feudel et al., 1996; Kuznetsov et al., 2008-I). It seems quite interesting to investigate the model of the nearly conservative coupled systems. The coupling should be conservative because phenomena typical for the systems with very weak dissipation are the subject of our interest. The present work is concerned to the dynamics of the coupled Henon maps

\[ x_{n+1} = \lambda_1 - x_n^2 - by_n + \varepsilon(x_n - u_n), \]
\[ y_{n+1} = \lambda_2 - y_n^2 - bx_n + \varepsilon(y_n - x_n), \]
\[ u_{n+1} = \lambda_3 - u_n^2 - b\varepsilon_y + \varepsilon(u_n - x_n), \]
\[ v_{n+1} = \lambda_4 - v_n^2 - b\varepsilon_x + \varepsilon(v_n - x_n), \]

The Jacobian of this map is equal to \( b^2 \), hence this map is conservative when subsystems are conservative. Parameter \( \varepsilon \) is further fixed and equal to 0.4.
Evolution of the \((\lambda_1, \lambda_2)\) parameter plane while the dissipation decreases is shown in the fig. 1. When \(b=0\), system (1) turns into the system of two logistic maps with the symmetric coupling. For this system two ways to chaos coexist (Kuznetsov et al., 2008-II). – transition via period-doubling bifurcations and via the destruction of the quasiperiodic motion. We can see that the decrease of dissipation leads to the sufficient changes of both these scenarios. The region of quasiperiodic dynamics, which for the logistic maps is located near the diagonal of the parameter plane, becomes very narrow and shifts into the region, where \(\lambda_1\) and \(\lambda_2\) are sufficiently unequal. The synchronization tongues also undergo some transformations. The transition to chaos via period-doubling bifurcation undergoes more sufficient changes. Starting from certain dissipation level period-doubling lines begin to flex and then the Feigenbaum line ruptures (fig. 2). It causes the formation of a big number of bifurcation lines and bifurcation structures such as crossroad area and spring area. The phase space divides into several multistability sheets. We call this situation “bifurcation burst”. In fact, the transition to chaos becomes two-parameter. Fig. 3 shows the enlarged fragment of the chart of the dynamical regimes. Accumulation points for the sequences of so-called FF and R2-points (points with multipliers (+1, +1) and (-1, -1) respectively) are marked by rings and squares. The existence of such sequences allows us to expect the existence of critical points of C and H-type as their limit.

We have carried out a search of the critical point of the H-type. We have calculated the sequence of the R2 points for the first periods of the period-
doubling cascade with the help of the *Content* program package (table 1). *(Content* was developed by Dr. Yu. A. Kuznetsov for bifurcation analysis of dynamical systems.)
<table>
<thead>
<tr>
<th>Period</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>0.280808946</td>
<td>3.268918021</td>
</tr>
<tr>
<td>32</td>
<td>0.280380626</td>
<td>3.269091236</td>
</tr>
<tr>
<td>64</td>
<td>0.280292623</td>
<td>3.269104448</td>
</tr>
<tr>
<td>128</td>
<td>0.280284972</td>
<td>3.269106342</td>
</tr>
<tr>
<td>256</td>
<td>0.280283942</td>
<td>3.269106559</td>
</tr>
</tbody>
</table>

One can see, that the parameter values converge to the point $\lambda_1=0.280284\ldots$, $\lambda_2=3.269106\ldots$ and allow to appreciate the scaling constant as $\delta=8.79$ which is similar to the theoretically known for this criticality type value $\delta_H=8.7210662\ldots$ (Kuznetsov et al., 1997). To certify our assumption about the type of critical behavior we have calculated the multipliers of cycles of different periods in the critical point. This method is based on the fact that in the critical point all cycles of the period-doubling cascade should be unstable, and their multipliers are to be equal to the universal values, which are theoretically calculated for each type of the critical behavior. We can predict the location of the critical point by the scaling law and calculate the values of cycle multipliers in this point. In our case we calculated the multipliers for cycles of period 32 and 64 in the point $\lambda_1=0.280283808$, $\lambda_2=3.269106587$ and have obtained values $\mu_1=-2.06$ and $\mu_2=-0.48$ which approximately coincides with the theoretically known values: $\mu_1=-2.0574783\ldots$ and $\mu_2=-0.4860318\ldots$ (Kuznetsov et al., 1997). So, we can state that the critical point of the H-type exists as the terminal point of the Feigenbaum line in the system (1). Moreover, the symmetry of the structures on the parameter plane allows us to assume the existence of such critical point in the vicinity of the point $\lambda_1=0.1381$, $\lambda_2=3.2031$.

For investigation of the dynamics of the weakly dissipative system in the phase space we used the method of drawing bifurcation trees for a set of initial conditions on one diagram. Such bifurcation diagrams were drawn along the diagonal of the parameter plane (fig. 4). It turned out that the transient time does not increase so strong as for the 2D systems (e.g. for the Ikeda map, which was investigated in (Kuznetsov et al., 2008-I) in the case of the very weak dissipation). So, even at $b=0.999$ the transient time does not exceed 100000 iterations while for the Ikeda map it is near 1000000.

On these diagrams one can see the birth of new attractors while the dissipation decreases. E.g., at $b=0.7$ there is a number of attractors coexisting in the large range of parameters, and the decrease of dissipation leads to the growth of their number. Also we can see the chaos extinction in the
weakly dissipative system: the regions, where chaos exists, become narrow enough both in the phase and parameter space. On the other hand, one can see the chaotic attractors at the smaller values of $\lambda$, but their basins are rather small.

So, the investigation of the system of the coupled weakly dissipative maps was carried out in the present work. It was shown that the decrease of dissipation leads to the sufficient transformation of both bifurcation scenarios, which are typical for the coupled logistic maps. The Feigenbaum line ruptures, and a big number of the bifurcation lines birth. The existence in such system of the H-type critical behavior was shown.

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References:

SIMULATION OF THE ELECTRON MOTION IN A SEMICONDUCTOR SUPERLATTICE UNDER THE INFLUENCE OF THE EXTERNAL ELECTRIC AND TILTED MAGNETIC FIELDS

A. Selskii

Saratov State University

Semiconductor superlattice, drift velocity, tilted magnetic field, Bloch oscillation, collective behavior, dynamic chaos

In this work the dynamics of the electron in a semiconductor superlattice under the influence of the external electric and tilted magnetic fields is considered. The system of the differential equations describing the movement of the electron is derived. The trajectories and drift velocities of electron are computed. The results obtained in this work can be used for the detailed analysis of the dynamics of electron in the superlattice.

This work is devoted to study the non-linear processes in the semiconductor superlattice, namely, the simulation of the electron motion in the superlattice under the influence of the external electric and tilted magnetic fields. The most interesting result is the dependence of the drift velocity on the tilt angle of the magnetic field, since it allows to study the collective behaviour of the electrons.

The semiconductor superlattice is a complex nanostructure, which contains several interlaced subtle layers of the different semiconductor materials, for example GaAs and AlGaAs [1]. Due to the difference of the widths of the forbidden bands of used materials, conduction band of ideal semiconductor superlattice has the periodic structure. As a result, the tight energy band (mini-band) for charges is formed, with the charges moving in the direction orthogonal to the layer surface [2].

In Figure 1 the structure of semiconductor superlattice is shown schematically. The coordinate system illustrates the orientation of magnetic displacement vector $B$, placed in $x$-$z$ plane and tilted on angle $\theta$ about $x$-axis. The electric field $F$ is vectored in the direction being opposite to the $x$-axis [3].

The idea of the creation of the one-dimensional semiconductor superlattice was introduced by L. Esaki and R. Tsu in 1969 [4,5]. The superlattice may be considered as the structure for the experimental study of the various quantum-mechanical phenomena related with the resonance tunneling and Bloch oscillations.

Recently a new approach for application of semiconductor superlattice to the generation and controlling of terahertz signals has been proposed. The complex dynamic transport regimes associated with the dynamic chaos are supposed to be used.

The ratio of Bloch and cyclotron frequencies, which equivalent of the ratio of the magnitude of the electric and tilted magnetic fields (projective $z$-axis) plays the important role in the study of the semiconductor superlattice.
The system of dimensionless differential equations describing the movement of the electron has been derived
\[
\begin{align*}
\frac{dX}{d\tau} &= V_0 \sin(-P_z \tan \theta + f \tau + \varphi), \\
\frac{dZ}{d\tau} &= S P_z, \\
\frac{d^2 P_z}{d\tau^2} &= -\Omega^2 \cos^2 \theta P_z + A \Omega^2 \sin 2\theta \sin(-P_z \tan \theta + f \tau + \varphi).
\end{align*}
\] (1)

where \(X, Z\) are the electron coordinates; \(P_z\) – the component of the electron momentum; \(\tau\) – time; \(V_0, \theta, \varphi, S, \Omega, f\) – dimensionless parameters being defined by the dimensional parameters of the semiconductor superlattice and the external fields.

Having used system (1), we obtain the trajectories of the electron movement. Depending on the ratio of Bloch and cyclotron frequencies the periodic, quasi-periodic and chaotic dynamic regimes may be observed. The chaotic regimes may be localized or unlimited (in the case of the strong resonance) in the space. The different regimes are observed when the angle of magnetic field is changed.

The drift velocity of the electron in the semiconductor superlattice may be calculated with the help of the following expression:
\[
\nu_d = \left\langle \nu_x(t) \exp\left(-t/\tau_{sci}\right) \right\rangle/\tau_{sci},
\] (2)

where \(\nu_d\) is the drift velocity; \(\nu_x\) – the velocity along \(x\)-axis; \(\tau_{sci}\) – the electron scattering time; \(t\) – time.
The result of the study of the collective behaviour of the electrons is the dependence of the drift velocity on the ratio of Bloch and cyclotron frequencies, the magnitude of the electric field and tilt angle of the magnetic field.

The results of this work may be used for the detailed analysis of the dynamics of the single electron in the superlattice and for obtaining the general conclusion about the collective behaviour.

This work has been supported by Federal special purpose programme “Scientific and educational personnel of innovation Russia (2009–2013)”.

References:


INTERELECTRON CORRELATIONS IN THE DOUBLE PHOTOIONIZATION OF ATOMS AND IONS WITH STRONGLY ASYMMETRICAL INITIAL STATE CONFIGURATION

T. Sergeeva, V. Serov, V. Derbov
Saratov State University

Ionization, interelectron correlations, time-dependent Schroedinger equation

Though interelectron correlations have been exploring for many years, they stay a subject of growing interest. Understanding the role of interelectron correlations in the simple systems, such as two electron atoms, provides representation of more complex processes proceeding details in systems containing many electrons. The interelectron correlations are defined as deviations from the Hartree-Fock model in which each electron motion is assumed independent and moving in the averaged field of both all other electrons and nucleus.
Problem we consider is the simultaneous double photoionization of the atom affected by ultraviolet radiation. Ionization is the electron ejecting from the atom after this atom absorbs the ultraviolet radiation photon (Fig.1). In our case of double ionization the target A is: helium atom \( \text{He} \), negative hydrogen ion \( \text{H}^- \) and helium in its excited state \( \text{He}(2s\,{}^1S) \), \( \text{He}(3s\,{}^1S) \).

Phenomenas like the one we consider here are studied by the scattering theory. The possibility of the scattering process is measured in cross section which defined as the number of some events by the time unity and unitary ingoing particles flux and by the one target atom. In our case the integral cross section is the number of double ionization events by the time unit divided to photons flux and by the number of target atoms.

However, the integral cross section doesn't contain information about velocity distribution and the outgoing electrons directions. To define this the differential cross section is introduced. The latter is the cross section of first electron energy lying in the range \([E_1, E_1 + dE_1]\) and its ejecting in the direction of the solid angle element \(d\Omega_1\), which is at \(\theta_1\) angle by the ingoing radiation direction, and the second electron ejecting in the direction of the solid angle element \(d\Omega_2\) at \(\theta_2\).

The simultaneous double photoionization can proceed if only photon energy is enough for two electrons ejecting, such minimal energy is called the threshold. For the helium in its ground state it is equal to 79 eV, for the hydrogen negative ion it is equal to 14.36 eV, and for the excited helium atom in the \((2s\,{}^1S)\) state it is equal to 58.4 eV. Near the threshold the double photoionization proceeds through photon absorption by one electron and the subsequent residual ion ionization as its collision with the first electron. The double photoionization process is the most possible if the photon is absorbed by the inner electron which subsequently ejects outer electron since in such configuration the recoil momentum is transferred to the nucleus by the easiest way.

When the photon energy slightly exceeds over the threshold and outgoing electrons energy is very small, the electrons outgo quite in opposite directions, i.e. it’s a strongly correlated process. Wannier proved 50 years ago that the ejection possibility dependence on the angle between directions of the electron
ejection should be described by Gaussian distribution with the maximum at 
\[ \theta_{12} = 180 \text{ degrees} \]:
\[ \frac{d^2 \sigma}{dE_1 d_1 \sigma (E_2, \theta_{12}) = a_g(E_1, E_2, \theta_{12}) (\cos \theta_1 + \cos \theta_2)^2 + a_u(E_1, E_2, \theta_{12}) (\cos \theta_1 - \cos \theta_2)^2} \],
where \( a_u = 0 \) for \( E_1 = E_2 \), correlation parameter at the small energies \( a_g(E_1, E_2, \theta_{12}) \approx Ae^{\frac{1}{2} \ln^2 \left( \frac{\theta_{12} - \pi^2}{\gamma^2} \right)} \), and \( \gamma \) is the angular correlation width [2].
Wannier established that it should be \( \gamma \sim E^1 \). The smaller \( \gamma \) corresponds to the stronger correlation, and when \( \gamma \) goes to infinity its denote that there is no correlation. The \( \gamma \) value is convenient since this single parameter describes approximately the angular distribution in generally therefore it is convenient for using in angular distribution dependence on the photon energy treatment.

For our calculations we used the time-dependent scaling (TDS) approach [5]. It is based upon the solution of time-dependent Schroedinger equation,
\[ i \frac{\partial}{\partial t} \psi(r_1, r_2, t) = \hat{H}_0 \psi(r_1, r_2, t) \]  
with the initial condition [3]
\[ \psi(r_1, r_2, 0) = (e_1 r_1 + e_2 r_2) \psi_0(r_1, r_2) \].
in the extending coordinate system \( r = a(t)x \) [4] (2) can be written for the transformed function
\[ \psi(r, t) = \frac{1}{a(t)^2} e^{\frac{i a(t)^2}{2}} \psi(\xi, t) \]  
in the form:
\[ i \frac{\partial}{\partial t} \Psi(\xi, t) = \left[ \hat{H}_0(a(t), \xi) + \frac{1}{2} a(t)a(t)\xi^2 \right] \Psi(\xi, t), \]  
where time-dependent scaling factor is \( a(t) = \sqrt{1 + (a_n t)^2} \). The idea of the method is the coordinate system extending with the extension of the ionization wave packet [4], and the differential cross section is simply proportional to the squared wave function modulus at the large time value \( t \):
\[ \frac{d(3)\sigma}{dE_1 d_1 \sigma (E_2, \theta_{12}) = \frac{4\pi^2 \omega c}{k_1 k_2 a_\infty^6 \lim_{t \to \infty} |\Psi(\xi_e(k_1, t), \xi_e(k_2, t), t)|^2} \],
where \( \xi_e \) meets the relation \( a_\infty \xi_e = \frac{r_0(k, t)}{t} = k + Z \frac{1+ln(1+\frac{k^2}{Z})}{k^2} k \).

To testify the reasonability of our method in energy interval which is in our interest, we calculated the Gaussian width dependence on the outgoing electrons total energy, which is equal to E, for helium atom originally in its ground state double photoionization. Then we compared our results to experimental data and other authors’ theoretical calculations which was performed by using other methods.
One can see from the figure that our results are in the best agreement with experimental data in the whole energy range. At the small energies calculated Gaussian width decreases due to Wannier law.

Further we calculated the Gaussian width for the negative atomic hydrogen ion.

It is clear from the Fig.3 that $\gamma$ increases and reaches its maximum as the energy decreases in despite of Wannier law, and only after that it begins to decrease. We proposed that the cause of this strange curve behavior is connected with the fact that the most possible negative hydrogen ion configuration is weakly bounded electron in the neutral hydrogen atom short-ranged field. This means that electrons states are strongly different unlike the electrons in the helium atom. Moreover, Gaussian width calculated through different methods is notably different, especially near the maximum.

Further, we calculated $\gamma$ for helium which originally was in the excited singlet 2s-state and therefore was characterized by electron states strong difference (the first electron is in the 1s-state, and the second electron is in the 2s-state).

![Fig. 3. The angular correlation Gaussian width for the negative hydrogen ion](image)

![Fig. 4. The angular correlation Gaussian width for the helium in its (2s $^1S$) state. CCC results are taken from [1]](image)
As can be seen from Fig.4, at small energies $\gamma$ dependence obeys to Wannier law. Also, we can see the maximum which is similar to the one for $H^-$ plot and absents on the first plot (He in its ground state); this maximum appearance seems to be inherent to targets with asymmetrical configurations. However, at large energies $\gamma$’s calculated using cross section approximation and correlation parameter approximation begin to vary strongly.

The origin of this effect is clear from the Fig.5. The cross section dependence on the angle differs strongly from the Gaussian distribution, particularly, we observe two maximums instead of one maximum. At small energies one of the maximums recedes, so the distribution slowly turns to Gaussian (Fig.5(a)), and at large energies it grows becoming equal to the main one (Fig.5(b)) and then begins to dominate.

We propose that the differential cross section angular distribution structure reproduces the initial state radial structure. Preliminary results for the Helium in the 3s-state ionization confirm that, in the differential cross section dependence on the electrons scattering angle three maximums are observed. However, results in the large enough energy range and with the enough precision are not obtained yet. If our hypothesis is true, it will perhaps allow developing the new method of atoms electronic structure experimental studying. Such method already exists and is called (e,2e) spectroscopy [6], but our method could allow to simplify the experiment.

In the current work the angular correlation Gaussian width and the differential double photoionization cross section for the helium in the ground state, the negative atomic hydrogen ion, and for the helium in its excited states $(2s^1S)$ and $(3s^1S)$ were calculated using the time-dependent scaling method. The problem explored became especially actual in the recent decade that connected to the technical possibilities development of experimental studying of the process we study in theory. Our results indicate that the number of the minimums in the angular distribution matches with the number of the initial
state wave function knots. In the future we are planning to perform similar and more accurate calculations to verify or to adjust this hypothesis. This perhaps will allow developing new method of experimental studying of the atoms electron structure.

References:


**USING MESSAGE PASSING INTERFACE TECHNOLOGY FOR SOLVING MATHEMATICAL PHYSICS PROBLEMS ON PARALLEL CALCULATING SYSTEMS**

*P. Shilovsky, D. Atmakin, I. Khvatov*

*Saratov State University*

MPI, parallel computing, high-performance, python, mathematical physics, integral equation

MPI is a library specification for message passing, proposed as a standard according to the consensus of MPI Forum which has over forty organizations. Research discovers how MPI can be used for solving general mathematical physics problems on parallel calculating systems.

Message passing parallel programming model is very flexible, universal, and can be highly efficient. In message passing paradigm your computer program can be logically split into as many different processes as you need. You can even have more processes than you have CPUs, but usually you try
to match these two numbers together. The processes can all run quite different codes and they can run on CPUs that are geographically distant.

A list of model's concepts follows.

1. Distributed memory. Every processor has its own local memory which can be accessed directly only by its own CPU. Transfer of data from one processor to another is performed over a network. Differs from shared memory systems which permit multiple processors to directly access the same memory resource via a memory bus.

2. Process. A set of executable instructions (program) which runs on a processor. One or more processes may execute on a processor. In a message passing system, all processes communicate with each other by sending messages— even if they are running on the same processor. For reasons of efficiency, however, message passing systems generally associate only one process per processor.

3. Message Passing. The method by which data from one processor’s memory is copied to the memory of another processor. In distributed memory systems, data is generally sent as packets of information over a network from one processor to another. A message may consist of one or more packets, and usually includes routing and/or other control information. [2]

4. Explicit Parallel model. The programmer is fully aware of implementing parallel algorithm and all the costs of interactions between processes.

5. Different architectures. It can be efficiently implemented on a wide variety of architectures.

Message Passing Interface (MPI) is a specification for message passing libraries, designed to be a standard for distributed memory, message passing, and parallel computing. MPI addresses primarily the message-passing parallel programming model, in which data is moved from the address space of one process to another process through cooperative operations of each process. The standard has been defined through an open process by a community of parallel computing vendors, computer scientists, and application developers.

The goal of the MPI simply stated is to provide a widely used standard for writing message-passing programs. The interface attempts to establish a practical, portable, efficient, and flexible standard for message passing.

A complete list of goals follows.

• Design an application programming interface.
• Allow efficient communication: avoid memory-to-memory copying, allow overlaps of computation and communications, and offload to communication co-processor, where available.
  • Allow implementations that can be used in a heterogeneous environment.
  • Allow convenient C, C++, Fortran-77, and Fortran-95 bindings for the interface.
• Assume a reliable communication interface: the user need to cope with communication failures. Such failures are dealt with by the underlying communication subsystem.
• Define an interface that can be implemented on many vendor’s platforms, with no significant changes in the underlying communication and system software.
• Semantic of the interface should be language independent.
• The interface should be designed to allow for thread safety. [1]

MPI provides a rich range of capabilities. The following concepts are useful for understanding and providing context for all of those capabilities.
• Groups. It defines an ordered collection of processes with scope for processes names in point-to-point communications and scope of collective operations.
• Communicator. These are objects that provide all communication operations in MPI. Within each communicator each contained process has an independent identifier and the contained processes are arranged in an ordered topology. Communicator are divided into two kinds:
  o intra-communicators, that allows communication between processes from single group of process.
  o inter-communicators, that allows communication between two groups of processes.
• Point-to-point basic. It provides communication between two processes from group. A much used example is MPI_Send which allows sending data from one process from one group to another process from the same group.
• Collective basic. It provides communication among all processes in a process group. The typical example is MPI_Bcast, which takes data from one identified process and send it to other processes from the same group.
• Derived Datatypes. Many MPI operations require that you specify the type of data which is sent between processes. While MPI has predefined datatypes (MPI_INT, MPI_DOUBLE, etc) it allows users to create their own ones.

There are a lot of different free and vendor's implementations of MPI standard. There are two of the most common free ones follows.
• MPICH2 from Argone National Laboratory. It provides efficiently support of different computation and communication platform and enables a cutting-edge research in MPI through an easy-to-extend modular framework for other derived implementations. [4]
• Open MPI from a consortium of academic, research, and industry partners. It is a successor of LAM/MPI, LA-MPI, FT-MPI and PACX-MPI projects and it provides many advantages for system and software vendors, application developers and computer science researchers such as component based design, network and process fault tolerance, support of network heterogeneity, etc. [3]

Mathematical physics is the scientific discipline concerned with the interface of mathematics and physics. The theory of partial differential equations (and the related areas of variational calculus, Fourier analysis, potential theory, and vector analysis) are perhaps most closely associated with mathematical physics. There is a close connection between differential and
integral equations, and some problems may be formulated either way. Integral equations are the most useful mathematical tool in both pure and applied analysis. I would like to take Fredholm integral equation of the second kind as a typical mathematical physics problem.

The algorithm of solving follows.

1. The linear integral equation $g(x) - \int_a^b K(x, y)g(y)dy = f(x)$, where $x \in [a, b]$ is given.
2. Get a system of linear equations by replacing integral with Simpson’s method:

$$g(x_i) - \frac{h}{6} \sum_{k=1}^{N} (K(x_i, y_k) + 4K(x_i, y_k + \frac{h}{2}) + K(x_i, y_k + h))g(y_k) = f(x_i),$$

where $N$ – number of nodes, $i = \frac{1}{N}$ and $h = \frac{b-a}{N}$.
3. Solve the system with Gauss method.

The most critical part is the third. In parallel variant we consider that one process operates with its own rows of input matrix.

An example integral equation is given by [5].

$$g(x) - \frac{1}{2} \int_0^1 (x + 1)e^{-xy}g(y)dy = ex - \frac{1}{2} + \frac{1}{2}e^{-(x+1)},$$

which has solution $g(x) = e^{-x}$.

Calculations were taken place at Intel Celeron Duo T3000 processor with 2 kernels. The program was written on python with mpi4py library using Open MPI implementation. Results are represented in Table 1 below.

<table>
<thead>
<tr>
<th>Number of nodes</th>
<th>Number of processes</th>
<th>128</th>
<th>192</th>
<th>256</th>
<th>384</th>
<th>512</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>1.37776s</td>
<td>4.41191s</td>
<td>10.18807s</td>
<td>36.42898s</td>
<td>77.64169s</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>1.01176s</td>
<td>3.01797s</td>
<td>7.58489s</td>
<td>20.78954s</td>
<td>39.88461s</td>
</tr>
</tbody>
</table>

According to the results, we can see that the parallel algorithm with two processes seeks to become two times faster than the sequential one while increasing number of nodes.

I would like to pick out two main parts of my research, which follow below.

• Overview of MPI technology, its main concepts and programming model.

128
• Efficiency of MPI technology for creating parallel solution of typical mathematical physics problem – linear integral equation.

References:


ON THE BEHAVIOR OF ONE OF THE POSITIVE LYAPUNOV EXPONENT IN MUTUALLY COUPLED CHAOTIC OSCILLATORS

S. Shurygina

Saratov State University

Generalized, lag, complete chaotic synchronization; Lyapunov exponent; coupling strength; unidirectionally and mutually coupled oscillators

In this work the dependence of one of the positive Lyapunov exponent on the value of coupling strength is considered. As the sample systems two mutually coupled Roessler oscillators and two mutually coupled tunnel-diode-based stochastic oscillators have been selected. It is shown that coupling strength values corresponding to the points of the sign reversal of this Lyapunov exponent are close to each other for the different frequency mismatches. At the same time, these critical values of coupling strength are not connected to the lag-synchronization regime onset.

Chaotic synchronization is one of the fundamental nonlinear phenomena actively studied recently [1]. Several different types of chaotic
synchronization of coupled oscillators, i.e. generalized synchronization (GS) [2], phase synchronization (PS) [1], lag synchronization (LS) [3], complete synchronization (CS) [4] and time scale synchronization (TSS) [5] are well known. There are also attempts to find a unifying framework for chaotic synchronization of coupled dynamical systems [6]. In our works [7] it was shown that phase, generalized, lag, and complete synchronization are closely connected with each other and, as a matter of fact, they are different manifestations of one type of synchronous oscillation behavior of coupled chaotic oscillators called time-scale synchronization.

One of the interesting and intricate types of the synchronous behavior of unidirectionally coupled chaotic oscillators is the generalized synchronization. The presence of GS between the response \( x_r(t) \) and drive \( x_d(t) \) chaotic systems means that there is some functional relation \( x_r(t) = F[x_d(t)] \) between system states after the transient finished. This functional relation \( F[\cdot] \) may be smooth or fractal. According to the properties of this relation, GS may be divided into strong synchronization and weak synchronization. There are several methods to detect the presence of GS between chaotic oscillators, such as the auxiliary system approach [8] or the method of nearest neighbors [2]. It is also possible to calculate the conditional Lyapunov exponents (CLEs) [9] to detect GS.

Other interesting type of synchronous behavior in coupled chaotic oscillators is the lag synchronization, which means that the interacting systems show identical oscillations, shifted by a certain time interval \( \tau \), i.e. \( x_1(t) = x_2(t+\tau) \). With the increase of the coupling strength value between the oscillators, the time shift \( \tau \) tends to zero, and the synchronous regime tends to be complete chaotic synchronization. To detect the lag synchronization, there are some methods, such as the comparison of states of interacting systems \( x_1(t) \) and \( x_2(t) \) in the Poincare mapping (e.g., with secant plane \( y = 0 \)) or the calculation of similarity function:

\[
S^2(\tau) = \frac{\langle |x_2(t+\tau) - x_1(t)|^2 \rangle}{\sqrt{\langle |x_1^2(t)| \rangle \langle |x_2^2(t)| \rangle}},
\]

(1)

If the interacting systems are in LS regime, the minimum of similarity function becomes zero, i.e. \( \min_{\tau} S(\tau) = 0 \), where \( \tau \) – time shift between the vectors of states of interacting systems. The regimes of LS and CS are also particular cases of GS.

It is known, that for unidirectionally coupled chaotic oscillators generalized synchronization can be analyzed with the help of conditional Lyapunov exponents, i.e. the Lyapunov exponents calculated for the response system. Since the behavior of the response system is governed by the drive system, these exponents are different from the Lyapunov exponents for the autonomous response system and are referred to as conditional Lyapunov exponents. A criterion for the existence of generalized synchronization in
unidirectionally coupled dynamical systems is the negativity of the highest conditional Lyapunov exponent.

For mutually coupled oscillators we know only, that the sign reversal of one of the positive Lyapunov exponent $\lambda_1$ precedes the lag synchronization and is close to this phenomenon [3]. At the same time, the difference in the parameter of coupling strength between the transition of $\lambda_1$ to the negative values and the onset of LS can be large enough. In this work we consider such problem in detail.

As the first sample system we consider two mutually coupled Roessler oscillators:

$$
\begin{align*}
\dot{x}_1 &= -\omega_1 y_1 - z_1 + \varepsilon(x_2 - x_1) \\
\dot{y}_1 &= \omega_1 x_1 + ay_1 \\
\dot{z}_1 &= p + z_1(x_1 - c) \\
\dot{x}_2 &= -\omega_2 y_2 - z_2 + \varepsilon(x_1 - x_2) \\
\dot{y}_2 &= \omega_2 x_2 + ay_2 \\
\dot{z}_2 &= p + z_2(x_2 - c),
\end{align*}
$$

(2)

where $\varepsilon$ is a coupling parameter. The control parameter values have been selected by analogy with Refs. [10] as $a=0.15$, $p=0.2$, $c=10.0$. The $\omega_2$ parameter, which determines the main frequency of the second system, has been selected as $\omega_2=0.95$, and the analogous parameter $\omega_1$ of the first system has been varied, providing the mismatch of the interacting oscillators.

The second sample system is the system of two mutually coupled tunnel-diode-based stochastic oscillators, which is described by the following equations [11]:

$$
\begin{align*}
\dot{x}_{1,2} &= \omega_{1,2}^2 \left[ h(x_{1,2} - \varepsilon(y_{2,1} - y_{1,2})) + y_{1,2} - z_{1,2} \right] \\
\dot{y}_{1,2} &= -x_{1,2} + \varepsilon(y_{2,1} - y_{1,2}) \\
\mu \dot{z}_{1,2} &= x_{1,2} - f(z_{1,2}),
\end{align*}
$$

(3)

where $x_{1,2} \sim I_{1,2}$, $y_{1,2} \sim U_{1,2}$, $z_{1,2} \sim V_{1,2}$, $h = MS/\sqrt{(LC)}$, $\mu = \tilde{C}/C$, $\omega_{1,2} = \sqrt{(L/L_{1,2})}$, $\varepsilon = \sqrt{L/(R \sqrt{C})}$ is the coupling parameter, and $L$ is a normalizing coefficient. The control parameter values have been taken from [11] as $h = 0.2$ and $\mu = 0.1$. As dimensionless characteristic $f(\xi)$ of the nonlinear element, we have used the function $f(\xi) = -\xi + 0.002 \sin(5\xi - 7.5) + 2.9$. The value of $\omega_2$ has been fixed ($\omega_2 = 1.02$), while $\omega_1$ and $\varepsilon$ parameters have been varied.

Studies of the behavior of one of the positive Lyapunov exponent $\lambda_1$ in both systems have shown that coupling strength values $\varepsilon$ corresponding to the points of the sign reversal of this Lyapunov exponent are close to each other for the different values of frequency mismatch $\Delta \omega$. At the same time, these critical values of coupling strength are not connected with the lag-synchronization regime onset, because the boundary value $\varepsilon$ of the lag
synchronization regime onset grows sharply with the frequency mismatch increasing.

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References:


HARDWARE-SOFTWARE SYSTEM FOR ANALYZING THE TEMPORAL CHARACTERISTICS OF REAL-TIME SYSTEMS

E. Sinelnikov
Saratov State University

Verification, methods of testing, temporal characteristics, real-time systems

Currently, there are several methods for analyzing real-time systems (RTS). Among them stand out analytical and empirical approaches. Analytical methods of analysis focused on the preliminary identification of worst-case execution time (WCET) by analyzing the source code or compiled object code of the RTS, and the construction of models for assessing the architecture of RTS and temporal predictability used in its algorithms. Empirical methods are aimed at testing the temporal characteristics of RTS with the help of specialized tools, allowing an analysis of the developed system or its prototype.

In this article considered method of constructing the hardware and software framework designed to enhance the analysis of RTS through the dynamic construction of analytical models using statistic data obtained in the process of empirical tests.
Methods of testing involves the study of time characteristics of the developed system or its prototype with the help of a hardware mechanism for measuring the time delays. Similar solution was presented in the open source project of device realization for measuring time delays (latencies), designed by the laboratory of the development of automation systems with open source software (OSADL, 2009). In contradistinction to the mechanism of the empirical analysis presented in the Latency Measurement Box project (Emde, 2009), the proposed method doesn’t involve the using of specialized 32-bit real time operating system (RTOS). In this article for realization of method assumed a using of a minimalist set of hardware controlled by 8-bit microcontrollers. In this case, the hardware implements only the predictable logic of the generation of external events and collection of data about the responses to these events (see fig. 1).

The investigated real-time system in this research will be called the **target system**. For implementation a hardware mechanism for measuring the latency, the delay test system is implemented in the form, that consists of two modules: a **system of measuring latencies** and **instrumentation** on the target system. Measuring the latencies system’s task is the generation of external events for the target system and the storing the data stream, which is represents the monitored flow of responses. Instrumentation on the target system represents an environment, that executes the logic of real-time system and performs responses to external events, that were generated by the measuring the latencies system.

In the simplest case, such scheme makes possible to estimate the time constraints of the target system generally. Thus, instrumentation of the target system is minimal and includes only a working in the **echo mode** mechanism of receiving data, that arising under the influence of external events. Echo mode represents the behavior, when each received message immediately sends a response. In this case, the analysis does not study the internal mechanisms of real-time system. With this approach there is an analysis of RTS, using the time of its reaction to external events. Such analysis can be useful both in selecting the hardware platform for realizing a real-time system in future, as to estimate the feasibility of current realizations.

Using the echo mode also can be applied for comparative analysis of the internal subsystems of different implementations of target RTS. This approach
allows us to estimate the applicability of different RTS for specific tasks. The results of comparative analysis will represent a necessary condition for the applicability of a system for problems in these temporal restrictions.

The using of measurement system in echo mode will be called the **method of response**. With the help of this method it is possible to statistically estimate the following set of parameters:

- latencies in the processing of interrupts for the drivers, installed in the target system;
- latencies in the processing of events in applications, running on the target system;
- latencies in task switching, during the processing of external events in the target system.

Except the echo mode, the instrumentation of target system can issue its status. This approach allows specify a set of specific variants for the functioning of the target system having the monitored data stream. Based on the set of events and order of transitions between them, the automaton model of the system can be given. Options for obtaining the temporal characteristics using automatic models obtained through analysis of empirical tests presented in the paper of Andrés Terrasa (Terrasa, 2003).

Fig. 2 shows the general scheme of the functioning of the complex to analyze RTS. In the present scheme is to provide a separate method of constructing automaton models based on the data collected. Set of states formed from the number of states are returned in response to the generated events. Transition function is formed from the order of responses to generated events. Furthermore automaton model can be accompanied by marks the transition time between states. This extended model is known as a model of Timed Automata (Alur, 1994).
This article was reviewed the method construction the analysis framework of the real-time systems. Implementation of this framework is held within the projects of the course and graduate works of students from Saratov State University. Continued work on the use of the considered hardware-software framework is planned towards the development of tools for building models based on temporal characteristics and the application of this approach in practice.

References:


OCT MONITORING OF DIFFUSION OF WATER AND GLYCEROL THROUGH TOOTH DENTINE IN DIFFERENT GEOMETRY OF WETTING

N. Trunina, V. Lychagov, V Tuchin

Saratov State University

Optical coherence tomography, diffusion, clearing agents, water, glycerol, tooth, dentin, OCT signal slope, permeability coefficient

In our previous work optical coherence tomography (OCT) has been proved to be a useful tool for monitoring of diffusion of chemical agents (water, glycerol) within human tooth dentine. Such diffusion studies are interesting for tooth therapy (diffusion of medicinal preparations) and cosmetics (chemical whitening agents). Here we compare different wetting schemes in which the sample is either merged in the liquid agent so that the probe beam is to pass through a layer of liquid, or subjected to wetting through a special window from the back side. In spite of certain difference revealed, the order of magnitude of the diffusion time constant and the permeability coefficient are shown to be the same in both cases.
In our previous paper [1] we have reported the first application of optical coherence tomography (OCT) to monitoring of diffusion of water and glycerol through samples of human tooth dentine in vitro. The diffusion process has been proved to manifest itself via optical clearing of the tooth tissue, the process that reduces both the attenuation of the OCT signal and the backscattering responsible for the OCT signal as such, via the equalizing (matching) of the refraction index of a randomly inhomogeneous medium. As a result the mean slope of the OCT signal versus depth demonstrated temporal decrease with the characteristic time constant associated with the diffusion time constant.

The study of dentinal permeability with respect to different chemical agents is of interest both for tooth care and treatment. Dental bleaching, which is of primary importance in cosmetology, involves diffusion of such agents as hydrogen peroxide into the tooth tissue [2].

In the abovementioned studies [1] the tooth sample was placed into a cell filled with a liquid agent, so that the OCT probing beam had to pass through a layer of liquid before and after travelling inside the dentine sample. The presence of this layer was seen to affect the probing process. Since the full measurement time was measured by hours, we had to periodically refill the cell because of the agent evaporation. This caused additional oscillations of the temporal dependence of the mean OCT slope. Hence we developed an alternative scheme of the agent application free of probing passing the layer of agent. In this scheme the agent is applied through a special window from the back side of the sample. Here we report the results of these new measurements. First we recall some necessary information about the samples, experimental setup and data processing. Then we compare the results obtained in the two application geometries.

The measurements were carried out using a portable time-domain OCT system (THORLABS Spectral Radar OCT Systems). The light source used in this system is a low-coherence broadband superluminescent diode (SLD) with the central wavelength 930±5 nm, spectral bandwidth of 100 nm and coherence length, defining axial resolution of the system, is 6.2 µm, output power of 2 mW.

The samples of human tooth tissue were prepared as follows. Teeth were extracted in dental clinic during an elective operation. They were kept in saline of physiologic concentration at 4°C in a sun-protected place. Water-wet tooth was cut with a diamond disk either along or across the dentinal tubules. Tooth tissue sections were then grinded and washed with 37% orthophosphoric acid and then placed into an ultrasonic bath to get rid of the dust and splinters left after sawing. The thickness of the samples was about 1mm.

At the preliminary stage microscopic images of the samples (see an example in Fig.1) were obtained using an optical microscope (Axio Imager, Carl Zeiss, and magnification 32). These images allowed us to evaluate the dimension of dentinal tubules and their distribution density and to select the windows of better surface quality, absence of defects and more homogeneous tubule
distribution for further OCT observation of the chemical agent diffusion. All sample surface, except the window chosen (2x2 mm), was covered with transparent fast-drying varnish and dried in an air flow. This was necessary to prevent the agent diffusion through the side and bottom faces of the tooth tissue section.

Fig. 1. Example of microscopic images of sections of human tooth dentin. Dentinal tubules, more dense and homogeneous peritubular dentine, and less dense and less homogeneous intertubular dentin are seen. The tubular diameter is estimated as (2.40 ±0.55) μm.

The experiments were carried out in two geometries. In the first case (Fig. 2 (a)) the samples were placed in a metallic cuvette connected with an injector providing the proper filling of the cuvette with the agent. OCT-scanning of the sample was performed through the liquid layer covering the sample. In the second case (Fig. 2 (b)) the samples were glued to the window of cuvette. Then this cuvette was filled by the agent. Wetting of the sample was implemented through the back side of the sample with respect to the OCT-probing beam. In this case two windows free of varnish coating were left on the opposite sides of the sample (Fig. 2(b)). In both cases OCT-scanning was performed repeatedly during a few hours.

Fig. 2. Schemes of diffusion agent application and OCT registration. (a) – front wetting, (b) – back wetting. OCT – optical coherence tomograph; 1 – cuvette with diffusion agent, 2 – sample, 3 – layer of transparent fast-drying varnish.

Two agents were used in the diffusion experiments, namely, glycerol (water solutions 44%) and pure water. Glycerol was chosen because it is a widely-used clearing agent for numerous biological tissues. Water is important
for the metabolism of a living tooth, moreover, it was shown [3] that water affects the mechanical resistance of the tooth tissue.

The data processing was carried out following the procedure described in detail in our previous paper [1]. The raw data of the OCT measurements were digitized and stored as produces a 2D array in the computer memory. Each column of this array presents an A-scan, i.e. the OCT signal in logarithmic scale versus the depth of probing. Averaging over a set of adjacent A-scans provided substantial noise reduction. The averaged A-scan was used to calculate the mean slope which was the fingerprint of optical clearing caused by the diffusion of the agent. We traced the temporal variation of this slope in the course of diffusion (during a few hours). Exponential fit of the obtained dependence gave an estimate of the diffusion time constant. To obtain the permeability of the tissue we used the simple formula $P = z_{\text{reg}} / t_{\text{reg}}$, where $z_{\text{reg}}$ is the sample thickness, while $t_{\text{reg}}$ is the diffusion time constant.

The comparison of the experimental results for water diffusion in two geometries is presented in Fig.3. In case of front to back diffusion (Fig.3(a,c)) the diffusion process manifests itself in the reduction of the OCT signal slope in which, obviously, the contribution of the mean attenuation coefficient is dominant. In the case of back to front diffusion (Fig.3(b)) the temporary order of A-scans is opposite to that of Fig. 3(a), which can be associated with primary reduction of the backscattering coefficient reduction of the probed layer first subjected to the agent action. The reduction of the OCT signal slope is not so apparent, but the data processing shows that it actually takes place (Fig. 3(d)). A remarkable finding is that in both cases of agent application geometry the ultimate time constants of the process appear to agree very well. From the practical point of view, back-to-front wetting is preferable due to the lack of artifacts introduced by the liquid layer covering the sample.

Similar measurements were carried out with different samples. For 44% glycerol solution an example of A-scans and time dependence of the OCT mean slope is presented in Fig. 4. The results for different samples are summarized in Tab.1. These results also demonstrate the correlation between the diffusion rate and the sample structure, particularly, the diameter and distribution density of tubules. Further studies are planned to clarify this correlation and to develop practical models for appropriate extraction of the tissue optical and diffusion parameter from the OCT measurements.

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Fig. 3. Manifestations of water diffusion in human tooth dentine (sample 1). (Top) Averaged A-scans taken at different moments of time for front (a) and back (b) wetting. (Bottom) The resulting plots of the OCT signal slope versus time for front (c) and back (d) wetting. The probed depth intervals are 150-300 µm for (c) and 60-300 µm for (d).

Fig. 4. Manifestations of 44% glycerol solution diffusion in human tooth dentine (sample 4). (a) Averaged A-scans taken at different moments of time for back wetting. (b) The resulting plots of the OCT signal slope versus time for back wetting. The probed depth interval is 60-300 µm.
Tooth tissue structural parameters and diffusion parameters obtained from microscopic images and OCT

<table>
<thead>
<tr>
<th>Sample number</th>
<th>Sample thickness, $d_{\text{sample}}$, mm</th>
<th>Mean tubule diameter, $\mu m$</th>
<th>Agent</th>
<th>Time of saturation, min</th>
<th>Permeability coefficient, cm/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9</td>
<td>0.60±0.10</td>
<td>water</td>
<td>78</td>
<td>(3.04±0.13)x10^{-6}</td>
</tr>
<tr>
<td>2</td>
<td>1.3</td>
<td>2.30±0.15</td>
<td>water</td>
<td>9</td>
<td>(4.02±0.24)x10^{-5}</td>
</tr>
<tr>
<td>3</td>
<td>1.2</td>
<td>1.60±0.13</td>
<td>water</td>
<td>154</td>
<td>(2.09±0.65)x10^{-6}</td>
</tr>
<tr>
<td>4</td>
<td>0.8</td>
<td>2.4±0.55</td>
<td>44% glycerol solution</td>
<td>54</td>
<td>(4.91±0.67)x10^{-6}</td>
</tr>
</tbody>
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References:

ANALYSIS OF FEMALE AND MALE GAMETOPHYTES LINE 2098 OF TRITICUM DURUM

V. Ulyanova

Saratov State University

Embryology, pollen, embryo sac, hard wheat, Triticum durum

*Triticum durum* is one of the most important agricultural crops in the world. It is 2nd among the soft wheat after wheat in planted area (Dorofeev, 1979). *Triticum durum* is used for the production of pasta, semolina and improves baking quality of flour of soft wheat (Gushin, 1984). On breeding new varieties data on the embryology of plants should be taken into account, as embryological material is the necessary theoretical foundation for broadening and deepening of research in genetics and selection. (Batygina, 1987). This work is devoted to the study of cytoembriologic line 2098 of *Triticum durum* in Saratov selection.

Line of *Triticum durum* in 2098 obtained in the laboratory of *Triticum durum* of South-East Agricultural Research Institute by complex multistep hybridization with local varieties, such as Valentine, Elizabeth, Golden Saratov, Saratovskaya 59 and others served as the studied materials (Vasilchuk, 2001).

Inflorescences of 10 plants were recorded using a powl Clarke (3:1) before and at the beginning of flowering under conditions of open pollination. The pollen was examined in temporary glycerine-gelatin preparations, stained by acetocarm. The structure of the female gametophyte was studied on specimens prepared by enzymatic maceration, followed by dissection of ovaries and ovules, and allocation of entire embryo sacs (Kupriyanov, 1989).

The pollen of plants line 2098 of *Triticum durum* varied in size from 36.5 to 54.8 microns. The average size of pollen grains was 44.4 microns. Along with plump and well-stained pollen grains (fig. 1A) there was pollen (40%) with different degrees of plasmolysis (fig. 1B). Abnormalities in morphological structure of the pollen grains have not been identified.

![Fig. 1. The pollen grains of Triticum durum.](image1)
A. Plump and well-stained pollen grains.
B. Different degrees of plasmolysis pollen grains
The pollen had three-celled structure. There was a large vegetative nucleus with one nucleolus, and two sperms. The shape of sperms was various: round, oval, crescent. In some cases, pollen grains on the prophase of division of the generative cell were found. There were also empty pollen grains (2%).

![Image](image.png)

Fig. 2. Male gametophyte line 2098 of *Triticum durum*. A. Three-celled structure of pollen. B. Prophase of division of the generative cell. C Empty pollen grains

All the embryo sacs of the lines were differentiated. Their structures were morphologically consistent with Polygonum-type, which is characteristic for embryo sacs of sexual species of cereals. The mature embryo sac (Fig. 3) was pear-shaped, 2 / 3 of which were taken by a well-developed antipodal complex. It consisted of 16 or more cells.

![Image](image.png)

Fig. 3. The same female gametophyte of *Triticum durum* in different planes:
A – Two synergids in the egg apparatus. B – One agg in micropylar area

Antipodal nuclei contained 1 or 2 nucleoli. In the central part of the embryo sac there were two polar nuclei with large nucleoli. The polar nucleus could be in various degrees remote from the egg apparatus, which shows the various stages of development of the female gametophyte. The nuclei were located either close to each other or overlapped. The egg apparatus consisted of a spherical egg with the nucleus in the basal part, and two located on its sides sinergid. Smaller in size and elongated in length sinergides contained one nucleus in the apical part.
Along with mature embryo sac gametophytes with undifferentiated egg apparatus were also found. In that case, three identical in size and shape cells as well as their nucleoli were in micropylar area.

Despite the fact that the investigated line was obtained by crossing a large number of varieties, it shows the stability of the structure of the generative structures. Fertility of pollen grains, the presence of normal differentiated embryo sacs and the absence of structural abnormalities in male and female gametophytes suggest plants line 2098 of *Triticum durum* to be promising for selection of new varieties.

References:


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**UTILIZATION OF MICROSTRIP PHOTONIC CRYSTALS FOR MEASUREMENT OF ELECTROPHYSICAL PARAMETRES OF LIQUIDS**

* D. Usanov, A. Skripal, A. Abramov, A. Bogolubov, M. Kulikov, D. Ponomarev

*Saratov State University*

Microwave radiation, photonic crystal, microstrip line, complex permittivity, reflection and transmission spectra, polar liquids, non-polar liquids, reverse problem

Among various types of planar circuits microstrip ones are the most often used in microwave electronics. Microstrip circuits are rather often used in implementations of microwave methods of measurement of parameters of material, in particular, materials of substrates for microwave circuits [1].

The intensive development of nanotechnologies had stimulated the creation of new type of periodical structures – photonic crystals. They consist of interlaced layers, which have thicknesses comparable with the wavelength of propagated electromagnetic radiation Yablonovitch, E. (1987) Inhibited spontaneous emission in solid-state physics and electronics. Phys. Rev. Lett., 58(20), 2059–2062. In the transmission spectrum of such structures there is a


Because of the high sensitivity of the frequency position of the low-loss transmission window to the parameters of irregularity it is promising to use microstrip photonic crystals for measuring the parameters of materials in the microwave band.


In this work we show the possibility of utilization of microstrip photonic crystals for implementing the method of measurement of parameters of liquids, which play as the irregularity in the microstrip photonic structure, in
the wide range of their values. We considered the microstrip photonic crystal consisted of concatenated sections of the microstrip line with interlacing permittivity of the substrate. Even sections were implemented on the ceramic \((Al_2O_3)\) substrate. Odd sections were aerial: they did not have the substrate; the strip conductor was strained in the air between two neighbouring sections with ceramic substrates. The drawing of the microstrip photonic structure is shown in fig. 1.

![Fig. 1. Microwave photonic crystal with cuvette for measuring parameters of liquid dielectrics. 1 – measured liquid, 2 – strip conductor, 3 – ceramic section, 4 – measuring cuvette, 5 – aerial section](image)

To calculate the reflectance and the transmittance of the electromagnetic wave propagated through the microwave photonic crystal in the quasistatic approximation we used the transmission matrix of the complex quadripole. Such quadripole can be represented as the cascade connection of elementary quadripoles with known transmission matrixes:

\[
T = \begin{pmatrix}
T[1,1] & T[1,2] \\
T[2,1] & T[2,2]
\end{pmatrix} = T'_N \cdot \prod_{i=1}^{N-1} (T''_{i,i+1} \cdot T'_i),
\]

where is the transmission matrix of the quadripole for the \(i\)-th section, is the one of the quadripole for the connection of \(i\)-th and \((i+1)\)-th sections of the microstrip line.

After calculation of the transmission matrix of the microstrip photonic crystal from one can calculate the transmittance of the microstrip photonic crystal through the element of the transmittance matrix:
The reflectance can be calculated through the element of the scattering matrix:

\[ r = |S[1,1]|^2. \]  \hspace{1cm} (5)

Elements of matrix are connected with elements of the matrix by the known relation.

In computer simulation we considered the microstrip photonic structure which consisted of 9 concatenated interlaced sections of a microstrip transmission line with different permittivity of the substrate (fig. 1). The odd sections were aerial. The even sections were implemented on the ceramic (Al₂O₃) substrate. The width of the stripline conductor was 1 mm, thickness of the ceramic substrate was 1 mm. **Permittivity of the ceramic substrate was 9.6.** The microstrip photonic structure was inserted into the 50-Ω external transmission line.

The frequency dependency of the transmittance of the microstrip photonic structure under simulation in the frequency range 0–20 GHz was calculated using the described above theoretical model in quasistatic approximation. The structure had the irregularity introduced as changed length of some sections and changed dielectric permittivity of the 5th section. This dependence has frequency ranges which are forbidden for electromagnetic wave propagation. There is the narrow low-loss transmission window in the forbidden gap of the photonic crystal. It appears due to the existence of the irregularity in the photonic structure Yablonovitch, E. (1987) Inhibited spontaneous emission in solid-state physics and electronics. Phys. Rev. Lett., 58(20), 2059–2062. – Yoshino, K., Ozaki, R., Matsumoto, J., Ojima, M., Hiwatashi, S., Matsuhisa, Y., & Ozaki, M. (2006, June) Properties of Liquids and Liquid Crystals in Nano-Scale Space. IEEE Transactions on Dielectrics and Electrical Insulation, 13(3), 678–686. Frequency position of the low-loss transmission window can be controlled by changing the dielectric permittivity of the substrate in the disturbed section.

For performing experimental investigations the two structures had been manufactured. The structures consisted of concatenated sections of interlaced sections of the microstrip transmission line with interlacing permittivity of the substrate: even sections were implemented on the ceramic (Al₂O₃) substrate; odd sections were air strip lines. The width of the stripline conductor was 1 mm, thickness of the ceramic substrate was 1 mm. End sections of the structure, implemented on the ceramic substrates, had the 50-Ω impedance. One of the sections, which played as the irregularity, was implemented as a cuvette for measurement of permittivity of liquid dielectrics. For liquids with low losses the wide cuvette was used, for liquids with high losses the narrow cuvette was used.
The structure was inserted into the 50-Ω coaxial measuring section. Using the *N5230A Agilent PNA-L Network Analyser* the transmission spectra of the microstrip structure with empty cuvette and with cuvette filled with various liquids were measured. Measured transmission spectra are presented in fig. 2 and fig. 3 (dashed curves).

![Fig. 2](image1.png)

**Fig. 2.** Transmission spectra for the structure with the wide cuvette near the low-loss transmission window for the empty cuvette (curves 1) and the cuvette filled with dielectric oil (curves 2). Experimental spectra – dashed line, calculated spectra using obtained value of complex permittivity – solid line

![Fig. 3](image2.png)

**Fig. 3.** Transmission spectra for the structure with the narrow cuvette near the low-loss transmission window for the empty cuvette (curves 1) and the cuvette filled with polar liquids: deionized water (curves 2), ethanol (curves 3), glycerine (curves 4). Experimental spectra – dashed line, calculated spectra using obtained value of complex permittivity – solid line

To determine the unknown parameter, for example, the complex permittivity, of liquid the cuvette filled with, it is necessary to solve the inverse problem Usanov, D.A., Skripal, A.V., Abramov, A.V., & Bogolyubov, A.S.
(2006) Determination of the metal nanometer layer thickness and semiconductor conductivity in metal-semiconductor structures from electromagnetic reflection and transmission spectra, Technical Physics, 51(5), 644–649., Usanov, D.A., Skripal, A.V., Abramov, A.V., Bogolyubov, A.S., & Kalinina, N.V. (2006, September) Measurements of thickness of metal films in sandwich structures by the microwave reflection spectrum. in Proc. of 36rd European Microwave Conf., Manchester, UK.. If the reflection and transmission spectra have the pronounced frequency dependency, and the theoretical description of this dependency is known, then such problem can be solved using the least-squares method. In this method one finds the value of the parameter at which the sum of squares of differences between experimental and calculated from (4) values of the transmittance

\[ S(\varepsilon) = \sum_n \left( |D_{n,\text{exp}}|^2 - |D(\varepsilon; f_{n,\text{exp}})|^2 \right)^2 \]  

reaches its minimum value. The sought-for value of permittivity of the sample is determined using numerical methods as a result of solving the equation

\[ \frac{\partial S(\varepsilon)}{\partial \varepsilon} = 0. \]  

Using the mathematical model of the photonic crystal and the experimental frequency dependencies of the transmittance near the low-loss transmission window we determined the complex permittivity of a number of liquid dielectrics.

Table 1

<table>
<thead>
<tr>
<th>Material</th>
<th>$\varepsilon'$</th>
<th>$\varepsilon''$</th>
<th>$f$, GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>2.43</td>
<td>0.025</td>
<td>4.06</td>
</tr>
<tr>
<td>Dielectric oil</td>
<td>2.5</td>
<td>0.026</td>
<td>4.05</td>
</tr>
<tr>
<td>Vacuum oil MB-5</td>
<td>2.4</td>
<td>0.017</td>
<td>4.05</td>
</tr>
</tbody>
</table>

Table 2

<table>
<thead>
<tr>
<th>Material</th>
<th>$\varepsilon'$</th>
<th>$\varepsilon''$</th>
<th>$f$, GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deionized water</td>
<td>76.5</td>
<td>10.3</td>
<td>3.24</td>
</tr>
<tr>
<td>Ethanol</td>
<td>10.5</td>
<td>7.9</td>
<td>3.58</td>
</tr>
<tr>
<td>Glycerin</td>
<td>16</td>
<td>11.5</td>
<td>3.54</td>
</tr>
</tbody>
</table>

Also the results of measurements of real and imaginary parts of complex permittivity for ethanol/water mixtures with the various volume maintenance of ethanol are presented on fig. 4. With the increasing of
volume fraction of ethanol monotonously decreases from 76.6 to 10.5. With the increasing of volume fraction of ethanol changes in nonmonotonic way. It has clearly expressed maximum equal 18.2 at equal 40 %. Because parametres were defined in a narrow frequency range of the low-loss transmission window the change of and at frequency change was not considered.

![Figure 4](image.png)

Fig. 4. Experimental curves of and for ethanol/water mixtures depending on volume fraction of ethanol in mixture

It is necessary to note that the received results of measurements of real and imaginary parts of complex permittivity for ethanol/water mixtures are in good conformity with results of the developed model for the description of spectra of permittivity for such mixtures, which considers the change of relaxation time of polarisation for ethanol/water mixture depending on volume fraction of ethanol in mixture [14].

So, the method for measurement of parameters of polar and non-polar liquids, which plays as the irregularity in the photonic structure, created on the open microstrip transmission line, had been implemented. The method is based on solving the reverse problem using measured frequency dependencies of the reflectance near the low-loss transmission windows of the microstrip photonic crystal. The values of complex permittivity for a number of non-polar and polar liquids with big losses had been measured.

References:


Liquid crystals, electro-optical properties of liquid crystals, Frederiks transition, composite structures, liquid crystal composites, polymer-dispersed liquid crystals, Frederiks Transition threshold field in nematic polymer-dispersed liquid crystals

We have simulated the dependence of Frederiks transition threshold field in nematic polymer-dispersed liquid crystal (PDLC) on different parameters with the help of MathCAD software package. Our results confirm the essential influence of the finite azimuthal surface anchoring energy, drop radius and effective dielectric anisotropy on its value and can be used by elaborating of PDLC-based systems with required characteristics.

As a rule, new materials appear because of scientists’ natural wish to improve characteristics of devices we use but when produced these new materials often open up a new world of possibilities to elaborate some essentially new devices and technological processes. One of the brightest examples is connected with composite materials [1] which have a wide range of applications for different areas of technics.

Composites with liquid crystals (so called liquid crystal composites or LC composites) in comparison with homogenous LC layers are characterized by more complex display of physical effects. In the field of application one of the most promising composite structure is a polymer-dispersed liquid crystal (PDLC), in which micrometer droplets of LC are embedded in a solid polymer matrix [2]. These compounds successfully combine properties of polymers with their ability to form films, fibers and coverings, as well as unique properties of liquid crystals capable of orientational reconstructions and optical characteristics changing under the influence of external electric or magnetic fields. Liquid crystal in PDLC is well protected from external destructive influences, but by the same time keeps a lot of its initial properties. That’s why it is necessary to examine physical bases of liquid crystals for correct understanding of PDLC properties.

Liquid crystals are substances which under some special conditions (such as temperature, pressure, concentration in a solution) are able to transform into liquid crystal state of aggregation intermediate between the solid (crystalline) and the liquid one. As for structure, they are similar to jelly and consist of extended molecules definitely ordered in volume. Depending on the molecule arrangement there are three basic types of liquid crystals compounds (fig. 1): nematics, cholesterics and smectics [3, 4].
The molecules in *nematics* can be assimilated to pencils in a box: they can rotate and slide back and forth but have to stay parallel to each other. The direction of the primary orientation of molecule axes is called *the director*. In *cholesterics* and *smectics* molecules form some layered structure. Within each layer of *cholesterics* the structure is equal to nematics, but moving from one layer to another the director turns on a small angle. As a result, a spiral layered structure is formed. In *smectics* the director within each layer does not lay in its plane: the long axes of molecules in each layer form some angle to it.

In the investigation of physical systems much attention is devoted to behaviour of solids under the influence of external fields. Changing of a parameter’s value under the influence of external field is called *response of the system*. There are situations when this response is possible only with fields which exceed some limiting value. Such phenomena are called *threshold* phenomena.

Indeed the ability of *liquid crystals* to change the molecule orientation under *the influence of external field* opens wide range of possibilities for their application in industry (*displays, LC indicators*): if we direct a ray of light to a LC, it will be transparent; if we take away external field, the molecules will come back in their initial conditions and LC will become again muddy. The basis of this ability is the so-called *Frederiks transition* [3, 5]. The Frederiks transition consists of ability of some liquid crystals molecules to be oriented *along* the field (for *nematic* liquid crystals with a positive dielectric anisotropy: \(\Delta \varepsilon > 0\)) after it overcomes some threshold value and becomes strong enough to block action of the rotate torque which, on the contrary, tried to constrain molecules in their initial conditions. Initially PDLCs were created to use their unique electro-optical properties. All of them are essentially determined by *the structure of nematic in droplets* (fig. 2) – i.e. by the arrangement of molecules in droplets [5, 6] which is connected with boundary conditions on the droplet surface defined by physical and chemical features of the pair LC – polymeric matrix. The bipolar structure is of the greatest interest for us.
It turns out, that under the influence of external electric or magnetic field the *structure of droplets changes* (molecules of nematic in droplets with bipolar structure are transforming and the droplet axes are orienting along the field – fig. 3), *that leads to occurrence of new properties in the PDLC*. The basis of such structural changes is the above mentioned Frederiks Transition, which also has a threshold character [5, 6, 7].

An important aim in PDLC-based devices elaboration is to find methods to reduce the Frederiks transition threshold field value and, as a consequence, to define its dependence on polymer’s and nematic’s parameters.

![Fig. 3. Droplet location in nematic PDLC before (left) and with (right) the application of electric field](image)

O.A. Afonin and V.F. Nazvanov [8, 9] took into account the finite azimuthal surface anchoring energy and worked out a formula for *Frederiks transition threshold electric field*:

$$E_c = \frac{1}{R} \times \left( \frac{5.7 \times K \times \delta^2 + 2.2 \times W a \times R^{1/3}}{\varepsilon_0 \times \Delta \varepsilon'} \right)^{2/3}$$

where $R=(a^2 b)^{1/3}$ is a radius of the equivalent-volume sphere; $K=(K_1+K_2+K_3)/3$- elastic module (in one constant approximation); $\delta$ – *droplet eccentricity*; $W a$ – *coefficient of azimuthal surface anchoring*; $\Delta \varepsilon'$- *effective dielectric anisotropy of the bipolar droplet*; $\varepsilon_0$ – the absolute dielectric constant.

The droplet shape was approximated by the elongated ellipsoid of rotation with semiaxes $(a, a, b \geq a)$ and a small eccentricity $(\delta \ll 1$, where $\delta=1-(a/b)^{1/2})$.

With the help of MathCAD software package we have simulated the dependence of Frederiks transition threshold field in nematic PDLC on finite azimuthal surface anchoring energy by fixed values of other parameters (table, fig. 4).
Values of polymer’s and nematic’s parameters which determine the Frederiks transition threshold field value in nematic PDLC.

<table>
<thead>
<tr>
<th>$\varepsilon_0$, F/m</th>
<th>K, 10^{-11}N</th>
<th>R, $\mu$m</th>
<th>$\Delta\varepsilon$</th>
<th>Wa, 10^{-6}N/m</th>
<th>$\delta$</th>
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<tr>
<td>8.85*10^{-12}</td>
<td>1</td>
<td>1,32</td>
<td>10</td>
<td>1</td>
<td>0,4</td>
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<td>5</td>
<td>2</td>
<td>12</td>
<td>20</td>
<td>0,6</td>
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<tr>
<td></td>
<td>100</td>
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</tbody>
</table>

Fig. 4. Dependence of Frederiks transition threshold field in nematic PDLC on finite azimuthal surface anchoring energy by fixed values of other parameters: 1) elastic module K; 2) droplet eccentricity $\delta$; 3) effective dielectric anisotropy of the bipolar droplet $\Delta\varepsilon^*$, and 4) radius of the equivalent-volume sphere R

Our results confirm the significant influence of a finite azimuthal surface anchoring energy of the polymer and nematic on Frederiks transition threshold
field value in nematic PDLC, and also indicate that the threshold field is largely determined by the radius of the equivalent-volume sphere and the effective dielectric anisotropy.

References:

out. Photosensitized fatty cells were irradiated with the radiation at a certain wavelength leading to the photocytotoxic effect. In photodynamic method low-energy lasers are used. The irradiation dose is selected not to exceed level of a thermal action. Efficiency of photodynamic action was provided with correspondence of radiation spectrum of source with absorption spectrum of photosensitizer. These methods can be used to develop technology removal of fat deposits in cosmetology.

Studying of optical methods for adipose tissue destruction in vitro, including photodynamic and selective photothermal methods, requires the development of a method allowing to estimate influence of different drugs and doses of laser radiation on cell viability of an investigated biotissue (Tuchin, 2009). The cell death can occurs under the influence of various physical, chemical and biological factors (Yanina, 2008). Depending on inductor occurs an apoptosis or necrosis cell. These two forms of cell death differ on biochemical and morphological signs. Biochemical changes occur quickly enough and difficulties of their detection are connected with it. Morphological sign of apoptosis is cell reduction in size, and necrosis is increasing in the cell size (Prints, 1999). This sign is simply enough defined visually by means of a digital video camera attached to microscope. The basic advantages of photodynamic and photothermal methods are their minimum invasiveness. There methods are approved enough, but require further development and adaptation to different drugs.

The goal of this work is development of photodynamic and photothermal methods, using various drugs (brilliant green, indocyanine green) and carrying out of experimental and theoretical researches of interaction of these agents with a adipose tissue, and also definition of a laser radiation dose required to induce apoptosis (or necrosis) cells of biological tissues. Within the limits of this work the problem of search of way the registration of lipolysis and apoptosis cells changing of their morphology, selection of pair dye-light source which provides “soft” operated technology of photodynamic influence which does not kill cells directly, but promotes it lipolysis (process can be stopped, having kept a cell live) or apoptosis.

The NIR transmittance spectrum of a layer of lipid mixture identical for the human adipose tissue, showing the absorption bands of lipids, and diffusion transmittance spectra for the 0.2 mm layer of abdominal fat of the female subject under surgery and for the 0.2 mm subcutaneous fat slab of male subject (post mortem, 48 hrs) are presented in Figs. 1 and 2. These spectra allows for prediction of light transportation of different wavelengths through adipose tissue and for providing of direct heating of fat by laser light of the corresponding wavelength. To study cell lypolysis (cell dimensions) and cell damage, the 100-150 μm adipose tissues slices were used in experiments in vitro. Water-ethanol solutions of indocyanine green (ICG) and brilliant green (BG) (440 and 650 nm) of 1 mg/ml and 6 mg/ml concentration, respectively, were used for adipose tissue staining. CW laser diode (AC-
CULASER, 812 nm) and dental diode irradiator Ultra Lume LED 5 (442 and 597 nm) were used for irradiation of tissue slices (table 1 and 2). Alterations of tissue morphology was studied using digital microscopy with attached Digital Camera for Microscope DCM500 (USB2.0), resolution 5 M pixels, connected to the PC, where images, where images were processed.

![Graph](image1.png)

Fig. 1. The NIR transmittance spectrum of a layer of lipid mixture identical for the human adipose tissue, showing the absorption bands of lipids

![Graph](image2.png)

Fig. 2. Diffusion transmittance spectra for the 0.2 mm layer of abdominal fat of the female subject under surgery (1) and for the 0.2 mm subcutaneous fat slab of male subject (post mortem, 48 hrs) (2)
Table 1

<table>
<thead>
<tr>
<th>Light source</th>
<th>Wavelength, nm</th>
<th>Power density, mW/cm²</th>
<th>Irradiation time, min</th>
</tr>
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<tbody>
<tr>
<td>LED</td>
<td>442</td>
<td>121</td>
<td>5, 7, 10, 13, 15</td>
</tr>
<tr>
<td></td>
<td>597</td>
<td>70</td>
<td>5, 7, 10, 13, 15</td>
</tr>
<tr>
<td>Diode Laser</td>
<td>810</td>
<td>250, 375, 500, 625</td>
<td>1, 2</td>
</tr>
</tbody>
</table>

Table 2

<table>
<thead>
<tr>
<th>Dye</th>
<th>BG</th>
<th>ICG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration, mg/ml</td>
<td>6</td>
<td>1</td>
</tr>
<tr>
<td>Absorption maximum, nm</td>
<td>440 and 650</td>
<td>700 – 805</td>
</tr>
</tbody>
</table>

Measured absorption spectrum of 0.1 % BG in ethanol and radiation spectrum of diode lamp (Ultra Lume LED 5) are presented in Fig. 3. Good correspondence of diode lamp radiation and BG absorption bands are well seen. Absorption spectrum of ethanol-glycerin solution of 1 mg/ml ICG and transmittance spectra of tape strips of the human skin stained in vivo by ICG solution are presented in Fig. 4 (Genina, 2002). Important to note that tissue staining leads to transformation of ICG spectra – strongest absorption maximum is moved to longer wavelengths to 805-810 nm. Fortunately, ICG binding to biomolecules makes diode laser with 810 nm more effective in interaction with the stained sites.

![Fig. 3. a) absorption spectrum of 0.1 % BG in ethanol; b) radiation spectrum of diode lamp (Ultra Lume LED 5)](image-url)
Optical (laser) radiation under control of its temporal, power and wavelength can induce different thermal effects via: 1) “sub-hyperthermia” (temperature lower than the customary hyperthermic cell-killing temperatures, metabolic and cell apoptosis temperatures); 2) hyperthermia (prolonged cell-killing temperatures); or 3) “high-level -hyperthermia(snapshot cell-killing temperatures, tissue selective thermolysis) in conjunction with localized specific fat tissue staining, and/or lipolytic, and/or apoptotic agents application resulting in body shape/contour improvement during the appropriate for a patient duration of the procedure.

The control tissue samples, which were not stained and exposed to light, were shown a good stability against environmental conditions without noticeable changes in structure during the characteristic time of any experiments. Images of adipose tissue sample stained by BG dye before and after irradiation during 15 min by Ultra Lume LED 5 (442 and 597 nm) at constant temperature of the sample of 39°C illustrate the efficiency of adipocytes damage using medical dye BG and corresponding light with power density of 70-121 mW/cm² (Fig. 5).

Fig. 6 represent images of subcutaneous adipose tissue sample stained by ICG before and after irradiation by the diode laser at 810 nm with power density of 500 mW/cm² during 1 min at constant temperature of 40°C. It is obvious that there was a cell lipolysis, which contributed to the optical clearing of adipose tissue. Cell lipolysis was seen as optical clearing effect of the upper cell layers of the photodynamically/photothermally modified adipose tissue slices. As a result of lipolysis, which is happened due to light induced cell membrane porosity, the intercellular content of the cell (free fatty acids (FFA))
percolates through these temporal pores into interstitial space. Thus refractive index of the interstitial fluid (initially equal to \( n_i = 1.36 \)) becomes close to the refractive index inside the adipocytes (fat refractive index, \( n_a = 1.44 \)) and due to refractive index matching effect the optical medium becomes optically homogeneous and more transparent to light.

![Fig. 5. Images of adipose tissue sample stained by BG dye before (a) and after irradiation during 15 min (b). Temperature of the sample was kept as 39°C. Ultra Lume LED 5 (442 and 597 nm), see Fig.3 and Table 1](image)

The optimal time for cell effective lipolysis and destruction could be found by variation of light exposure, temperature and ICG incubation time. Besides, it is possible to control cell destruction pathway – via either necrosis or apoptosis.

For the temperature of 40°C and light irradiation for 1 min and a power density of 250 mW/cm² observed morphological features of apoptosis (decrease in the amount of cells) and formation of apoptotic cells, and then also happened clearance tissue (Fig. 7).

![Fig. 6. Images of a subcutaneous adipose tissue sample stained by ICG before (a) and after (b) laser irradiation during 1 min. Time delay between image capture and irradiation finishing is 240 min (b). Temperature of the sample was kept at 40°C. Diode laser, 810 nm, power density 500 mW/cm²](image)

![Fig. 7. Images of adipose tissue stained by ICG dye before (a) and after laser irradiation during 1 min. Incubation time of 38 min (b), 74 min (c), 80 min (d) and 100 min (e). Temperature of the sample was kept at 40°C. Diode laser, 810 nm, power density 250 mW/cm²](image)

With increasing power density (500 and 625 mW/cm²) and the temperature of the sample (42 and 43°C) leads to the complete destruction of cell membranes and the cell dies by path necrosis.
The optical methods described in this paper may provide reduction of regional or site-specific accumulations of abdominal or subcutaneous adipose tissue least-invasively by inducing of cell apoptosis and controlled necrosis of small amounts an adipose tissue. In particular, it relates to the employment of localized optical (laser) radiation of the appropriate wavelength and power, which also may be integrated in conjunction with localized specific adipose tissue staining or lipolytic agents application, to noninvasive and non- or least-destructively downsize adipose tissue volume and thereby modify contour/shape local target adipose tissue. Behind fat reduction the major mechanisms are the enhancement of lipolysis of cell triglycerides due to expression of lipase activity and cell release of FFAs due to temporal cell membrane porosity, and delayed cell self-killing due to apoptosis caused by the induced adipocyte stress and/or limited cell necrosis.

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