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Computer Modelling and New Technologies, 2011, Volume 15, No.4

CONTENTS

Editors' Remarks

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The Beauty of it All

by Celia Berrell

All we can touch, and all we see
began in cosmic history.
How long ago, came things to be?
Perhaps it was infinity.

All our surroundings hold in store
the clues to what has gone before.
A fascination long prevails
to understand time's every tale.

Our tiny earth holds precious gifts
as through the universe it drifts.
With organisms varied, rife.
Are we alone in having life?

This special form of energy
enduring in its frailty,
bestows such beauty, all admired.
Intelligence is awe-inspired.

October, 2011

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Celia Berrell♣

This 15th volume No.4 presents the special issue, which puts forward the materials of NATO Advanced Research Workshop **Nanodevices and Nanomaterials for Ecological Security** (June 20–23, Riga–Jurmala, Latvia). This issue demonstrates the ARW general scientific report and short annotations of key-speakers' papers including problems formulations and general results and conclusions. It should be considered as a kind of promotion of forthcoming publication of the book **Nanodevices and Nanomaterials for Ecological Security**, Editors Yuri Shunin and Arnold Kiv, **Springer Science and Business Media** – NATO Science for Peace and Security Series – B: Physics and Biophysics.

♣**Celia Berrell** - Born in England, her literary icons include Edward Lear, Alan Milne, Roald Dahl and Isaac Asimov. Celia pursued a career in teaching maths and science for four years before travelling to Australia. That was thirty years ago. She has regarded her life in Australia as a working holiday ever since. Environmental poem *The Beauty Of It All* was selected for publication in the secondary school textbook *MacMillan English 7,* released in October 2011. *Battle of the Bulge* has been incorporated in a Science Presentation on gravity by the Australian Science and Mathematics School at Flinders University SA. Celia's articles and poetry have been published in magazines such as *Get Ahead Kids* and *Toastmaster*. A selection of her poems regularly appears in the CSIRO's children's science magazine *Scientriffic* and *The Helix.* They are found in anthologies such as the *Tropical Writers Raining On The Sun* (2008) and *Cracks in the Canopy* (2010). Award-winning poems include *Fat Chance* in the *Cairns Post Inaugural Writing Competition* January 2008 and *Replanting Neurons* in the *California Institute of Regenerative Medicine*'s stem-cell awareness contest in October 2010.

The main part of the program is concerned with the application of nanomaterials for the creation of novel nanodevices and sensor systems that are necessary for prevention of technogenic catastrophes and terrorist attacks. Multifunctional applications of these nanodevices were thoroughly considered in key lectures. The ARW participants have discussed the relevant scientific, technological and economic problems including fundamental problems of organic-inorganic hybrids improvements and their applications in the creation of novel nanodevices. The innovative approaches not only in the search for new combinations of organic and inorganic compounds, but also in the advanced engineering of materials with bioelectronic design principles have been discussed by ARW participants as well. The innovative approaches to the creation of biosensors for detecting pathogen microorganisms with radically lowered measurements time and detection limits were also a subject of key lectures.

Lectures devoted to the problems of radiation modification of nanomaterials, on the one hand, and to the defence against the radiation danger, on the other hand, have been included into the program.

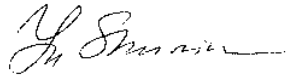
General problems concerning further advancement of nanotechnologies have been considered. Unexpected obstacles in the creation of novel nanodevices that have been recently revealed are a subject of intensive discussions among qualified experts from different countries. In particular, the problem concerns the nature of electronic noise in deeply scaled nanodevices. This problem is closely linked with the creation of the efficient lower-powered devices, including new sensor systems. A critical factor that puts on the further progress in nanotechnologies is the slowing speed of signal propagation within the chip. New approaches to the creation of nanomaterials that can ensure progress in the solution of chip interconnect problem have been presented by the leading laboratories.

Novel nanodevices based on a new direction of electronics – **"track electronics"** – have been considered from the point of view of the creation of principally new generation of electronic systems. All the aforementioned innovations have been considered in the light of the creation of novel nanodevices and electronic systems for special purposes of ecological security.

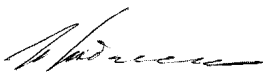
Our journal policy is directed on the fundamental and applied sciences researches, which are the basement of a full-scale modelling in practice.

This special edition we consider as a possibility to attract the attention of our readers and authors to the actual problems of nanotechnologies. We also hope our journal will be interesting for research community, and we are open for collaboration both in research and publishing. We hope that journal's contributors will consider the collaboration with the Editorial Board as useful and constructive.

EDITORS



Yu.N. Shunin



I.V. Kabashkin

Computer Modelling and New Technologies, 2011, Vol.15, N .4, 7–15
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QUALITY CONTROL SYSTEM AS A TOOL FOR COMPETITIVENESS ENHANCEMENT IN PRIVATE HIGHER EDUCATION MANAGEMENT: *THE SYSTEMIC CRITERIA ASSESSMENT*

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Strategies to deal with competitiveness enhancement in private higher education should start with its performance assessment. The importance to carry out such an evaluation is determined by a vast array of factors. The major ones include the requirement to develop innovative approaches to competitiveness increase, to compile new programs to capture the customer perception and to enter new education marketplaces, to construct effective and flexible assortment and education fee policies. All the aforementioned measures are directed to define the place of a higher education institution on the market. The possibility to attain this goal gains grounds in integration of operational and objective methods implemented for competitiveness assessment that will allow evaluating institutional performance and outcomes as well as offering particular ways to improve competitiveness.

Keywords*: system approach, intelligent system structure, quality system, higher education management*

1. Compatibility: a Common but Flexible Educational Framework

The higher educational sector globally is more competitive than it has ever been. Private educational establishments are under closer scrutiny than ever before, budgets are tight, job markets are enormously competitive and students are becoming increasingly discerning in the establishments and courses they choose.

Against this background, the need for educational organizations to carry out market research and keep a close check on internal and external offerings is self-evident. Competition in the education marketplace is constantly increasing.

We define an education market as a system that provides the freedom for knowledge producers and knowledge consumers to voluntarily associate with one another, as well as the incentives that encourage people to be loyal consumers, and educators to innovate, control education fees, and expand their services. It is a system in which institutions can offer instruction in any discipline, using any method, for which consumers are willing to pay.

As the economy becomes more global, a European educational-labour market grows more real. Private higher education systems and institutions are not just being asked to ensure that the people they are educating are employable, but also that they are employable on a European (or world) scale.

Private higher education institutions, as higher education in general, drive and are driven by globalisation. They ‘produce’ properly educated, qualified and highly skilled manpower and contribute to the research base and capacity for innovation that determine competitiveness in the knowledge-based global economy. They facilitate international collaboration and cross-cultural exchange. Cross-border flows of ideas, students, faculty and financing, coupled with developments in information and communication technology, are changing the environment where private higher education institutions function. Co-operation and competition are intensifying simultaneously under the growing influence of market forces and the emergence of new consumers. How will private higher education evolve over the following decades? How can governments and institutions meet the challenges and make the most of the opportunities?

In this paper we address these issues both from a quantitative and qualitative standpoint. The key issues under research include the Systemic approach to human resources management at a private higher education institution, to comparing the criteria and indices of its study programmes and their compatibility. Sociometric matrix method applied to institutional complex ratings is the factor that integrates all the elements.

The paper explores significant trends in private higher education provision, human resources management, including a specific focus on the role of market forces, mobility, and quality assurance in higher education. Taking into account specific economic, social and cultural contexts, an essential challenge for private higher education systems is to combine the encouragement of efficiency and excellence with the promotion of equity and access.

The overall emphasis on quality assurance has started to move towards assessing educational and labour market outcomes instead of inputs, but there are still notable differences between audit and evaluation approaches across regions. At the same time, one can observe the emergence of cross-border accreditation and a general strengthening of co-operation across borders: several regional networks of quality assurance agencies have been established and there is an increasing interest in establishing common regional criteria and methodologies, particularly in Europe. The emergence of a common quality assurance framework on a global scale does not, however, seem likely in the near future.

Private higher education institutions are aware that they face increasing competition when carrying out their core missions of teaching and research, when developing and implementing innovative education marketing programs, and when they are providing additional privileges and services to society, the amount and range of which is now vast. In order to exploit external educational opportunities (cooperation) accompanying the threat of external competition from other providers of research, education and training – some coming from other parts of the world – institutions need within their systems to establish the image of the institution and evaluate both internal and external awareness and perceptions. It provides insight as to how your institution is positioned against competitors on the attributes that drive positive image and perceptions of the institution.

Compatibility of the institution and its brand image are determined by the ability to attract and retain students offering them a variety of qualifications, the state-of-the-art education and training, advantageous education fees, innovative methods of teaching, flexible forms and full-scale levels of education, comfortable educational environment and conditions, convenient education location site, attractive image of the institution, advertising and numerous other factors.

Higher education institution is an open system permanently experiencing the influence of the external environment. To attain sustainable development, the institution needs to reach a well-balanced integration of internal capacities and constantly changing external demands. Changes in the external environment inevitably cause changes in the internal educational environment. Major external factors influencing the institutional functioning include:

- external environment complexity: the amount and variety of factors to be reflected by the institution is huge and their analysis is time-consuming;
- external environment mobility: major factors and key processes undergo constant changes there, bringing considerable or even fatal consequences to the organization;
- external environment fluctuation: the changes in the external environment are difficult to define and their pace is unpredictable.

Thus, the analysis of the internal environment is directed, first of all, to elucidating institutional strengths and weaknesses. A solid marketing strategy can, therefore, directly affect the bottom line of a private higher education institution through measurement and understanding of its position in the marketplace and by eliminating weaknesses and building upon strengths. The system of external and internal educational environments integration on different levels of functioning, and the impact of the external environment upon the quality and educational activities of a private higher education (Figure 1) result in changes not only in the performance quality and outcomes of particular educational departments, but in education quality in general.

Vigorously competitive education industry poses the necessity for careful and skilful construction of the internal educational environment and the system of its quality control that has a direct continuous impact on the functioning of the whole educational establishment. Under the present circumstances, private higher education has to consider the inner factors and processes even closer from a variety of perspectives. Internally, institutions must manage costs, similar to traditional educational services, while at the same time there is a growing need to specialize and communicate a unique message to an expanding marketplace. From the applicant's vantage, student prospects are faced with more education options than ever before

Private higher education institutions must be free to make strategic choices, to concentrate on their core areas, to develop individual identities, to choose their partners, and to position themselves to compete to deliver quality education, research and services. Private higher education institutions are taking responsibility for the preservation of their core values — as well as their adaptation to changing times.

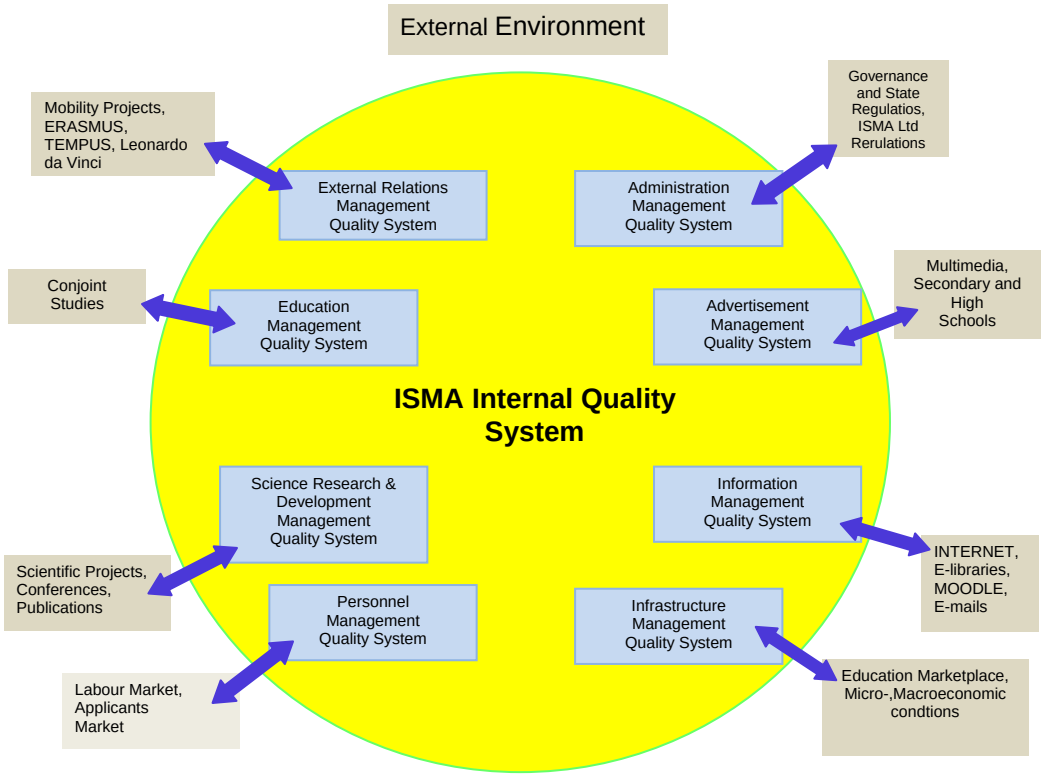

Figure 1. The system of external and internal educational environments integration on different levels of functioning

When the pace of change accelerates, institutions need even more autonomy to steer their course of action. Quality control system (Figure 2) has to become a focal point of competitiveness enhancement in these circumstances.

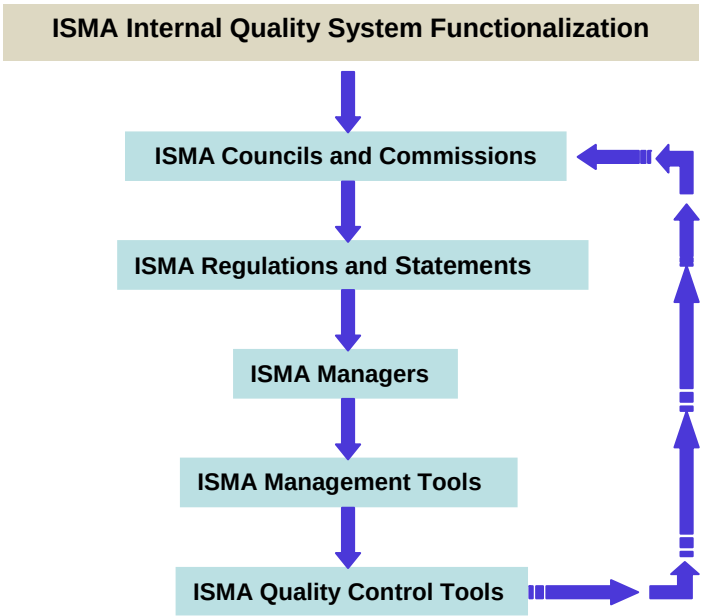

Figure 2. Quality Control System in a private higher educational institution

Since the functioning of the higher education institution is indispensable from the external environment, it is possible to distinguish between different levels of environmental influence:

- *local* (the direct impact environment) – these are factors that have a straight effect on the inner processes of the organization. The components of this environmental level include consumers, competitors, laws, governmental structures;
- *intercultural* (multicultural business environment) – these are factors contributing to organization expansion and entering new cross-border marketplaces;
- *global* (the indirect impact environment) – these are factors that do not have the immediate influence on the institutional activities: sociocultural, technological, economic, ecological, political and legal factors.

Compatibility self-assessment is the initial and essential element of applying primarily qualitative criteria that assess the institution's current state of affairs in terms of quality and its effectiveness for undertaking measures directed to the enhancement of indices. A wide range of methods can be used to evaluate compatibility of higher educational institutions. One of the approaches is the so-called ratings evaluation or the method of ranking.

The institutional performance evaluation is conducted through a combination of several criteria: the quality of academic programmes and competence outcomes, faculty qualifications and numbers, quality oriented performance, the levels of scientific research and achievements, the size of the institution, and the number of applicants and graduates. However, the major factors envision the perspective institutional quality potential and its relevance to national needs.

Institutional quality self-assessment is a disciplined, coordinated, systematic, and sustained effort to achieve the institution's mission and goals through decisions and actions that shape and guide what the institution is, what it does, and why it does it, with a focus on the future.

The institution regularly evaluates its actions and achievements in conformity with its mission and goals. The evaluation results provide a fair and systematic set of information to help in intuitional improvement with emphasis on academic programmes. Evaluation enables an institution to verify with reliable means its achievement in accomplishing its goals and objectives inside and outside the institution both in a quantitative and qualitative manner.

The Institutions face the challenge of maintaining a balance among its goals, directions from the Government, expectations of all those to whom it is accountable, and the availability of resources. The sustainable development of an effective institution depends upon a rational and consistent inbuilt process of self-assessment and planning. The nature and quality of planning conducted by an institution is considered to be the best indicator of its effectiveness which is further linked up with its capability to achieve its own goals and flexibility to simultaneously respond to the dynamics of the prevailing environment. Thus, with efficient planning, regular self-assessment, along with clarity of mission and strategic thinking, an institution continues to meet its purpose and goals, while creating equal opportunity for further development and compatibility.

The effectiveness of the institution's organizational structure and governance system is improved through reviews and assessments on periodic basis. These evaluation results are conveyed to administrators and faculty members and integrated in planning for the purpose of quality improvement and increased effectiveness of governance practices at the institution to raise its rating on the international marketplace.

2. Rating Assessment Model of Institutional Performance

The rapid growth of competition among private and public higher education institutions in response to high demand in education is a comparatively recent phenomenon in the higher education market in which a public and a private universities compete for students offering similar academic programmes in the presence of borrowing constraints.

Students differ in their unobservable ability and in their income endowment, and choose whether to attend a public or private institution with a lower tuition fee in order to maximize their lifetime income. Therefore, institutions strive to compete to offer up-market educational services and to guarantee extra privileges and additional advantages.

Rating assessments of higher education institutions (HEIs) and programs are a global phenomenon. They serve many purposes: they respond to demands from consumers for easily interpretable information on the position of higher education institutions; they stimulate competition among them; they provide some of the rationale for allocation of funds; and they help differentiate among different types of institutions and different programs and disciplines. In addition, when correctly understood and interpreted,

they contribute to the definition of 'quality' of higher education institutions on the national level and internationally, complementing the rigorous work conducted in the context of quality assessment and review performed by public and independent accrediting agencies. This is why rankings of higher education institutions have become part of the framework of national accountability and quality assurance processes, and why more institutions are likely to see the development of ratings or rankings in the future.

Given this trend, it is important to start with consecutive stages of compatibility self-assessment. The first stage provides a market-based research, formulation and systematisation of consumer demands towards the higher education or the academic programme, which allows designing indicators of competitiveness to consumer requirements.

The designed indicators can be divided into three major categories: economic, quality, and indicators of external representation, which, in their turn, are subdivided into the following sub-groups:

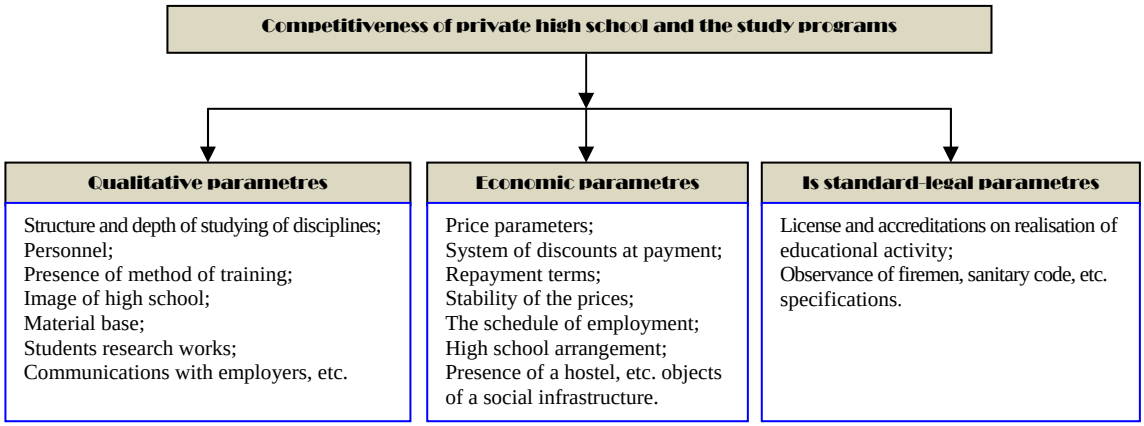

Figure 3. Competitiveness indicators for higher education and academic programmes

Special systemic criteria/factors are necessary to determine to carry out competitiveness assessment. A method of sociometric matrices can be applied for this purpose. One of the best-known techniques of sociometric analysis is that outlined by Moreno in *Who Shall Survive?* [1]. Sociometry, by definition of its founder – Jacob L. Moreno, measures the 'socius' – the interpersonal connections between people. The basic data for this matrix analysis are derived from the sociometric test which consists in eliciting positive (choose/acceptance/attraction) or negative (not-choose/rejection/repulsion) choices for associates of any group which an individual might become a member of.

The techniques for administering a sociogram consist of five basic stages: 1) criterion selection, 2) matrix formation, 3) sociogram charting, 4) analysis, and 5) application. The criterion for sociometric utilization refers to the 'what' one wishes to measure, and usually a question about some aspect of social interaction. For an academic programme the criteria/factors will be the following:

- the number of students per academic staff unit,
- the number of professors per academic staff unit,
- the number of granted student places per total number of students,
- the number of student loans per total number of students,
- specific programmes of payment,
- social benefits for particular specializations.

For a higher education institution the criteria/factors will be the following:

- the number of students per academic staff unit,
- the number of professors per academic staff unit,
- the number of granted student places per total number of students,
- the number of student loans per total number of students,
- the number of accredited programmes,
- tuition fees,
- social benefits offered by the institution.

All the aforementioned criteria can either increase or decrease. A sociometric matrix is a data summary sheet which systematically organizes the choices and/or rejections as presented by each respondent [3, 4]. It is a multicellular chart with two margins: one at the left vertical margin and the other at the top, proceeding horizontally. A matrix is completed based on the initial data (Figure 4), in which all

the choice patterns appear simultaneously – a visual representation of the psychological situation in the group seen from the viewpoint of each individual – the so-called a *matrix of domination – D*.

Competitiveness of higher school

1. **Number of students per academic staff units**
2. Number of professors per academic staff units
3. Part of budget places per total student number
4. Part of social credit places per total student number
5. Number of accreditated study programmes
6. Average Cost of Study
7. Social priority of the higher school

Typical Table of Comparison Factors

Higher School	1	2	3	4	5	6	7
1	16	0,2	0,2	0,5	7	2200	0,5
2	20	0,4	0,1	0,6	10	1200	0,6
3	12	0,3	0,1	0,7	20	1500	0,7
4	14	0,1	0,4	0,5	4	1600	0,4
5	10	0,15	0,6	0,3	8	2500	0,3

Domination Matrix of the 1st factor

$$D_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Figure 4. Sociometric Matrices Approach or Complex Ranking of Private Higher Education Institutions

Further on, a ranking matrix according to the first criteria is calculated (that is the sum of dominants) and the symbols are recorded in the cells of a conventional vertical margin (Figure 5).

Competitiveness of higher school

1. **Number of students per academic staff units**
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4	14	0,1	0,4	0,5	4	1600	0,4
5	10	0,15	0,6	0,3	8	2500	0,3

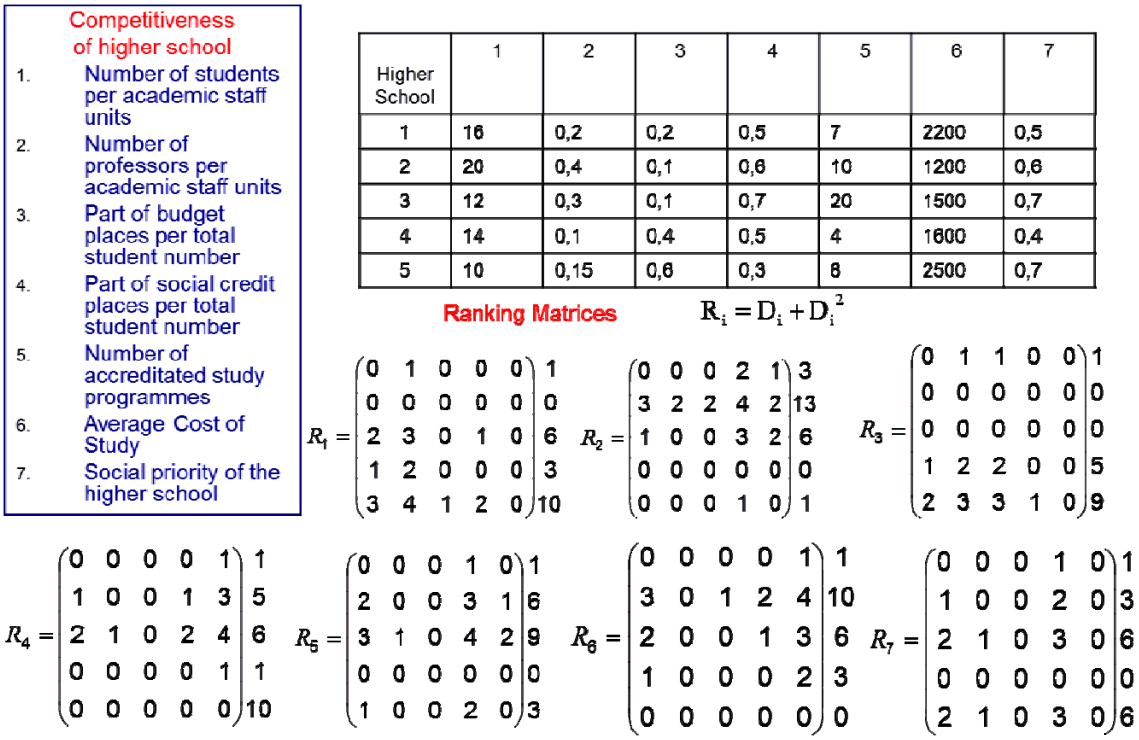
$$\mathbf{R}_1 = \mathbf{D}_1 + \mathbf{D}_1^2$$

Ranking Matrix of the 1st factor

$$R_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 2 & 3 & 0 & 1 & 0 \\ 1 & 2 & 0 & 0 & 0 \\ 3 & 4 & 1 & 2 & 0 \end{pmatrix} \begin{matrix} 1 \\ 0 \\ 6 \\ 3 \\ 10 \end{matrix}$$

Figure 5. Sociometric Matrices Approach for Complex Ranking of Private Higher Education Institutions

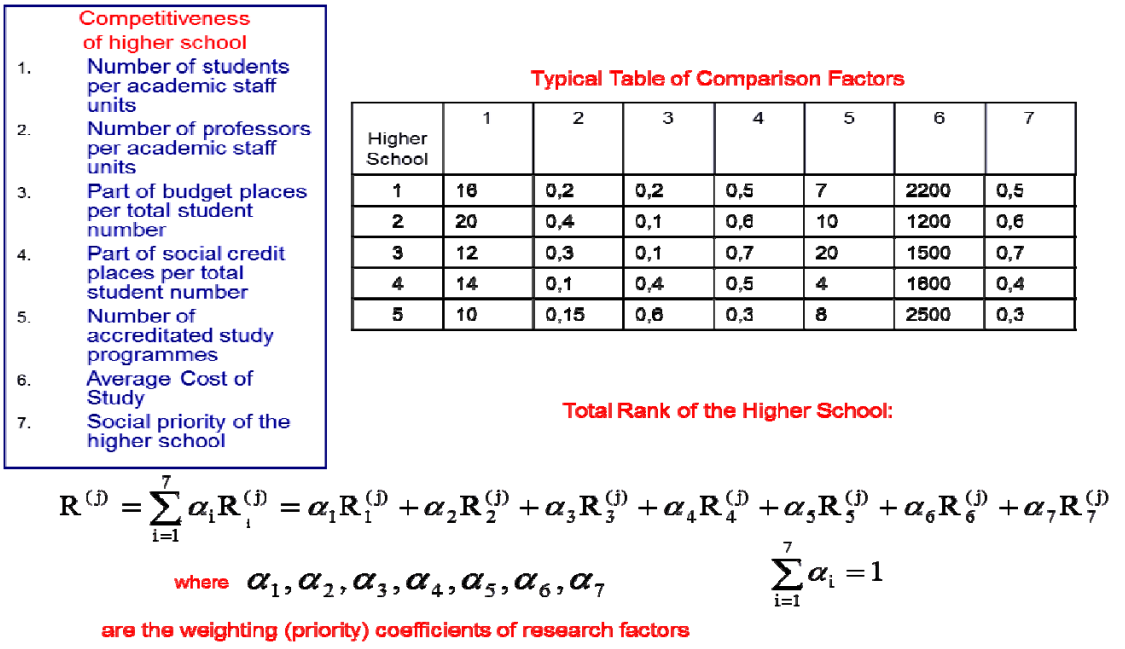
In the same way a ranking matrix according to each criteria/factor is calculated and the results are registered in the appropriate cells (Figure 6).



Higher School	1	2	3	4	5	6	7
1	16	0,2	0,2	0,5	7	2200	0,5
2	20	0,4	0,1	0,6	10	1200	0,6
3	12	0,3	0,1	0,7	20	1500	0,7
4	14	0,1	0,4	0,5	4	1600	0,4
5	10	0,15	0,6	0,3	8	2500	0,7

Figure 6. Sociometric Matrices Approach for Complex Ranking of Private Higher Education Institutions

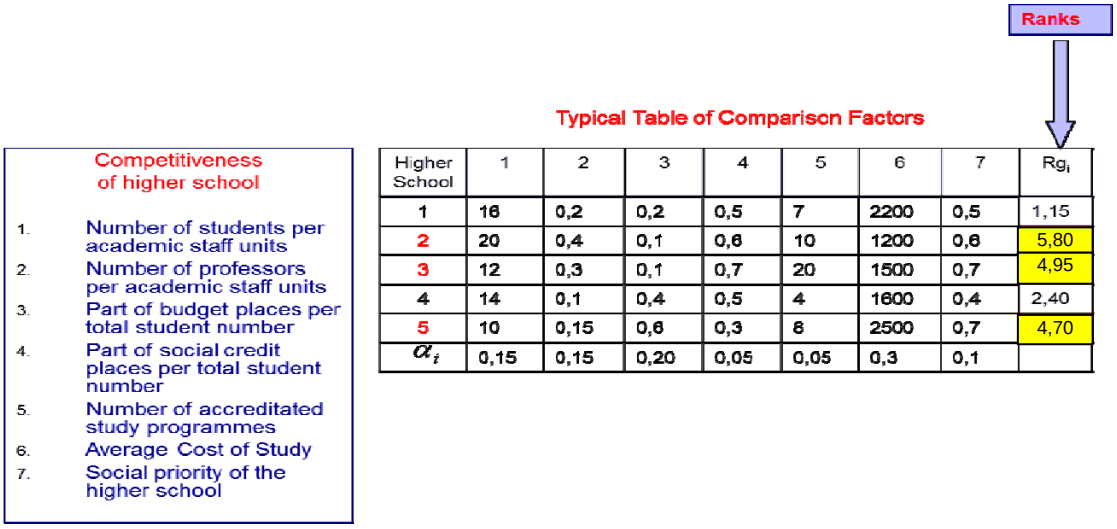
As a result, it is possible to calculate the final institutional rating coupling the obtained data with the importance factors (weighting/priority factors), where R – is the general rating of a particular institution, j – is the number of the institution, *a* – is the weighting (priority) factor, and *i* – is the number of criteria/factor. Thus, we can get a typical table of comparison factors/criteria (Figure 7).



Higher School	1	2	3	4	5	6	7
1	16	0,2	0,2	0,5	7	2200	0,5
2	20	0,4	0,1	0,6	10	1200	0,6
3	12	0,3	0,1	0,7	20	1500	0,7
4	14	0,1	0,4	0,5	4	1600	0,4
5	10	0,15	0,6	0,3	8	2500	0,3

Figure 7. Sociometric Matrices Approach for Complex Ranking of Private Higher Education Institutions

It is very economical to use the matrix to locate the sociometric stars, rejectees, and isolates, which makes it possible to see the share of a certain criterion's weighting (priority) in the institutional rating (Figure 8). Sociometric stars are those institutions that have received the largest number of positive responses according to the defined criteria/factors. The sociometric rejectees receive the largest number of negative responses. The sociometric isolates are those institutions that have received no positive or negative responses; they have not been chosen at all.



Higher School	1	2	3	4	5	6	7	Rg_i
1	16	0,2	0,2	0,5	7	2200	0,5	1,15
2	20	0,4	0,1	0,6	10	1200	0,6	5,80
3	12	0,3	0,1	0,7	20	1500	0,7	4,95
4	14	0,1	0,4	0,5	4	1600	0,4	2,40
5	10	0,15	0,6	0,3	8	2500	0,7	4,70
α_i	0,15	0,15	0,20	0,05	0,05	0,3	0,1	

Figure 8. Sociometric Matrices Approach for Complex Ranking of Private Higher Education Institutions

The research results have demonstrated that the model of sociometric matrices can be successfully applied for the purposes of compatibility assessment of higher education institutions, since it provides the possibility:

- to design methodologies for compatibility assessment of higher education institution and its academic programmes based on differentiation of compatibility factors/criteria applied to educational services and the institution in general;
- to determine the most essential factors/criteria that influence compatibility of educational business;
- to work out recommendations on strategic approaches for compatibility enhancement.

The Rating Assessment Model of Institutional Performance offers the methodology for Higher Education Institutions (HEIs) that helps to direct efforts to get recognition for maintaining and improving the academic quality by evaluating and demonstrating that high standards are being met and academic activities are also in accordance with the national policies striving to further enhance the standards according to international practices and development and international compatibility.

3. Conclusions

It is to be understood that an institution may be stronger than others while serious weaknesses in a particular area may negatively affect the institution's performance evaluation status and, consequently, its rating among the competitors. Also, meeting institutional performance evaluation standards will not assure the quality of its academic programs, courses or graduates. These standards are primarily qualitative criteria that assess the institution's current state of affairs in terms of quality and its effectiveness.

Therefore, the Rating Assessment Model of Institutional Performance can be considered an essential tool for competitiveness enhancement, since it helps the institution decide on appropriate mechanisms to increase the share of a certain weighting (priority) criterion/factor in the institutional rating, prioritisation for particular criteria/factors, means to generate the desired rating, financial control, utilization of allocated resources and elimination of weaknesses.

Implementation of the obtained research results can contribute to the development of scientifically grounded concept for higher education institution management, stimulate compatibility self-assessment, eliminate weaknesses and build upon strengths.

In the present conditions of stiff competition for students, private higher education institution functions, first of all, as the subject of entrepreneurial activities, being an autonomous economic system with a classical management framework. The unique equilibrium in which the public institution is different from the private institution, thus, appears a totally eliminated concept. In terms of management, the key factor becomes economic effectiveness. The research highlights the interdependence of the elements of the institutional management system with key economic indices of its performance and outcomes.

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SUPRAMOLECULAR COMPLEXES OF CARBON NANOTUBES WITH DOXORUBICIN AND POLY (ETHYLENE GLYCOL) STUDIED USING THE MOLECULAR DOCKING AND DYNAMIC METHODS

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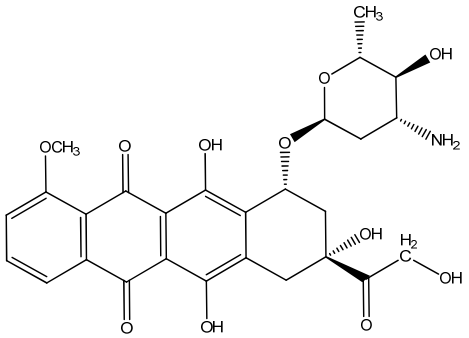
Using the molecular dynamic and docking techniques, the binary and ternary complexes of antitumour drug doxorubicin, carbon nanotubes, and poly (ethylene glycol) are studied. On this basis, we determine the hydrophilic/lipophilic behaviour, the structures and stabilities of supramolecular complexes in water and organic (octanol) solutions and give recommendations on what type of nanotubes should form the most perspective compositions for delivery of the doxorubicin. It is shown that coupling between the nanotube and solvent molecules results in a regular approximately circular alignment of both water and octanol molecules in the outer region and in the inner cavity of the nanomaterial. Both solvents influence the doxorubicin conformation. In water, the conjugated core of doxorubicin is orientated almost parallel to the nanotube surface favouring a surface complexation of the drug and tubule. In organic solvent, the core and the nanotube surface are orientated virtually perpendicular, pointing on the absence of π-π-stacking coupling. In the case of water, increase of distance between the tubule and drug results in energy increase, but in the organic solvent, the lager distance between tubule and doxorubicin the smaller is energy. The stable nanotube-doxorubicin supramolecular complexes being formed in water solutions are to be destroyed in biological tissues resulting in drug release. For nanotubes of small diameters $d < 12.5$ Å of any chirality (armchair or zigzag), the doxorubicin molecule is located on the outside of the nanotube, but for nanotubes of larger diameters it is to be located inside the tube. The tubule diameter dependence of the doxorubicin bond energy is nonmonotonic: the complexes with nanotubes having $d \sim 13.5$ Å are the most stable, the doxorubicin molecule being located inside the nanotube. The external or internal location of poly (ethylene glycol) in the complexes with nanotubes is dictated by the tube diameter too; however, the boundary diameter is different ($d \sim 11$ Å). This fact makes it possible to predict that in the ternary supramolecular complexes of (8, 8) and (14, 0) nanotubes the poly (ethylene glycol) molecule is to be located inside and the doxorubicin molecule outside the nanotube. These complexes should be the best water soluble doxorubicin carriers on the basis of the water soluble nanotubes.

Keywords: *Molecular dynamic; molecular docking; nanotube; doxorubicin*

1. Introduction

Despite the success of current treatments for several types of cancer, all known treatments have major limitations. The conventional chemotherapy or radiotherapy damage many cells, and both have significant side effects. In addition, tumour cells develop resistance to many chemotherapeutic agents, and most chemotherapeutic drugs kill dividing cancer cells and not dormant ones. The carbon nanotubes are the aromatic cylindrical molecules with inner cavity. The unique physical properties of carbon nanotubes allow for a range of novel cancer therapies including photothermal therapy, photoacoustic therapy, and radiofrequency ablation treatment of tumours [1, 2, 3, 4, 5].



During the last decade single-walled carbon nanotubes have been extensively explored as nanoscale drug carriers for potential applications in cancer treatment [6, 7, 8]. The doxorubicin ($C_{27}H_{29}NO_{11}$) is

the drug for chemotherapeutic treatment of some forms of cancer [9, 10]. Unfortunately, doxorubicin suppresses hematopoiesis and exhibits gastrointestinal toxicity [11] and cardiotoxicity [12]. This drug can be more widely and efficiently used in clinical practice if it is delivered directly to the diseased tissues. This can be provided by using nanotubes since they accumulate in diseased tissues, on the one hand, and form complexes with doxorubicin, on the other [13]. The nanotubes are almost insoluble in water, which hinders their direct use as the medicinal drug carriers. However, complexation of nanotubes with a poly (ethylene glycol) leads to water soluble nanotube derivatives. The experiments on mice have shown that the nanotubes functionalised with poly (ethylene glycol) are non-toxic [14, 15]. The circulation time of nanotubes complexes with poly (ethylene glycol) in the blood ($t_{1/2}$ equal to 22.1 hours) sharply increases as compared with the circulation time of free nanotubes (5.4 hours) [16]. This is responsible for higher transport characteristics of the nanotubes poly (ethylene glycol) complexes as compared with free nanotubes. Finally, *in vivo* experiments have confirmed that the supramolecular doxorubicin complexes with nanotubes functionalised by poly (ethylene glycol) are efficient in cancer therapy [17]. In these studies, mixtures of nanotubes of different structure (diameter and chirality) were used. The therapeutic efficiency of the composition can be enhanced by choosing a nanotube that would provide its best binding to poly (ethylene glycol) and doxorubicin.

The present study is aimed at estimating the hydrophilic/lipophilic behaviour of the nanotubes, doxorubicin, and their complexes and determining the energies of complex formation of nanotubes with doxorubicin and poly(ethylene glycol) using molecular dynamic and docking techniques. On this basis, we determine the structures and stabilities of supramolecular complexes of nanotubes with doxorubicin and poly (ethylene glycol) in water and organic solutions and give recommendations on what type of nanotubes should form the most perspective compositions for the doxorubicin delivery.

2. Simulation Methods

The doxorubicin and nanotubes are coupled through the non-covalent intermolecular forces. In the supramolecular complexes of single-walled nanotubes with poly (ethylene glycol), a chemical bonding is also intermolecular one. Therefore, to assess the structure and stability of the complexes, one should use the methods of computational chemistry adapted for the calculation of intermolecular forces. Nowadays, the molecular dynamics and docking techniques are direct approaches and the most popular to solving such problems. In both methods, a total potential energy of system is evaluated as a sum of several individual contributions, namely, the bond stretching, angle bending, torsion, stretch-bend, torsion-stretch, bend-bend, electrostatic, and van der Waals energies.

In this study, the nanotube and ligand molecules were arranged in a cell with the geometry of a rectangular parallelepiped, and the free space in this parallelepiped was filled with solvent molecules. The molecular dynamic simulations were carried out using a Tinker package [18], which previously had been applied to studies the polymer composites with nanotubes [19, 20, 21, 22]. The molecular docking studies were performed using an Autodock 3.0 computer program [23]. Both methods are essentially empirical and depend on the applied parameters scales. In our molecular dynamics simulations, we used the so-called OPLSAAL force field [24] widely used in the studies of common organic and inorganic materials, a TIP3P model [25] being applied for water. In case of molecular docking technique, we used the potential parameters specified in the form of tables for basic chemical elements and presented in Ref. 23.

In the molecular dynamics calculation, the velocity form of Brook's "Better Beeman" method [26] was used to integrate the equations of motion with a basic time step of 1.0 fs, and the Nose-Hoover thermostat algorithm [27] was used for temperature control. All the molecular dynamics simulations were implemented at 300 K. A cutoff distance of 10 Å was used for all potentials, and *NVT* (the number of particles (*N*) and the volume (*V*) of system in the ensemble are constant and the ensemble has a well-defined temperature (*T*), given by the temperature of the heat bath with which it would be in equilibrium) ensemble has been applied.

In molecular docking calculations, the nanotubes were taken to be the rigid host macromolecule with fixed geometry and position in space, and the ligand molecules [poly (ethylene glycol) and doxorubicin] were taken to be guests that executed random walks in the vicinity of the rigid nanomaterial and were considered as the nonrigid systems with large number of possible conformations. In each step of simulation, the ligand executed small random displacements along each degree of freedom: the displacement of the centre of gravity, orientation of the molecule, and rotation about nonrigid bonds with the changes in

internal dihedral angles. These displacements lead to the formation of a new configuration of the ligand and of the macromolecule ligand complex. For each configuration of complex thus generated, the energy of interaction of the ligand with the macromolecule was calculated as the sum of the interaction energies of atoms of the ligand and macromolecule. Among the vast number of possible conformations, the most stable conformations of complex were selected with the use of genetic algorithms and annealing procedure [23].

3. Hydrophilic/Lipophilic Behaviour of the Nanotube and Doxorubicin

Let us discuss the results of the molecular dynamics simulations of the hydrophilic/lipophilic behavior of carbon nanotubes and doxorubicin. To study the lipophilic interaction, we take octanol as a typical non-polar solvent. It is shown below using molecular docking that the (8, 8) tubule forms stable ternary complexes with doxorubicin and poly (ethylene glycol) in water. Correspondingly, we take the particular cases of the pure and poly (ethylene glycol) functionalised tubules (8, 8) in the molecular dynamics study of hydrophilic/lipophilic behaviour.

Figs. 1 shows a distribution of the water and octanol molecules in a neighbourhood of the (8, 8) tubule. One can see that the intermolecular coupling between the nanotube and solvent molecules results in a regular approximately circular alignment of both water and octanol in the outer region and in the inner cavity of the nanomaterial. Possibly, due to a formation of H-bonds between the H_2O molecules, the cylindrical layer-type structure of the water molecules arrangement is more pronounced in comparison with that of the organic solvent; for example, one can note some circular ordering of the H_2O molecules beyond the first layer too. The H_2O molecules in the first layer are aligned so that their OH bonds are directed to the outer and inner cylindrical surfaces of tubule, the distance between carbon cylinder and the nearest hydrogen atoms being equal to 2.0 Å approximately. Note that similar regular water distribution in region of the (16, 0) nanotube was observed previously on basic of molecular dynamics simulations with another force field parameter scale in [28].

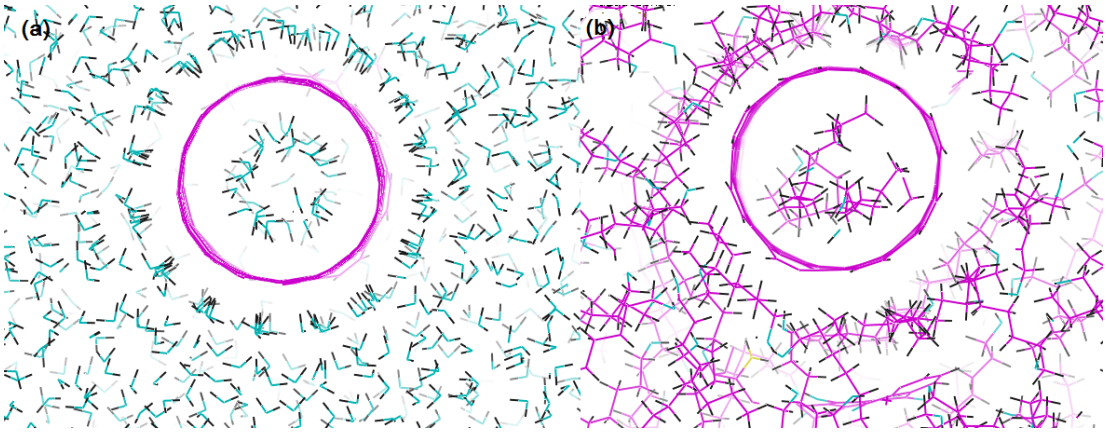


Figure 1. Distribution of solvent molecules in the region of (8, 8) nanotube: (a) water, (b) octanol

The coordination of the octanol on the outer cylindrical surface of (8, 8) nanotube is characterized by wrapping of the tubule by rather long organic molecules, manifesting the lipophilic coupling between the components. The average distance between the carbon cylinder and the nearest H atoms of octanol equals 2.5 Å is longer than in the case of water.

Figure 2 shows that water and octanol solvents influence the doxorubicin conformation. There is some change of planarity of rigid conjugated core of drug. The OCH_3, $COCH_2OH$, and $OC_6O_2NH_3$ groups vary their orientation relative to the core due to the coupling with solvent. The geometry of doxorubicin changes due to the coupling with the nanotube too, the orientation of doxorubicin relative to the tubule being sensitive to the solvent. In the case of water, the conjugating core is orientated almost parallel to the nanotube surface favouring a surface complexation of the drug and tubule. In organic solvent, the core and the nanotube surface are orientated virtually perpendicular, pointing on the absence of π-π-stacking coupling.

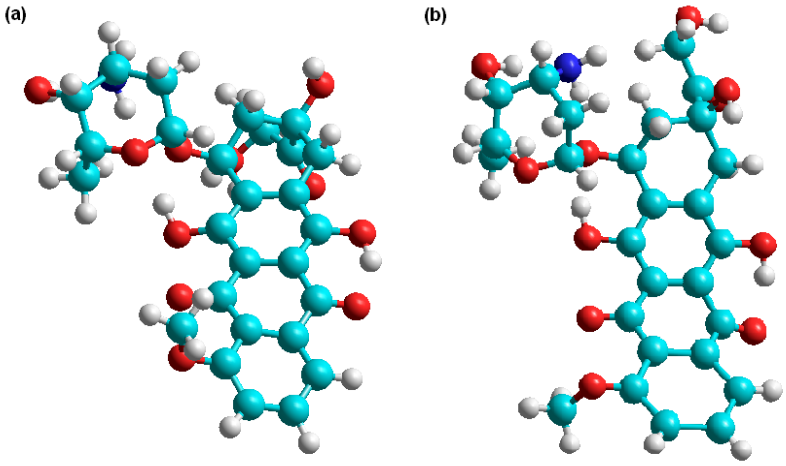


Figure 2. Conformation of the doxorubicin molecule in water (a) and octanol (b) solutions. Solvent molecules are not shown

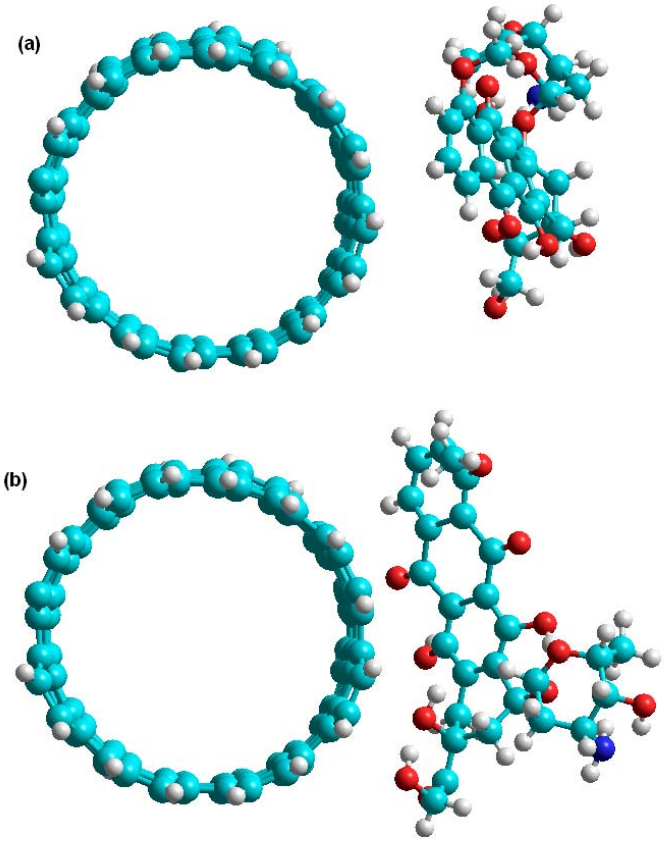


Figure 3. Conformation of the doxorubicin molecule near nanotube in solutions. In water (a), the conjugating core is orientated almost parallel to the nanotube surface. In octanol (b), the core and the nanotube surface are orientated virtually perpendicular. Solvent molecules are not shown

The differences between the solvents effects on coupling of doxorubicin and nanotube is most pronounced in the dependences of total energies on the distance between the tubule and drug (Fig. 4). In the case of water increase of this distance it results in energy increase. On the contrary, in the organic solvent, the lager distance between tubule and doxorubicin the smaller is energy. These data show that

the complex under consideration is stable in water but not in the octanol. Thus, the molecular dynamic calculations support an intuitive idea that the stable nanotube-doxorubicin supramolecular complexes being formed in water solutions are to be destroyed in biological tissues resulting in drug release.

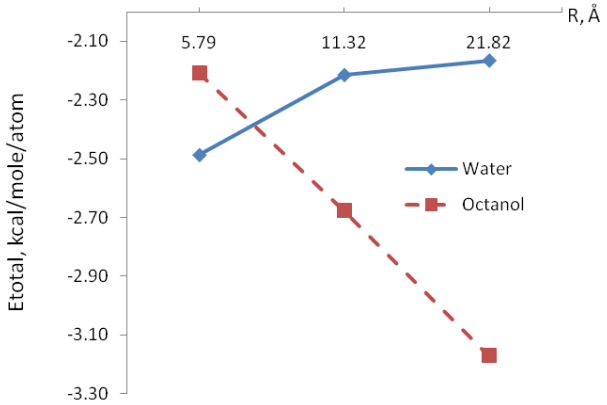


Figure 4. Total energy versus distance between doxorubicin and (8, 8) nanotube in water and octanol solution

4. Doxorubicin and Poly (Ethylene Glycol) Docking with Nanotubes

Now, let us discuss in detail the nanotube diameter and chirality dependences of the structure and stability of the nanotubes supramolecular complexes with doxorubicin and poly (ethylene glycol) in water, because it is the stabilization of appropriate complexes between doxorubicin and vehicle in this solvent that is of great importance for the drug delivery.

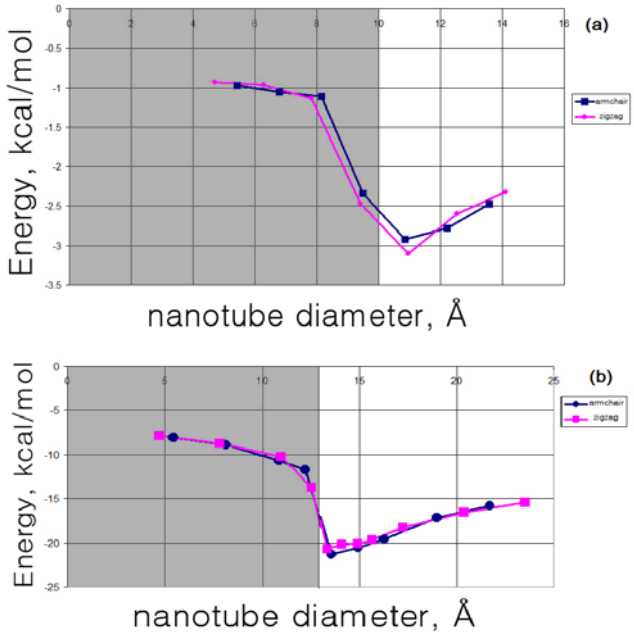


Figure 5. Formation energies of the complexes of (a) doxorubicin and (b) poly (ethylene glycol) with armchair and zigzag nanotubes

The docking results show that, for nanotubes of small diameters $d < 12.5$ Å of any chirality (armchair or zigzag); the doxorubicin molecule is located on the outside of the nanotube in energetically most favourable conformations (Fig. 5a, shaded area). For nanotubes of larger diameters, doxorubicin is to be located inside the tube. The dependence of the doxorubicin bond energy on the tube diameter is nonmonotonic: the doxorubicin complexes with (10, 10) and (19, 0) nanotubes ~ 13.5 Å in diameter are the most stable, the doxorubicin molecule being located inside the nanotube. It is clear that the bond

energy of the complex of poly (ethylene glycol) with a nanotube depends on the poly (ethylene glycol) chain length. Calculations showed that this energy is directly proportional to the number of units in the polymer. Therefore, it is convenient to recalculate this bond energy per unit (Fig. 5b). As in the case of doxorubicin, the external or internal location of poly (ethylene glycol) is dictated by the tube diameter; however, the boundary diameter is different ($d \sim 11$ Å). This fact makes it possible to obtain ternary supramolecular complexes with the poly (ethylene glycol) molecule being inside and the doxorubicin molecule being outside the nanotube. These complexes will be excellent doxorubicin carriers on the surface of the water soluble nanotubes since doxorubicin and poly(ethylene glycol) do not compete with each other for binding to the same (internal or external) tube surface (Fig. 6). This pertains to the complexes of (8, 8) and (14, 0) nanotubes.

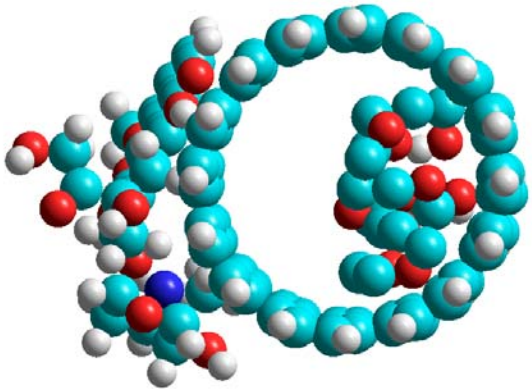


Figure 6. Supramolecular complex of the (8, 8) nanotube with doxorubicin (on the outside) and poly (ethylene glycol) (inside) according to molecular docking data

Thus, for any nanotubes of small diameters, the arrangement of doxorubicin on the outside of the nanotubes is energetically more favourable. For nanotubes of more than 12.5 Å in diameter, both doxorubicin and poly (ethylene glycol) should be located inside the nanotubes. For nanotube diameters 11 Å $\leq d \leq$ 12.5 Å, in energetically favourable complex conformations, doxorubicin is located on the nanotube surface while poly (ethylene glycol) is inside the nanotube.

5. Conclusions

Using the molecular dynamic and docking techniques, the binary and ternary complexes of antitumour drug doxorubicin, carbon nanotubes, and poly (ethylene glycol) are studied in water and organic (octanol) solutions. The hydrophilic/lipophilic behaviour, the structures and stabilities of supramolecular complexes are determined. We predict that in the ternary supramolecular complexes of the (8, 8) and (14, 0) nanotubes the poly(ethylene glycol) should be located inside and the doxorubicin molecule outside the tubules and these complexes should be the best water soluble doxorubicin carriers on the basis of the water soluble nanotubes.

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The calculations have been performed using the Joint Supercomputer Center of the Russian Academy of Sciences.

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E-LEARNING IN THE ENVIRONMENT OF THE UNIVERSITY UNIFORM INFORMATION SPACE

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The results of application of the modern approaches of e-learning (EL) in the university teaching process are discussed. EL is considered in the university uniform information space. It is concluded that today the optimal variant of application of EL is a realization of "mixed learning" that unites EL with a traditional teaching.

Keywords: *uniform information space, e – learning, mixed learning*

1. Introduction. Information Space of University

The problem of creation of a uniform information space in university attracts an increasing interest. However there is a lack of integrated solutions and infrastructure approaches to informatization of universities. The solutions obtained within universities are not compatible.

In this paper we consider in general the questions linked to organization of the university uniform information space (UIS) and to implement e-learning into the environment of UIS[1]. The main stages of creation of UIS are as follows:

- creation and maintenance of databases for all categories of University users without any duplication of information;
- provision of internal and external users with a single entry point into the corporate network of the University;
- automation of all processes of users interactions in the University through the application systems that support modern and uniform protocols of information exchange;
- creation of conditions for official and informal association of the University with other educational institutions to implement joint educational activities in the Internet on the basis of common standards, conventions and technologies. We keep in mind a joint teaching and a use of the common content.

2. Problems of Electronic Learning

Currently, the terms "distance" and "electronic (e) learning" are not well defined in spite of the fact that the term "e-learning" (EL) is widespread in education. It is often equated with the concept of "distance learning" (DL). Without going into the history of the appearance of these two terms, we understand EL as any educational process that is conducted with using the Internet and multimedia.

The introduction of EL in the teaching process of university requires along with the development and application of new information technologies, changing the general approach to the teaching process, significant organizational changes, staff training, improving the normative and methodical bases of the educational process and development of new pedagogical tools.

Analysis of the existing learning portals and systems of management of virtual environments, also known as the Learning Management Systems (LMS), showed that in some universities learning portals and LMS are integrated, while in others they operate separately.

Analysis of the functions of learning portals and LMS in university showed that the LMS are important for administration management of schedule and tracking the performance of all activities [1]. LMS has such architecture and implementation that provide a possibility in any moment to know who, what and when did; who, what and when can do and either everybody is going to do what he supposed to do.

[1] The results are based on the experience obtained in South-Ukrainian National Pedagogical University after K. D. Ushinskiy

Modern learning portals are examples of a "single window service" for the user, where you can ask a question, have an access to experts and the knowledge base, view the latest training materials (courses, lessons, notes, articles, snippets, videos from "YouTube", etc.), and interact with lecturers or students. Learning Portal is actually much smaller than LMS.

Analysis of the most promising environments for EL showed that currently there are three of them:

- systems for management of the virtual environment (VLE);
- personalized learning environment driven by students, built on the service Web 2.0;
- "Cloud computing" or simply "Cloud".

There are no final definitions of VLE-systems. These systems in the process of their development were adapted to new tools, such as blogs and wiki-resources. Just like "VLE" the term "cloud computing" has many definitions.

Experts examined more than twenty of them and came to the following common formulation: "Cloud" is a large pool of easily usable and accessible virtualised resources (such as developed hardware, platforms and/or services). These resources can be dynamically reconfigured to serve the varying loads (scalability), which allows optimising the use of resources. This pool is usually operated on the basis of the model of "pay only for what you are using".

All three environments are used for EL at the university. On the world market of platforms for distance learning (DL) there are more than 125 management systems of VLE [2]. Analysis of statistical data on the use of platforms for DL in Ukrainian universities shows that in 42 high schools the platform Moodle is used, 18 high schools use the platform "Prometheus". Several other platforms are used by 2–3 universities [3].

We have an experience of using the following environments:

- systems for management of virtual environment VLE (LMS) Moodle and Adobe Connect 8/4 /;
- services Web 2.0;
- services Microsoft Live@edu for e-learning in the "Cloud".

Each of these environments has its advantages and disadvantages. VLE-systems are mostly criticized for a weak possibility of generating and storing user-produced content and a low level of integration with social networks. These systems are primary praised for some specific features (for example, the ability to provide specific content and functionality for "closed" groups of students that study a course in a certain period of time).

The services Microsoft Live@edu have the main advantage that is a way to use cheaper the resources of cloud providers. There is not a necessity to purchase and maintain corporate hardware and software for providing these services. The main disadvantages in the last case are the lack of guarantees that the service will be continued for a long time, or that it will be for free further. Significant changes in the service (software update) can result in high costs for the university that will lead to lose the control over the software or data.

Despite the search for alternative environment for e-learning, LMS will remain the main medium for delivery of training courses in the nearest future. Specialists and educators have not yet found an answer to the question how to structure the learning through social networks. The introduction of cloud computing is in its initial stage.

3. Mixing Learning

Analysis of the EL model shows some its disadvantages. For example, teaching of students of physical-training departments, art or language departments is impossible without real training using the appropriate instruments and communication with lecturers and peers. During EL it is difficult to teach students to perform tolerant debates, to learn critically to think and to express thoughts aloud. In EL there are problems of psychological perception. EL is devoid of sensory, but is full of intelligence (in the text, graphics and charts, created by the participants of communication). Such learning is devoid of emotion, an example to follow and educational factor, etc. The webcam does not convey all the emotions, so you shall train to express your emotions by participating in virtual communities, using emoticons, etc. People with auditory and visual perception are more adaptive to EL, than kinaesthetic people.

The structure of e-learning environment in a uniform information space of the university is represented in Fig. 1. The algorithm of users' work in Adobe Connect Pro environment is shown in Fig. 2 and the algorithm of users' work in Moodle environment is shown in Fig. 3.

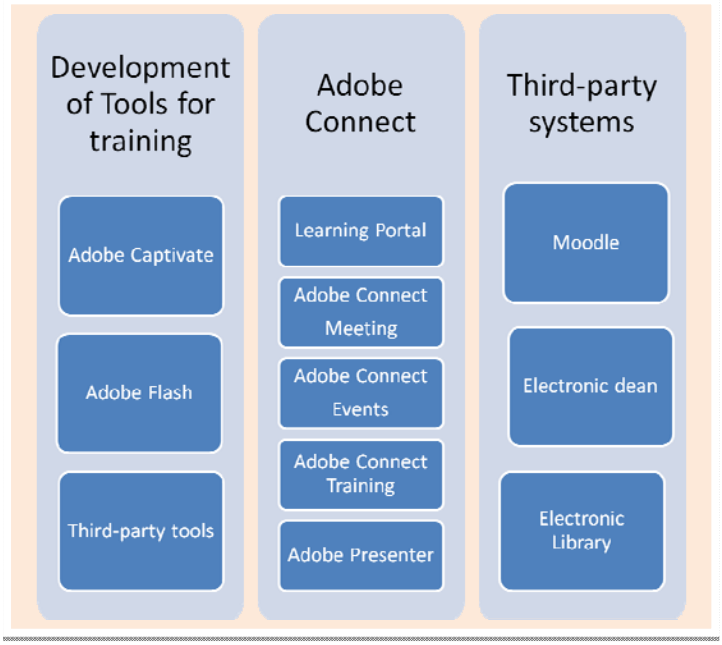

Figure 1. The structure of e-learning in the environment of the university information space

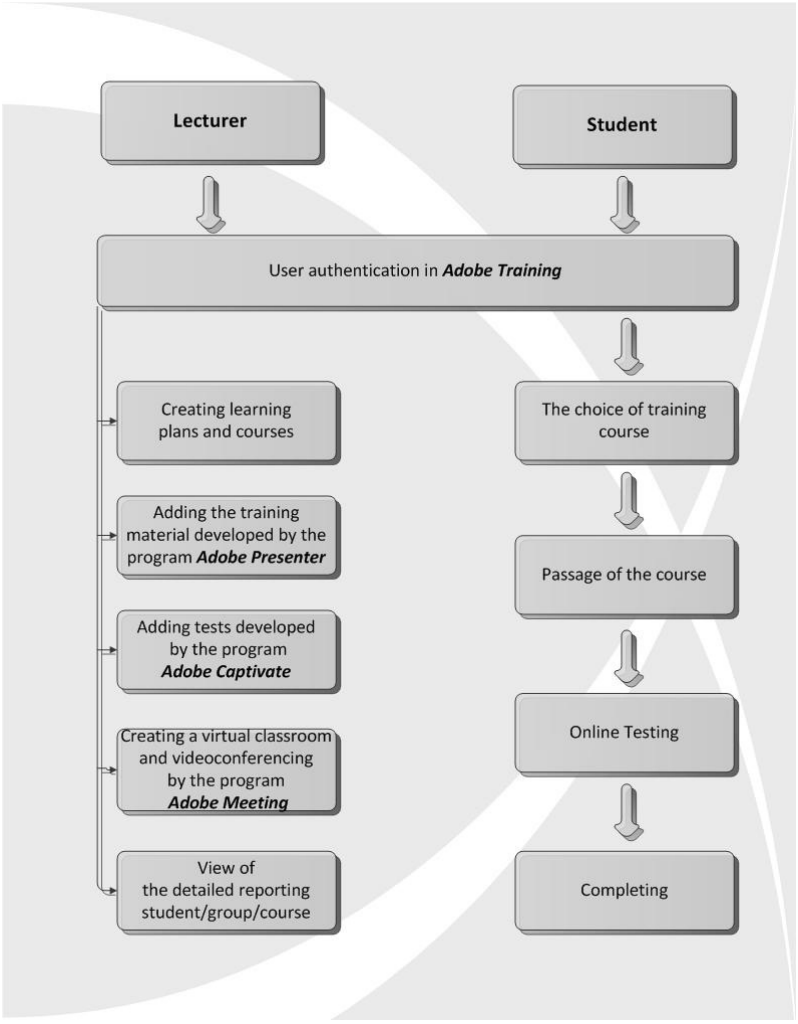

Figure 2. The algorithm for the program "Adobe Connect PRO"

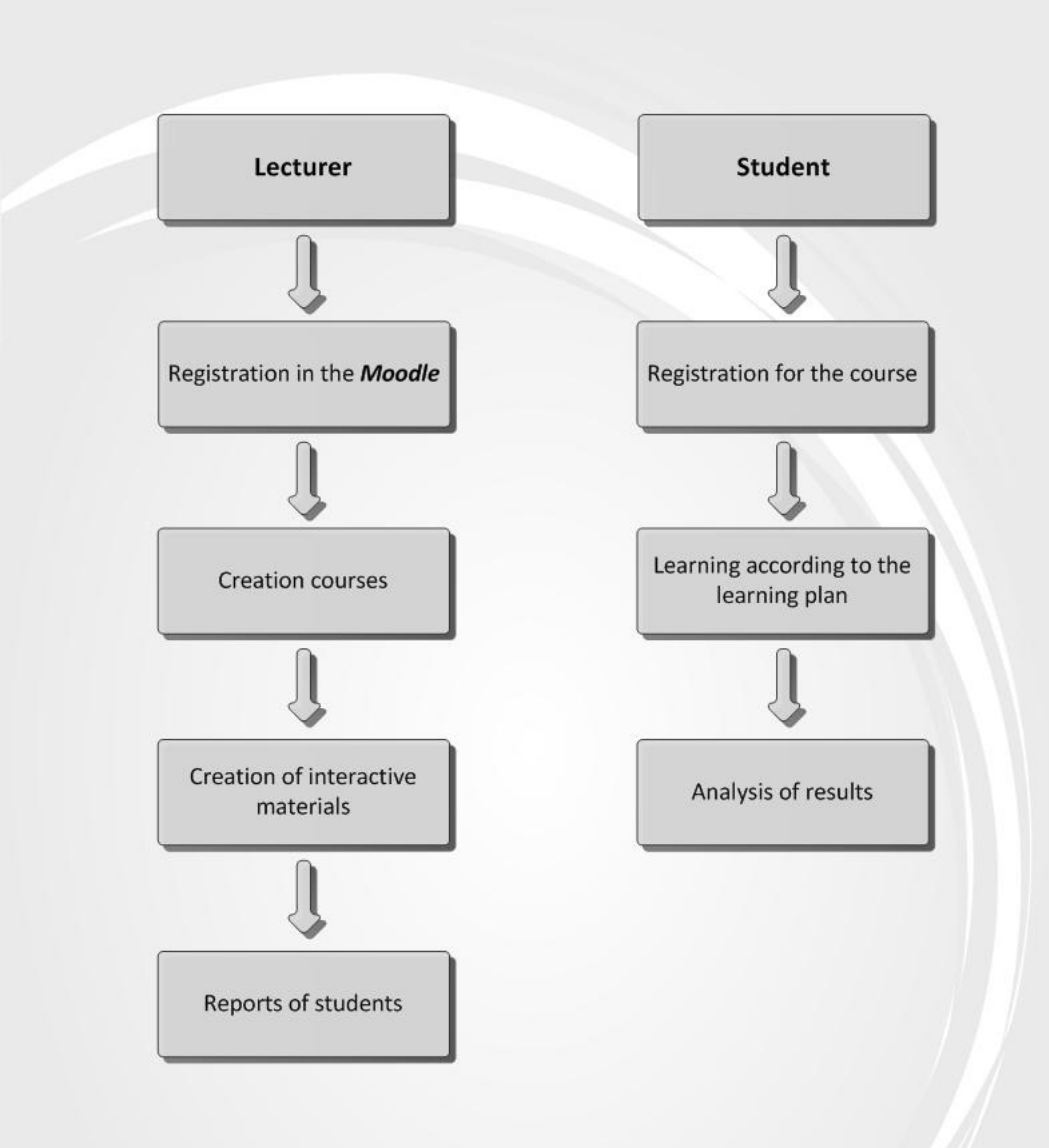

Figure 3. The algorithm for the program "Moodle"

4. Conclusions

The model of 'mixed (*combined*) learning' is the most attractive, which is defined as the organization of educational process, where EL technologies are combined with traditional teaching in the classroom in full-time schedule. Mixed learning is an effective learning technique, where the constituent components of full-time and e-learning process interact harmonically.

On condition that this interaction is methodologically well-organized, a high level of knowledge of trainees is its result. Thus, the model of mixed learning is not just the using of information and communication technologies in the individual work of students at home or in the electronic library. This is a unified, holistic learning process, which assumes that a part of the cognitive activity of students is carried out in the classroom under the direct supervision of the lecturer, and another part of the trainees' activities shall have an electronic form, with the predominance of individual or group individual work at home or in an electronic library.

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SOME PARTICULAR CASES OF MULTI-LAYER FEED-FORWARD NETWORKS MODELLING

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The paper considers an input data representation of the sequence for time series forecasting using the multi-layer feed-forward (MLFF) neural network with supervised learning. The values of input sequence are chosen in three different ways: using standardization in some interval, transferring to binary code and transferring to Gray code. To form the training set for the network learning the sliding window method was applied.

Each representation variant determines a rightness and speed of network learning with some network configuration using different values of window width. As a result it is possible to compare the rightness degree of forecasting for each variant of data presentation and to define the most preferable variant for this sequence.

Keywords: *multi-layer feed-forward neural network, time series forecasting, input data representation*

1. Introduction

Time series forecasting is an important problem in many branches of knowledge, in particular, in the modern financial and economic sciences. Forecasting of future events allows diminishing of making decision risk. The forecasting we understood as a result of determination of future values of indexes, based on some mathematical model with the use of data present in the moment of forecasting.

The forecasting problem actuality is confirmed by the amount of the written monographs and articles in different magazines, for example, International Journal of Forecasting, Journal of Forecasting and others. Different forecasting methods consist of the study of accumulated data with the purpose of development of models that can be effectively used in the future [1]. The suitable method can be determined by a kind and set of time series descriptions.

Time series is the well-organized sequence of numerical indexes that characterizes the levels of studied process in successive moments or time periods. Time series y_t can be presented as:

$$y_t = \chi_t + S + C + \varepsilon_t, \tag{1}$$

where χ_t is a trend that characterizes the substantial dynamics of process development, S is a seasonal constituent, C is a cyclic constituent, ε_t is a stochastic component of process that represents casual vibrations and noises of process.

Stationary time series signs are absence of trend and periodic constituent, systematic changes of vibrations scope and systematic changing dependences between the time series elements. Non-stationary time series signs are a presence of the above-stated components.

Time series recognition is possible by time series graphic presentation analysing on a presence or absence of tendency and periodic constituent, autocorrelation, by using tests on the trend presence, statistical descriptions constancy, etc.

Some of forecasting methods are the statistical methods that allow building dynamic series on a prospect, at what the methods of proceeding in the dependences used for prognostication go only out the set time series. In books and articles of different authors [1–4] the most often used statistical methods over are brought the prognostications applied to the temporal series. For example, this classic decomposition, regressive methods, exponential smoothing out, Box-Jenkins methods.

In [2] 6 models of data forecasting are compared: naive, non-parametric, combined, ARIMA, VAR, TF. Authors got that the naive and non-parametric methods owned the worst properties as compared to the prognoses on the basis of more difficult models.

In [3] authors generalized results of the numerous researches conducted within the different rows (3003 rows) analysis and comparison by different methods (24 methods). The results are alike with the results of other researchers: the difficult or complex forecasting methods do not give the best prognoses comparatively with more simple; the estimation of forecasting quality depends on the fact, what description of quality is chosen by standard and depends on forecasting length.

Comparison over of forecasting properties of time series different methods is performed in [4]. Authors concluded that linear methods give better prognoses as compared to nonlinear one. For example, prognoses with the use of neural networks, in all cases appear worse than the prognoses with the use of linear methods (autoregressive models). Such conclusion is probably caused by inaccuracy of evaluation of nonlinear model parameters, especially if such situation appeared off type for a teaching selection. But authors demonstrate that nonlinear models can give the best prognoses at short-term forecasting on one-two steps forward.

However in other sources [5] nonlinear methods, in particular neural networks, give better results as compared with linear ones. Neural networks give additional opportunities in the design of the nonlinear phenomena and recognition of chaotic behaviour. Due to the large flexibility (a neural network can carry out an arbitrary nonlinear reflection), networks can process the most different structures. Thus any dependence of type xt = $f\{x_{t\_1}, x_{t\_2},...,x_{t\_p}) + e_t$ with a continuous nonlinear function can be reproduced on a multi-layered network. Neural networks can be also applied for an un-dimensional and multidimensional analysis, properly forming the great number of independent entrances and depending on them exits.

Forecasting is a good example to demonstrate the power of various artificial intelligence techniques in teaching and learning.

The neural network capacities for prognostication straight ensue from its capacity for generalization and selection of the hidden dependences between input and output data. After teaching a network is able to predict the future values of the sequence on the basis of a few previous values or some existing presently factors. It should be noted that forecasting is possible when previous changes determine the future values.

Artificial neural networks are an information processing technology for modelling mathematical relationships between input and output variables. In recent years, artificial neural networks have become another important technique for predicting stock prices. Recently some studies have empirically forecasted macroeconomic variables such as inflation, interest rates and exchange rate. This approach is effective for input and output relationship modelling even for noisy data and has been demonstrated to effectively model nonlinear relationships such as related studies have estimated and forecasted stock prices and stock volatilities [11–14].

2. Neural Network Structure

A neural network is an interconnected network of simple processing elements (neurons) with a different weight associated with each connection.

With a proper network topology and appropriate weights between the connections, a neural network can be trained to approximate any function mapping between its inputs and outputs by using an appropriate learning algorithm.

The basic building block of a neural network is the neuron. The neuron consists of a propagation function g and an activation function f, where f takes the output of g as argument. The propagation function g is the weighted sum of inputs. The activation function f can be a linear function or non-linear function and it determines dependence of signal on the neuron output from the self-weighted sum of signals on his entrances. Thus, a neuron can be represented in the general form as $y(x) = f(g(x; w))$. Such neurons are assembled in layered structure to construct the artificial neural network (ANN).

Development of ANN model for any system involves three important issues:

1. Topology of the network,
2. Proper training algorithm,
3. Activation function.

For the output units an activation function suited to the distribution of the target values should be chosen. For binary targets the step function can be used. For targets with a bounded range the sigmoid and TANH functions can be used, provided either scale the outputs to the range of the targets or scale the targets to the range of the output activation function. For targets with no known bounds, the linear activation function is used.

At the use of step function until the self-weighted signal on the neuron entrance does not arrive to some level T — a signal on an output is equal to the zero. As soon as a signal on the neuron entrance exceeds the indicated level — an output signal saltatory changes to one.

$$f(x) = \begin{cases} 1 & if\ x \geq T \\ 0 & else \end{cases}. \qquad (2)$$

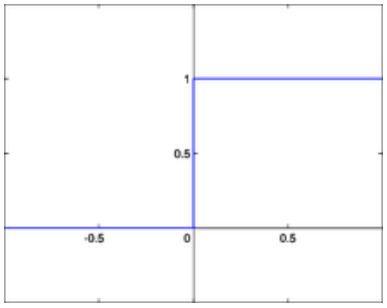

Figure 1. Chart of step function

A sigmoid activation function uses the sigmoid function to determine its activation, it only returns positive values. The sigmoid function is defined as follows:

$$f(x) = \frac{1}{1+e^{-x}}. \tag{3}$$

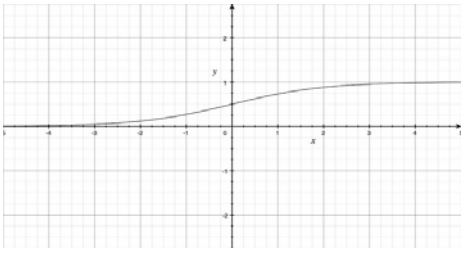

Figure 2. Chart of sigmoid function

The hyperbolic tangent function can be used to provide negative numbers:

$$f(x) = \frac{e^{2x}-1}{e^{2x}+1}. \tag{4}$$

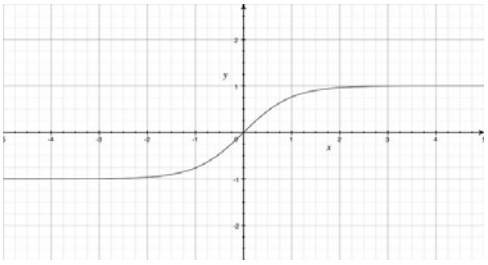

Figure 3. Chart of hyperbolic tangent function

The linear activation function is essentially no activation function at all. It is probably the least commonly used of the activation functions. The linear activation function does not modify a pattern before outputting it. The linear activation function might be useful in situations when you need the entire range of numbers to be output. Usually, you will want to think of your neurons as active or non-active. Because the hyperbolic tangent and sigmoid activation functions both have established upper and lower bounds, they tend to be used more for Boolean (on or off) type operations. The linear activation function is useful for presenting a range.

$$f(x) = x. \tag{5}$$

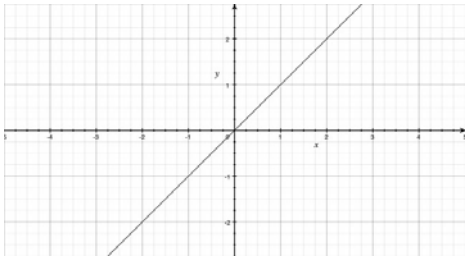

Figure 4. Chart of linear function

Basically an ANN involves an input layer and an output layer connected through one or more hidden layers. The network learns by adjusting the interconnections between the layers. When the learning procedure is completed, a suitable output is produced at the output layer.

The learning procedure may be supervised or unsupervised. In prediction problem supervised learning is adopted where a desired output is assigned to network beforehand.

Multi-layer feed-forward neural network (MLFF) is one the famous and it is used at more than 50 percent of researches that are doing in financial and economy field. This class of networks consists of multiple layers of neurons, usually interconnected in a feed-forward way. Multi-layer networks use a variety of learning techniques; the most popular is back-propagation algorithm (BPA). Each neuron in one layer has directed connections to the neurons of the subsequent layer. In many applications the neurons of these networks apply a sigmoid function as an activation function. It has a continuous derivative, which allows it to be used in back-propagation.

The BPA is a supervised learning algorithm that aims at reducing overall system error to a minimum. This algorithm has made multilayer neural networks suitable for various prediction problems.

Consider a feed-forward network with n input, m output units and it can consist of any number of hidden units. We are also given a training set $\{(x_1, t_1), \ldots, (x_p, t_p)\}$ consisting of p ordered pairs of n- and m-dimensional vectors, which are called the input and output patterns. The weights of the edges are real numbers selected at random. When the input pattern x_i from the training set is presented to this network, it produces an output o_i different in general from the target t_i. We want to make o_i and t_i identical for $i = 1, \ldots, p$ by using a learning algorithm. Thus we want to minimize the error function of the network, defined as

$$E\left(\{W_{i,j}\}\right)=\frac{1}{2}\sum_{i-1}^{p}\left(t_i-o_i\right)^2 . \tag{6}$$

After minimizing this function for the training set, new unknown input patterns are presented to the network. The network must recognize whether a new input vector is similar to learned patterns and produce a similar output. The back propagation algorithm is used to find a local minimum of the error function. The gradient of the error function is computed and used to correct the initial weights.

The weights in the network are the only parameters that can be modified to make the error E as low as possible. Because E is calculated by the extended network exclusively through composition of the node functions, it is a continuous and differentiable function of the l weights $w_1, w_2, \ldots, w_l$ in the network. An iterative process of gradient descent can be used to minimize E, for which we need to calculate the gradient

$$\nabla E=\frac{\partial E}{\partial w_1},\frac{\partial E}{\partial w_2},\ldots,\frac{\partial E}{\partial w_l} . \tag{7}$$

Each weight is updated using the increment

$$\nabla w_i=-\gamma\frac{\partial E}{\partial w_i}\ for\ i=\overline{1,l} , \tag{8}$$

where γ represents a learning constant, i.e., a proportionality parameter, which defines the step length of each iteration in the negative gradient direction.

3. Standardizing Input Data

Standardizing either input or target variables tends to make the training process better behaved by improving the numerical condition of the optimisation problem and ensuring that various default values involved in initialisation and termination are appropriate. Standardizing targets can also affect the objective function.

In theory normalizing or standardizing inputs is not necessary. The reason is that any rescaling of an input vector can be effectively undone by changing the corresponding weights, leaving the exact same outputs as had before. However, there are a variety of practical reasons why standardizing the inputs can make training faster and reduce the chances of getting stuck in local optima. Also, weight decay can be done more conveniently with standardized inputs.

Another reason to make normalizing or standardizing is a small coefficient of variation of inputs. Assume we have an MLP with one hidden layer applied to a classification problem and are therefore interested in the hyperplanes defined by each hidden unit. Each hyperplane is the locus of points where the net-input to the hidden unit is zero and is thus the classification boundary generated by that hidden unit considered in isolation. The connection weights from the inputs to a hidden unit determine the orientation of the hyperplane. The bias determines the distance of the hyperplane from the origin. If the bias terms are all small random numbers, then all the hyperplanes will pass close to the origin. Hence, if the data are not centred at the origin, the hyperplane may fail to pass through the data cloud. If all the inputs have a small coefficient of variation, it is quite possible that all the initial hyperplanes will miss the data entirely. With such a poor initialisation, local minima are very likely to occur. It is therefore important to centre the inputs to get good random initialisations.

In this paper the learning process of neural network based on the input sequence shown in three different ways:

- sequence becomes a standardized sequence in [0,1] interval;
- sequence becomes a sequence of bits transferring each number;
- sequence becomes a sequence of bits by transferring each number in Gray code.

This presentation of sequence elements will compare the learning speed and accuracy of the network's prediction and identify the advantages and disadvantages of each method of data presentation in predicting.

Binary code – means the data presenting as a combination of two characters, numbered 0 and 1. In general, the number of combinations (codes) n-bit binary code is equal to the number of placements with repetition:

$$A(2,n) = A_2^n = 2^n, \tag{9}$$

where $A(2,n) = A_2^n$ – number of codes, n – the number of binary digits.

To convert the original sequence of decimal numbers in a sequence of binary numbers, you must first present each number in the form of a nonnegative decimal number. Fractional part is removed by multiplying each of the original sequence by *10 * n*, where n – the maximum number of digits in the fractional part of numbers. Nonnegativity is achieved by adding a module to a minimum number of initial sequence numbers. These transformations are possible, because they do not affect the learning network.

Once obtained a nonnegative integer sequence, each number in the sequence can be represented in binary. The number of bits in each of those should be the same. To do this, choose the maximum order, convert it to binary code and fix the number of received bits. Since the network can predict the numbers are larger than input, one more bit should be reserved in binary form for such forecasts. As a result, we obtain the maximum number of bits for each binary representation of the number.

But this code is not without drawbacks. The main disadvantage is that adjacent numbers differ in the values of a few bits that could hamper operation. To avoid this problem it is better to use an encoding where adjacent numbers differ in fewer positions in the ideal value of one bit. This source code is Gray.

The Gray code may be got out of the binary representation, so you need to perform all operations to the original sequence for the binary case. Gray code can easily be obtained from the binary number by bitwise XOR with the same numbers, shifted right by one bit. Thus, i-th bit Gray code G_i is expressed through the binary B_i as follows:

$$G_i = B_i \oplus B_{i+1}, \tag{10}$$

where $\oplus$ – XOR operation; the bits are numbered from right to left, starting with the youngest.

4. Computer Experiment

For the research the network was created by 2 of the hidden layers of 30 and 15 neurons in the layer. The learning method is the feed forward back propagation algorithm and the step activation function. The step function may be used because the output takes on values of 0 or 1. The threshold of the function is 0, 5.

Parameters of the network training are the same for all cases: learn rate=0.1; momentum = 0.6. To form the training set, the sliding window method was chosen.

The sliding window method constructs a window classifier h_w that maps an input window of width w into an individual output value y. The window classifier h_w is trained by converting each sequential training example (x_i,y_i,) into windows and then applying a standard supervised learning algorithm. A new sequence x is classified by converting it to windows, applying h_w to predict each y_t and then concatenating the y_t's to form the predicted sequence y. The obvious advantage of this sliding window method is that permits any classical supervised learning algorithm to be applied.

Consider a sequence, which values variation is in a range [25, 5...103, 5].

Determine a rightness and speed of network learning with this network configuration using the different values of window width. As a result it is possible to compare the rightness degree of forecasting each variants of data presentation and to define the most preferable variant for this sequence.

Table 1. Time for one iteration passing according to window width

Input data presentation	Window width				
	Width 2	Width 3	Width 4	Width 5	Width 10
Normalized data	60-70	65-70	70-75	75-80	80-85
Binary data presentation	125-130	145-155	170-175	190-200	295-300
Gray code data presentation	125-130	145-155	170-175	190-200	295-300

The table shows that the window width for normalized data does not affect on time for the one iteration passing. What can not be said for the binary and Gray code representation. This is understandable, if a window step at a normalized representation the number of input data changes by one, in the binary and Gray code it changes by the number of bits.

Table 2. The speed of network learning using normalized input data for each window width

Iterations	Network error			
	Width 2	Width 3	Width 4	Width 5
1000	0.343471057431769	0.345319174821116	0.34622481212717	0.348586180901093
2000	0.343471057431561	0.345319174820865	0.346224812126758	0.34858618089768
3000	0.343471057431285	0.345319174820614	0.346224812126345	0.348586180894261

These results suggest that for normal network error we will have to perform much iteration except missing the local minimum.

Table 3. The speed of network learning using binary input data for each window width

Iterations	Network error			
	Width 2	Width 3	Width 4	Width 5
1000	0.0838191111771904	0.131531967033968	0.130759339370178	0.0794431268417932
2000	0.0562938427675918	0.128573964265933	0.120720971794628	0.0670068945670948
3000	0.0543685704609346	0.125269190220933	0.120165596542908	0.0665155863710945

Table 4. The speed of network learning using Gray code input data for each window width

Iterations	Network error			
	Width 2	Width 3	Width 4	Width 5
1000	0.131682178027423	0.123371454107763	0.116662328031173	0.122181287306132
2000	0.100599131102028	0.113918976541896	0.107810234859625	0.1209612977577
3000	0.0924150029893533	0.106972444908355	0.107416559727618	0.12071927208667

Using binary data presentation the network with a given configuration learns quickly. After spending quite a number of iterations the network error can be substantially reduced. Although after 1000 iterations the network error can fairly accurately predict the value.

Conclusions

Our results showed that the speed and the exactness of neural networks learning for the forecasting tasks can depend on the type of presentation of input data. *The expediency of normalizing and its type depend on the initial sequence (dispersion of values) and the configuration of the network.* We have found that for stationary time series with a small dispersion of values in the case of MLFF networks with supervised learning for forecasting the sequence can be represented by binary or Gray code.

During the data translation in a binary or Gray code as pluses it is possible to select a simple step activation function for network learning. At the greater value of threshold an output result is more precise. For normal work with binary sets it is necessary to have a large enough teaching base. The problem of such approach where even one of the values will be formed wrongly all subsequent values will be predicted with an enormous error.

To minuses it is possible to take a necessity in great numbers of neurons for presentation of input data vector, so it is necessary more time for one iteration passing, but it leads to the maximum allowable value of error after 500 iterations.

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THE ANALYSIS OF THE DATA OF GEOPHYSICAL RESEARCH OF BOREHOLES BY MEANS OF ARTIFICIAL NEURAL NETWORKS

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The analysis of geophysical research of boreholes in uranium fields is an important phase of deposits searching, exploration and mining. The method of pre-processing of data and training of artificial neural network is described. This method gives stable results. About 2000 calculation experiments have been made; software and templates for pre-processing of data and results interpretation have been developed. Different methods of normalization, smoothing, excluding shifting data, preparing of training samples were researched. These experiments showed the perspective of neural network approach to solving the problem of rock recognition on stratum-infiltration uranium deposits. Problems of the further experiments which will allow raising the degree of automation of recognition process and its accuracy have been formulated.

Keywords: *geophysical research of boreholes, artificial neural network, pre-processing data, normalization, smoothing*

1. Introduction

The method of acidic in situ leaching is widely used for uranium mining in Kazakhstan [1] (Fig. 1).

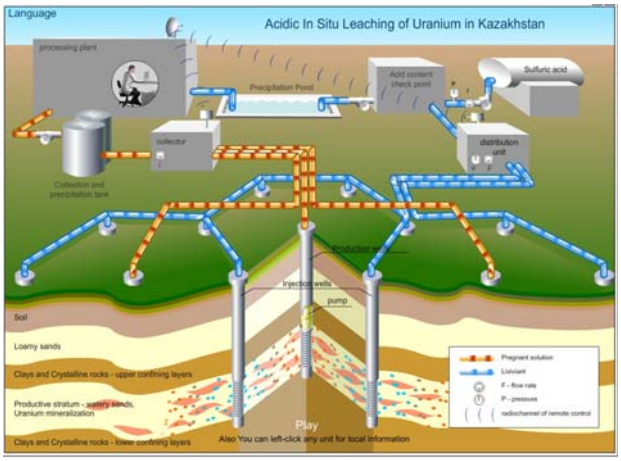

Figure 1. The method of acidic in situ leaching of uranium in Kazakhstan

In this case the efficiency of extraction depends of accuracy and timeliness of data interpretation of geophysical research of boreholes (GRB). The process of logging data interpretation can not be strictly formalized. Computer interpretation methods on the basis of expert estimates are necessary. Among these systems are artificial neural networks (ANN) which have already been used for a wide range of recognition problems [2–4] including GRB in oil field development [5], and their usage for rock recognition in uranium deposits is offered in [6]. Quality of network essentially depends on its configuration parameters and methods of data processing. The researches results of ANN configuration parameters and pre-processing data methods with using of data from deposit “Budenovsky” are described.

2. The Basic Scheme of Setting of Neural Net According Current Task

The neural network setting according current task includes four main stages: **Pre-processing, neural network configuration parameters selection, training of neural network and neural network model estimation** [1]. Pre-processing stage particularly includes normalization, smoothing and errors exception (in our situation it was borehole logs moving and anomalous values deletion).

Network architecture, neuron activation functions and learning algorithm are neural network parameters.

Results depend in considerable extent on chosen method of assessment. In real experiments neural network will work with new data. Thus, the estimation of results on same data set which fully or partially took part in training will not be right. For this reason the percent of correct answers (CCR) on "raw" boreholes (which haven't taken part in training) have been used as metrics of neural network quality.

3. Pre-Processing Methods of Data

After cleaning of data of abnormal values the next steps of work are the procedures of normalization and centring of data so that every component of initial vector will be within interval from 0 to 1 or – 1 to 1.

At a known size of changing of an input variable it is possible to use linear transformation $p = \frac{(x - x_{\min})(b - a)}{(x_{\max} - x_{\min})} + a$, where [a, b] – the range of acceptable input signals; [$x_{\min}, x_{\max}$] – variation range of input variable values; p – converted input signal.

Transformation by sigmoid function or hyperbolic tangent is used in cases of large size of changing of input variables. In some cases can be used modular, positional and functional pre-processing methods [2].

Wavelet data analysis and Fourier transform can be used for cleaning data from the noise.

4. The Technique Of Experiments

In the process of experiments the impact of following factors was investigated:

- Neural network training algorithm;
- Neural network architecture;
- The type of normalization;
- Smoothing method;
- Special methods of formation of learning samples;
- Exception of shifting of logging data.

About 2000 calculation experiments have been done. "Floating window of data" with parameters 5 + 1 + 5 (there were 5 points above and below the current one plus current point) was an input for network in experiments. Three types of logging data: IL – induction logging, AR – apparent-resistivity logging, NP – method of natural polarization logging were used. The complete size of input vector was 33.

Numerous computing experiments with the application of package Alyuda Neuro Intelligence (http://www.alyuda.com/companyinfo.htm), and with the special software and templates developed by using Python language, have been performed. To implement the wavelet smoothing WaveUtils library was used. Package Alyuda Neuro Intelligence allows selecting required network structure, training it by using correct and, in case of need, automatic partition of data into groups (training, validation and testing). Particularly experiments have shown results range on "raw borehole" would be 10%–15% even for minimum CCR variation on Validation set. Therefore in most cases each experiment was repeated up to 10 times and more in order to get statistically right set of results. The stages of pre-processing of data and formation of learning samples were included in experiments.

Stages of pre-processing of data:

- Deletion of abnormal values;
- Nonlinear (X) and linear normalization;
- Wavelet analysis (X);
- Removal shift of logging data (X);
- Data formatting into "floating window of data".

Note: stages which either had not influence to results or made it worse are marked with (X).

The stages of training data formation and network training are as follows:

1. The combining of boreholes data or using special data set (“ideal borehole”);
2. Network architecture selection;
3. Algorithm and training parameters selection.

5. The Analysis of Algorithm of Neural Network Training

Some algorithms of neural network training were investigated: Quick Propagation (Quick), Conjugate Gradient Descent (CGD), Quasi-Newton (QN), Limited Memory Quasi-Newton, Levenberg-Marquardt (LM), Online Back Propagation (OBP), Batch Back Propagation. The differences between algorithms are training speed, convergence (some algorithms, for example Leven-M, were not finished – “freeze”), dispersion of results.

As shown in Table 1, algorithm “Conjugate Gradient Descent” on the average gives closer to the best results and at the same time it has minimal dispersion. Therefore that algorithm was chosen as basic for all other experiments.

Table 1. Quality factors of learning algorithm

Parameter	Quick	CGD	QN	LM	OBP
Average	53.9	**58.6**	59.1	“Freeze”	50.8
Dispersion	195.4	**19.7**	42.0	“Freeze”	69.1

6. Effect of Neural Network Architecture

Neural network architecture is number of neuron in layers, quantity of layers and relations between neurons. The optimal number of neuron in hide layer/layers depends on quantity of input and output neurons. Unfortunately, formal method for determining the optimal number of neurons does not exist. Practically the only method is the exhaustive search and checking the various options [2]. However, obtaining an exact solution with any suitable quantity of neurons is impossible in practice, due to the combinatorial explosion in search of solutions. Therefore heuristic methods of package Alyuda were used for practical application. As a result of numerous experiments four-layer neural network architecture were selected. It included an input layer for enter “floating data window”, two hidden layers and output layer – [33-39-33-8].

7. Effect of Normalization

One of the most important methods of data pre-processing is normalization. Signal normalization can be linear and nonlinear.

Nonlinear normalization (sigmoid and hyperbolic tangent) had negative effect on quality of recognition (the average percentage of correct recognition decreased by 10%). A linear normalization, in contrast, significantly (15–20%), improved the quality of recognition.

8. Effect of Smoothing

Different methods of smoothing allowing removing of noise and other non informative data content could be used to improve the quality of recognition. There are two discrete transformations often used as methods of smoothing: Fourier analysis and wavelet transform [5].

As this existing selection had almost no high-frequency noise at this stage it was decided not to use the Fourier transform for data smoothing. At the same time, eliminating high-frequency component will lead to informativeness losing of signal (minor fluctuations of rocks will no longer are visible.)

Three (depth of decomposition / scale) variants of wavelet smoothing parameters were used (range of Daubechies wavelet and depth of decomposition / scale).

Table 2. Effect of wavelet smoothing of signal on quality of recognition

Wavelet (range of wavelet – scale)	CCR on set Validation	% on "raw" borehole
1-1	47,4	60,33
1-3	41,8	34,22
7-2	46,2	57,66
No smoothing	48,8	58

The experimental results show us it is no any significant improvements in recognition quality with application of wavelet smoothing. However, wavelet smoothing can be applied in the future, for example, to simplify the identification of AR extremum, which information requires the separation of the input data into categories.

9. Correction of Displacement of Logging Data

Factor affecting the quality of pre-processing data is shift of IL curve relative to AR and NP curves. Values of AR and NP are fixed one device, and IL another. Usually this displacement is not large and constant (within a single borehole to 0.5 meters up or down). Cross-correlation function was used to determine value of IL displacement relating to AR. As known it has such given form for two finite signals:

$$P(i) = \sum_j f(j) * g(i + j),$$

f – the main signal; g – linked signal; i – time shifting of one signal relative to another; $P\ (i)$ – correlation of shift i.

The most likely is displacement in which signals correlation reaches a maximum. Experiments have shown that the shift affects recognition results only slightly (less than 3%).

Table 3. Analysis of correction of AR data displacement on recognition quality (a part of results is shown)

Boreholes quantity	The number of "raw" borehole	CCR on Validation	CCR on "raw"
8 (n.c.)	9	62%	67%
8 (corr.)	9	59%	62%
8 (n.c.)	7	65%	45%
8 (corr.)	7	60%	43%
8 (n.c.)	7	65%	45%
8 (corr.)	7	68%	48%
8 (n.c.)	6	63%	68%
8 (corr.)	6	63%	68%

Notes:
(corr.) – The data adjusted to the maximum cross-correlation function.
(n.c.) – data with IL curve displaced relative to NP and AR curves (not corrected).
Training was conducted until the learning error (training error) = 90%;

10. Formation of Learning Sample

In the interpretation of log data it is very difficult to recognize scarce rocks: dolomite (carbonate rocks, lithotype code 9) and sand-gravel deposits (code 1), whose quantity in the training set is small (less than half a percent of whole data), which is insufficient for normal network learning.

After preliminary analysis, we decided to create the so-called "an ideal borehole" – a set of data, in which the number of examples of different rocks was the same, and themselves examples were uniformly taken from different boreholes at different depths (within the same horizon). In this case set of learning samples can be reduced significantly.

Note that total we can use 7000 learning samples, which provide an average level of CCR 60%. There were two thousand samples in developed "ideal borehole". Table 4 shows CCR with using some variation of "an ideal borehole", 1 + 2 – "ideal borehole" where combined first and second variant were used as learning samples (in this case data of scarce rocks were doubled).

Table 4. The part of recognition results with "an ideal borehole" application

The number of borehole	CCR 1	CCR 2	CCR 1 + 2
3	48	76	69
4	48	44	62
5	49	53	70
6	58	75	77
7	39	53	65
8	62	69	75
9("raw")	51	67	57

Table 5. Impurity content (in percent %)

The number of borehole	*% 3*	*% 123*	*% 4*	*% 12*	*% 7*	*% 74*	*% 47*
3	*25*	*31*	*18*	*4*	*9*	*10*	*2*
4	*19*	*39*	*5*	*16*	*9*	*6*	*2*
5	*30*	*25*	*6*	*19*	*13*	*7*	*1*
6	*24*	*25*	*15*	*17*	*4*	*6*	*9*
7	*25*	*30*	*20*	*5*	*0*	*10*	*11*
8	*26*	*26*	*24*	*10*	*5*	*2*	*6*
9("raw")	*20*	*17*	*13*	*24*	*3*	*9*	*13*

Note. Table columns show the contents of rocks (in percentage) in the corresponding boreholes (rounded to integers). For example column %7 shows the percentage of clay. The table uses the following codes litho-types: 3 – medium-grained sands, 123 – Sands inequigranular, 4 – from small-grained sands to super fine-grained sands, 12 – various-grained sands with gravel, 7 – clay, 74 – sandy clay, 47 – short-grained clayey sands.

It is evident that using of "ideal borehole" can achieve approximately the same level of recognition (60%) with three time's smaller data amount.

11. Conclusions

The set of experiments allows us to recommend the developed methodology for future experiments on the setting of neural networks for problems of uranium boreholes logging. But we have to take into account the following limitations.

Due to the random initialisation of weights of a neural network the difference of results are less than 5% can not be considered sufficient reason for choosing a particular method of data pre-processing due to the significant influence of random initial distribution of weights.

When we place data to network input as a floating window with parameters 5 + 1 + 5, small shift (up to 10 points) of IL curve relative to AR and NP curves had not affect the recognition results, because the network is "trained" to detect such shifts.

There are not significant improvements in recognition quality on application of wavelet smoothing.

The effective method of preparation of samples is formation of special learning sample ("an ideal borehole").

For achievement of the best result of recognition it is necessary to solve the following problems:

Problem 1. Estimate limits of accuracy of recognition of the data.

Problem 2. Study possibility of use of the general geological data to improve the quality of interpretation.

Problem 3. Develop methods and algorithms to eliminate anomalies in the initial data.

Problem 4. Develop methods of data pre-processing on the "acidified" boreholes, methods of predicting spreading of leach solutions, etc.

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ANALYSIS OF WEB-BASED APPLICATIONS FOR EXPERT SYSTEM

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Convergence of technologies in the Internet and the field of expert systems have offered new ways of sharing and distributing knowledge. However, there has been a general lack of research in the area of creating web-based application for expert systems (ES). Our work will address the issues associated with the analysis of design, development, and use of web-based ES from a standpoint of the benefits and challenges of developing and using them. As a case study, the architecture of a Web site/application will be presented. The benefits and challenges in developing and using web-based application for Expert System will be mentioned by comparing them with traditional and existent web-based ES. Based on the gained experience, useful tips will be given on the construction of such Web sites applications.

Keywords: *WEB-based applications, expert system*

1. General

Expert systems are computer programs that are used to solve problems and answer questions in a problem domain that ordinarily requires human expertise. This goal is usually achieved by combining a logical inference engine with a knowledge base. The information in the knowledge base contains a set of known facts and a set of production rules that allow if-then inferences on the facts and other acquired information.

Expert systems are part of artificial intelligence and dynamic trend in its area, where fuzzy logic and neural networks are implemented in knowledge database of expert systems. Thus, expert systems – it is a new trend to develop expert system using soft computing in audit of information security belonging to security standards (ITIL, COBIT, ISO 2700). Firstly, little scientific research has gone into them. Generally, there is having been done some research in area of neural fuzzy algorithms. But none of them were implemented in developing knowledge database of expert systems. More over it is another way of using web based approach of implementing expert system interface.

Since research into expert systems using soft computing is fairly new, only one area will be researched.

Moreover, expert systems have been applied in a wide range of industrial and commercial problems. Typical applications include diagnosis, planning, scheduling, decision support, and process monitoring and control. There are few research have been done in this area.

Consulting companies that do an audit of Information Security always meets problem with high rotation of employers. Expert systems that will be enrolled to auditing process will help to solve this problem. In addition they will develop their own “knowledge database” of expert’s experience. [4], [5].

2. Analysis of Web Based Expert Systems

First and foremost, the web based expert systems will be analysed by some criteria’s: usability, security, data processing and knowledge (database) base. As for usability, it consists of several parts: fit for use, easy of learning, task efficiency, easy of remembering, subjective satisfaction, and understand ability. In order to analyse Web-based expert systems, we took two good examples of them (WITS and Fish Expert System), which satisfy to large amount of other expert systems by their functionalities, design and logics.

Example 1.

WITS is a Web-based Intelligent Training and Support system. It is developed for providing training and intelligent support for Small and Medium sized Enterprises (SMEs) on the use of Information and Communication Technologies (ICT). The research was inspired by the evidence from the literature that lack of adequate skills and knowledge is one of major barriers for SMEs in successfully adopting and running e-commerce and e-business. As a result of this deficiency, there is an emerging need for better

education and decision support to SME managers who are eager to embrace the technology and afraid of being left behind. WITS advisor has three subsystems, which are designed to facilitate SME managers' decision making process in e-commerce and e-business adoption. [1]

Table 1

Analysis of Web-based intelligent Training and Support System (WITS)	
Usability	Generally, it satisfies usability test criteria (fit for use, ease of learning, task efficiency, and ease of remembering, subjective satisfaction, and understand ability). Web-based ES makes the evaluation and implementation of WITS much easier; Easy to collect feedback from online forms; Use of Web design software makes the user interface design easier; HTML-based user interfaces allow the incorporation of rich media elements; E-mails, feedback forms and other Internet communication functions allow users to question and comment on the system, thus making an expert system more interactive and personal; Useful links are incorporated in the system which can help the user to understand and interpret the expert system's recommendations; It has certain limitations. It does not have an easy to use knowledge updating facility.
Security	Any attempt to update and modify domain knowledge has to be done by the system developers using the original programs.
Data processing and access	No need to install the system in advance; Easy to collect feedback from online forms; Hyperlinks in HTML provide an extra facility in enhancing ES explanation and help; functions as users can access the relevant Web site easily.
Knowledge base	Useful knowledge source for knowledge acquisition in constructing the WITS knowledge base; With a Web-based knowledge base, any knowledge updating and maintenance can be handled centrally, and no reinstallation needs to be carried out.

According to the graph (Figure 1), there is a 'Knowledge validation', which validated and verified against test cases until its quality is acceptable, whereas 'Knowledge representation' prepare the knowledge map and encoding the given knowledge in the knowledge base. 'Inferencing' component allows the computer to make inferences based on the knowledge and the specifics of the problem. As for 'Explanation and justification', it is a program that allows the system to answer questions about a specific piece of information or how a certain conclusion was derived. Moreover, direct arrows mean just one-side relation; others identify two-side connections.

Example 2: Fish-Expert

Fish disease diagnosis is a rather complicated process in aquaculture production activities. Fish-Expert is a Web-based expert system for fish disease diagnosis in China. This Web-based expert system can mimic human fish disease expertise and diagnose a number of fish diseases with a user-friendly interface. A fish disease diagnosis expert system contains a large amount of fish disease data and images, which are used to conduct online disease diagnosis. The system has been tested and is in pilot use in certain regions of North China. [2]

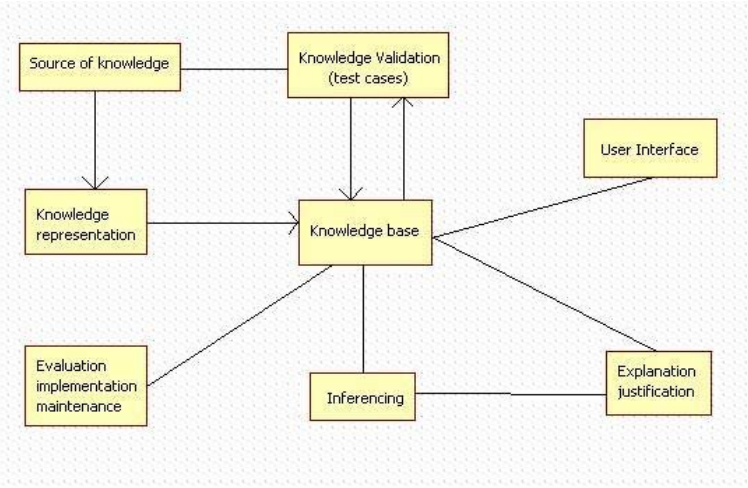

Figure 1. System Architecture of WITS

Table 2

Analysis of Web-based Fish Expert System	
Usability	Generally, it satisfies usability test criteria (fit for use, ease of learning, task efficiency, and ease of remembering, subjective satisfaction, and understand ability); The multimedia interface in Fish-Expert is effective in helping the user to query the system, but it slows down the access speed to it; A multimedia interface was used in the system. Matching of pre-defined text description and images of symptoms was provided to users who can choose text and/or images to describe the symptoms. Different interfaces were designed for pond inspection, fish inspection, etc. In the fish inspection interface, users can input information by selecting matching symptom pictures and descriptions from eight symptom groups (single or multiple selections are allowed); Online user feedback and evaluation of the ES was effective and popular.
Security	Knowledge engineer is still needed to check and transfer the knowledge into the knowledge base; the final responsibility of checking and updating the knowledge base still lies in his or her hands.
Data processing and access	Internet access speed is seen as a bottleneck for Web-based ES applications, especially in developing countries; Users can talk to a human expert via tele-diagnostic equipment in either a synchronous or asynchronous manner; Using HTML makes it easier to enhance the ES user interface. The multimedia interface was effective in helping the user query the system, but it slows down the access speed.
Knowledge base	Knowledge engineer is still needed to check and transfer the knowledge into the knowledge base; ES are known for their inability to deal with exceptions or complex problems due to the inflexibility and limits of the knowledge base; The knowledge base contains rules for disease diagnosis; Fish-Expert users can query the system using a forward chaining inference process that automatically matches facts against patterns to determine which rules are applicable.

The graph (Figure 2) consists of 6 main modules such as ‘Explanation System’, ‘Farming System and Information System’, ‘Inference Engine’, ‘Fish Disease Database and its management’, ‘Knowledge acquisition tool’, ‘Fish Disease Knowledge Base and its management’. Moreover, we have such components as ‘User’, ‘User Interface’, and ‘Human Expert’. Generally, the given graph is simple, because its relations are understandable; all connections are two-sided, instead of ‘Knowledge acquisition tool’.

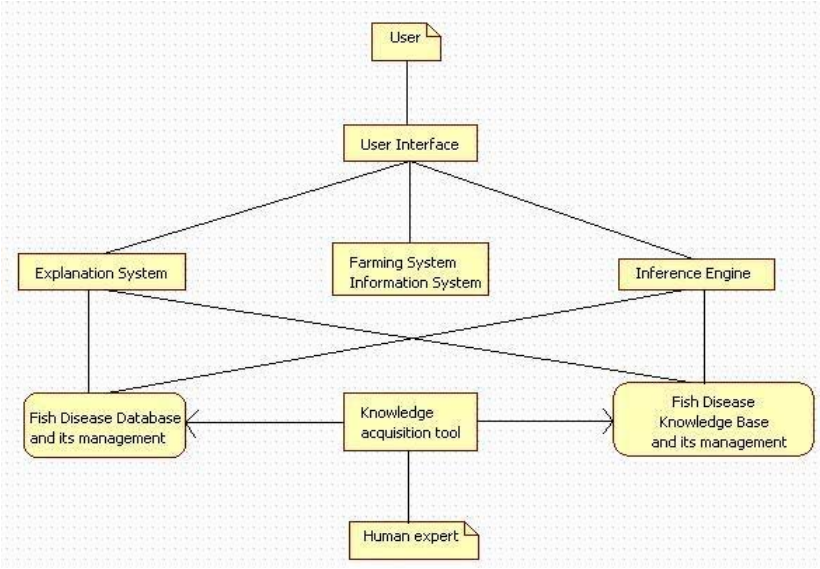

Figure 2. System Architecture of Web-based Fish ES

The main point of our issue is to clarify that Web based expert systems can be created by merging an expert system and a Web site/application developing subprojects. It means that in order to develop at least a rather “successful” Web based expert system the developer must follow basic expert system technology and Web engineering principals. The Web system consists of a Web based fuzzy expert system, databases and a set of dynamic and static Web pages. Moreover, we have analysed few Web-based Expert systems, and we want to provide an advice aiming to prevent the operational problems

occurrences and to minimize their unwanted effects of their consequences. Furthermore, some useful tips for the development of analogous Web systems will be given.

During developing your own web based expert system, you should satisfy some plan, which is given on the Figure 3.

Firstly, 'Identification of requirements and specifications' component is given, because all projects start from this point. Next, we have, Design of data, which is important for Web application notions in order to identify, analyse and describe data structures for displaying that for users. 'Design of Hypertext' component is necessary for html code to be written and some object, which are important for Web pages, are identified. The good examples of these are tables, frames, layers and images. The forth vital part of graph is 'Design of Architecture', where we can identify the main software and hardware components. Other components such as 'Implementation', 'Testing and assessment' 'Maintenance' also have to exist in developing process of Web Site for Expert System.

It is certainly true today that the developers of Web based Expert systems should spend more time on functional requirements, just after that on design, beauties and other factors of Web Site. So, there are some requirements in right creating the Web site for Expert System.

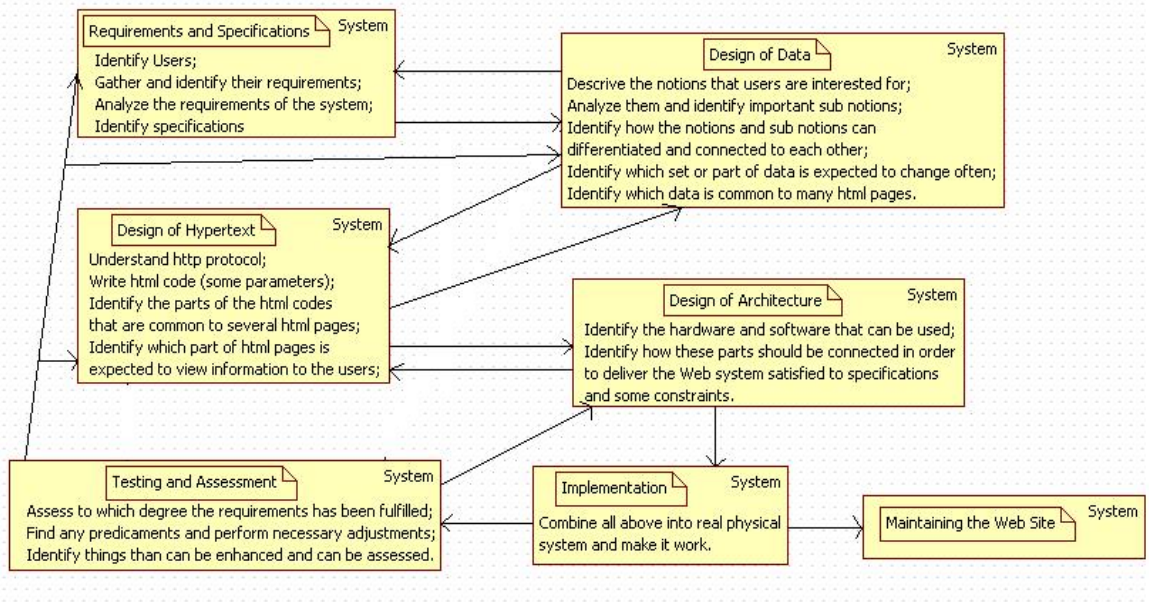

Figure 3. Architecture relating to Web Site developing process

3. Functional Requirements

1st fact: The Web application must provide the means that will allow to users to make queries regarding the direct extraction of a specific problem advice, without activating the Web based expert system.

2nd fact: Users would like to know and understand the reasoning of the expert system and based on which formula it calculates the operational problem occurrence possibility.

3rd fact: Users would appreciate and assess the fact that the Web application is providing information regarding the:

a) Knowledge acquisition process;
b) Tools that were used in the creating of expert system; c) Basic notions of the Web application (e.g. what is expert system, knowledge acquisition, etc.).

4th fact: The Web application must provide the means that will allow to users to make comments and to submit their proposals and experiences. Specifically, domain experts proposed to have the opportunity to describe how an operation problem/accident occurred in a landfill and based to their description the developer of the system to be able to update the knowledge base of the Web expert/knowledge based system. [3]

4. Non-Functional Requirements

The developers should know that the Web site/application must be as follows:

1. Aesthetically beautiful and at the same time serious and simple design.
2. Ease in use (easy of learning, task efficiency, easy of remembering, subjective satisfaction, and understand ability) and in navigation (usability).
3. Fast, regarding the time duration of the Web system response to a request (performance).

Moreover, the developers of the Web site/application should want it to be:

1. Constantly available to the users (availability).
2. Easy to maintain and to perform necessary changes (maintainability).

5. Conclusions

The aim of the article is to provide an overview of Web-based Expert Systems and present the developing process of those systems. Based on the fact that Web-based Expert System consists of two parts such as Expert System and large Web Site/Application, this issue is devoted to creating an appropriate Web Site for Expert System. The analyses of two such systems were given in the article and according to them it can be recommended aiming to prevent the operational problems' occurrences and to minimize their unwanted effects of their consequences. Furthermore, some useful tips for the development of analogous Web systems were given. Currently, we write our research work relating to development of Web-based Expert System for information security audit. All plans, schemes and tips given above we are trying to involve in our project.

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EARLY ESTIMATION METHOD OF SOFTWARE DEVELOPMENT

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In order to estimate the effort put into software development various models are used, which are basically based on some form of analysis specification of customer requirements or technical project. In particular, FP metrics that allow to estimate the effort based on the numbers of the function points is widely known [1, 2].

In our opinion, adaptive evaluation system based on formalized specifications of a customer can be used in established system of development (elaboration). This evaluation system can be named as "early", since it does not include the in-depth analysis methods of the projected system. This system of effort estimation should be based on some important parameters of formalized specifications and additional parameters, which include, for example, qualification of software developer, type of module, etc. For an assessment of basic applicability of formalized specification the analysis based on actual data was performed. The quantity of words and characters were used as the metrics of formalized specification (LFC).

The results of the technique based on the LFC metrics show that error of evaluation results compared with the actual data is relatively small (at least for one module). The maximum error value is 20%, the average is around 9% as compared to the actual data.

Keywords: *software engineering, labour effort estimation, formal specification, labour input estimation metrics, estimation methods*

1. Estimation of Labour Input of Software Development

Estimation of labour input of software development is one of the difficult tasks in software engineering. It is solved by different methods [1–5]:

1. Expert estimation;
2. Estimation using models.

1. Expert estimation. The method is designed for project estimation with an emphasis on the expert's knowledge and experience. The estimation is conducted for the whole project or its separate parts by the experts.

2. Estimation using models. This technique is designed for project estimation with the help of specific models.

"Estimation using models" technique has the following types:

2.1. Estimation by analogy;
2.2. Use Case Points (UCP);
2.3. Function points (FP);
2.4. Fast Function Points (FFP);
2.5. Early Function Points (EFP).

2.1. Estimation by analogy. Project estimation on the basis of historical data. In fact, it is an automated version of expert estimation method. Project estimation based on its "measurement" of forms, reports, subsystems, essence, etc. Conversion of measurement results to labour effort according to accumulated statistics.

2.2. Use Case Points (UCP). The method is designed to evaluate the projects, for which requirements definition is applied with the help of use cases (or precedents). The main point of this technique is to determine "actors" and use cases (precedents) and to estimate (evaluate) its complexity.

2.3. Function Points (FP). The method is designed to evaluate the project on the base of a concept called "function point". Its essence is as follows:

- Identification of all information objects and all operations on data exchange between the system and "actors" (users, other systems) and estimation of its complexity;
- Correction of the results – account of non-functional requirements;
- Using the result (in FP) in a COCOMO (Constructive Cost Model) calculator (conversion to labour effort with the partition according to project phases and processes) or conversion to code size, and further to labour efforts.

2.4. Early Function Points (EFP). Variety of a Function Points method allowing application in the absence of detailed requirements. The main point of this technique is:

- Identification of all information objects and all operations on data exchange between the system and "actors";
- Correction of the results – account of non functional requirements.

2.5. Fast Function Points (FFP). Variety of a Function Points method allowing application in the absence of detailed requirements. The essence is as follows:

- Identification of all information objects and all operations on data exchange between the system and "actors" (users, other systems) without estimation of their complexity (an average value is used).

In the case of the established software development process estimation of labour input can be conducted using the statistics based on the results of the previous tasks. Particularly, in this regard, size-oriented metrics has worked well. The given approach described in [1] is based on LOC (lines of code) estimation by analogy with COCOMO.

2. Software Development Input Estimation on the Basis of Formal Specification

The techniques considered above are not easy to implement, and in some cases, for example, when modifying system modules, their application can be redundant.

Here comes the question: is it possible to move away from the given techniques for input estimation and replace them with the simplified method that allows performing immediate estimation of software development input at an early stage, the stage of task formulation?

We assume that, in some cases, in the well-organized development process, in "conservative" environment, where specific statistics of software development is given and the groups of developers are stable, it is possible to use formal specification of software development (FC – formal specification) for calculation of labour input (WD – work days) in man-days.

FC = > WD.

In other words, it can be assumed that formal specification can be sufficient for relatively accurate labour input calculations of software development.

In this case, the task is to find a function

$$WD = fwc (FC, P), \quad (1)$$

where P is a vector of additional parameters, including, for example, a developer's qualification, a type of the designed module , etc. It is supposed that in some instances it is possible to perform convolution of P vector to the correction factor that depends on the specified parameters. The general model of a customisable (adaptive) system of input estimation is shown in Fig. 1.

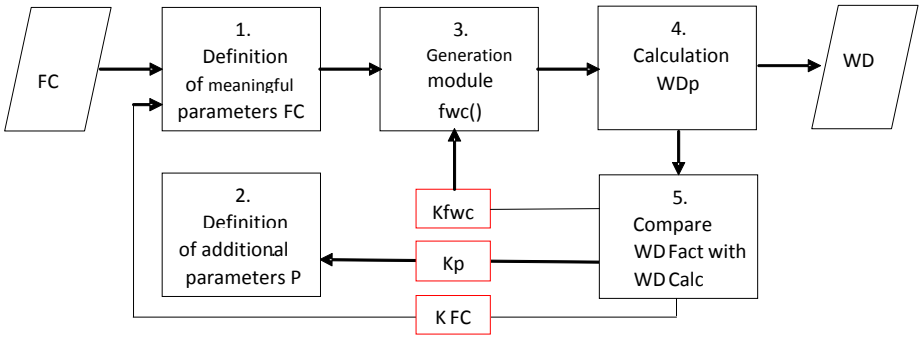

Figure 1. The generalized model of adjusted (adaptive) system of an assessment of labour input

According to Figure 1, block 1 is a block for definition of significant parameters of formal specification, block 2 is a block for definition of a vector of additional parameters, block 3 is a module for definition of fwc function, block 4 is used for calculation of predicted input, block 5 performs a comparison of actual indicators of labour input with the calculated ones, Kfc, Kp, Kfwc are corresponding correctors that ensures the system configuration to improve an accuracy of input calculations. The factor

analysis, clustering and pattern recognition algorithms, and also algorithms for semantic analysis can be applied in order to construct the correctors.

The experiments with an actual data were conducted in order to verify the possibility of using formal specification for software development input calculations.

At the same time, the number of words and symbols (which, in this case, plays the role of significant parameters) is used as a simple metrics of formal specification. In this instance, the expression (1) can be converted to the following form:

$$WD = LFC(w,c) * p, \quad (2)$$

where LFC is a function depending on the number of words (w) and symbols (c) in formal specification, p is a correction factor. In this case, a correction factor is a convolution of P vector.

At first glance, the described approach looks very formal, independent of the semantic content of specification to a software product. However, it can be recalled that the structure of formal specification developed by an expert gives necessary substantial sense to the whole technique.

3. An Example of LFC Metrics and Formal Specifications Application for Estimation of Software Development Labour Input

The applicability analysis of LFC metrics and formal specifications was conducted based on the data accumulated in an organization with an "HB" label. In this organization software development and modification is done as follows (Fig. 2).

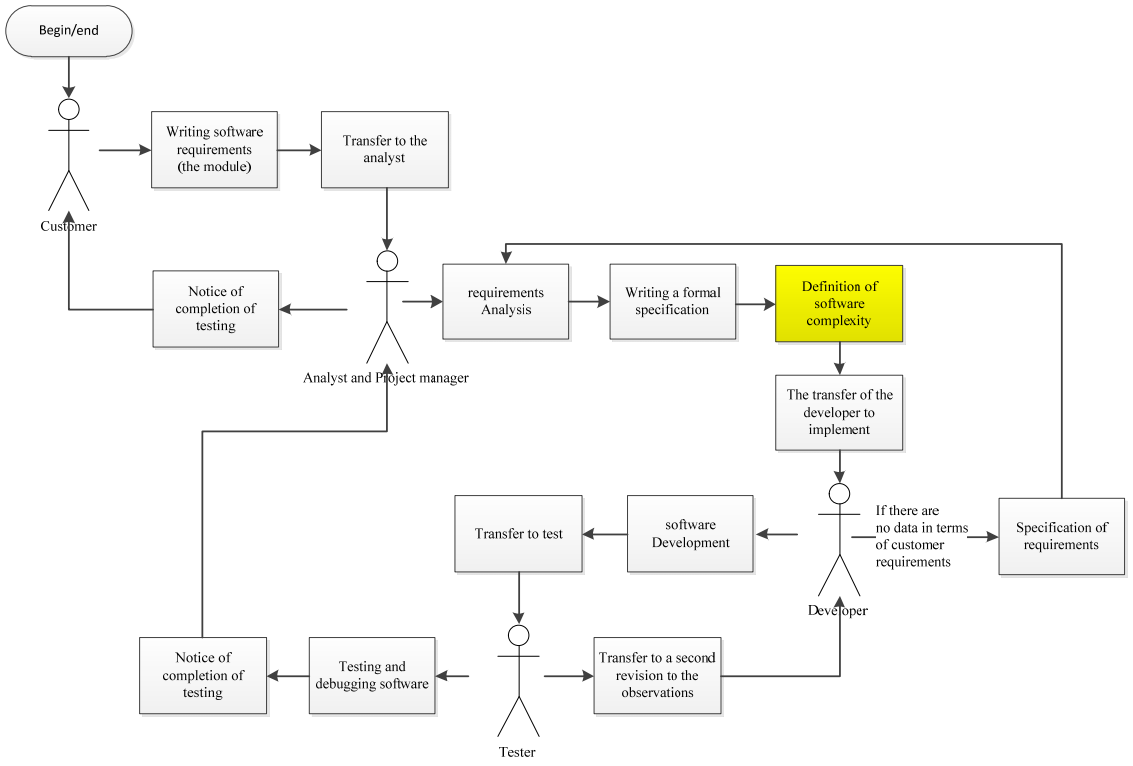

Figure 2. The development and modification of software in the organization of "HB"

At first, an application form written by a customer in a free form and related to the specific module of a system comes to an analyst.

Based on this application the analyst writes formal specification and passes it to the developer.

At this point, on the basis of the given specification the developer in the "HB" organization estimates his/her labour input. The calculation of labour effort is not formalized and based on expert estimation. But, as shown on Figure 2, it is proposed to calculate efforts at an analysis stage, without bringing up an application to the developer. To formalize the process of effort calculation empirically dependence LFC = f(w,c) was found in the following form

$$LFC = w1 + c1 + w2 + c2, \quad (3)$$

where w1 and w2 are the number of words in the application of the customer and analyst, respectively; c1 and c2 are the number of symbols in the application of the customer and analyst, respectively.

As a result formula (2) has the following form

$$WD = LFC * p. \quad (4)$$

In order to get the p factor, data about WD accumulated in the development process can be used. In other words, for each application Pi = WDi/ LFCi, where WDi is the developer's labour effort for i-th application, LFCi is LFC calculation using formula (3) for i-th application.

The generalized factor P is calculated as an average for all Pi.

Let's consider an application of the given technique in the "HB" organization when modifying modules in one system.

Formal specification for software development (modification) was designed for the use of the technique. Formal specification is based on GOST34 [8] (Fig. 3).

Application for revision of software

Customer: _____
Type of application: _____
Name of system: _____
Name of module: _____
Name of task: _____

Access level: _____
Purpose, objectives, expected results from the introduction: _____

Reason for work: _____
Basic requirements: _____
_____
_____
Interaction with other subsystems

A list of all the classifiers (directories)
The list of legal acts and regulations (including internal), regulating the order of execution of works –
Requirements for the ways and means of communication for information exchange between users of the subsystem: in accordance with the specifications.
The requirement to conduct the event log: Yes.
Number of users of the subsystem: _____
Availability of information included in the list of information to be protected:_____
The owner created an information resource_____
Aspirational deadlines –
Customer's representative_____
Authorized representative of the analysis _____
Head of Analysis

_____ _____ _____ **2012r**
(signature of the head)

Figure 3. Example, formal specification (the application) to refine the software

Table 1 contains the source data for calculation (w1, c1, w2, c2)

Table 1. Quantitative characteristics of applications for the module "Credits"

S/n	Name of application	WDi fact.	Customer application		Analyst application	
			Number of words, (w1)	**Number of characters, (c1)**	**Number of words, (w2)**	**Number of characters, (c2)**
1	Unblock	11	612	6685	568	4917
2	Stepped rate	15	853	7657	1058	7208
3	Calculation of the duration	5	240	1715	292	2564
4	Cancellation of deposit	13	688	6518	764	6087
5	Changes mortgage	4	234	1981	319	2722
6	Delivery of documents	4	127	1114	418	3372
7	Calculation of the homogeneity	9	130	1146	812	8205

According to the data given in Table 1, the following results are derived:

Based on the first application "Unblock" LFC = 612+6685+568+4917 = 12782

$$Pi = WDi/ LFCi = 11*60*8/12782 = 0.41,$$

where 11 is a runtime of the application in man-days. For accuracy improvement, calculations are done in minutes with account of 8-hour workday.

An average value of a correction factor for the module "Credits" calculated according to 7 applications is P = 0.44.

Using the values of p and data from Table 1, the developer's labour effort (WDi) is calculated according to 7 applications (Table 2).

Table 2. The results of calculations of labour input required for application processing by the developer according to the module "Credits"

S/n	Name of application	LFC	Pi	P	WDi (per.-min.)	WDi (per.-day)
1	Unblock	12782	0,38	0,44	5624,08	11,72
2	Stepped rate	16776	0,43	0,44	7381,44	15,38
3	Calculation of the duration	4811	0,6	0,44	2116,84	4,41
4	Cancellation of deposit	14057	0,68	0,44	6185,08	12,89
5	Changes mortgage	5256	0,27	0,44	2312,64	4,82
6	Delivery of documents	5031	0,48	0,44	2213,64	4,61
7	Calculation of the homogeneity	10293	0,23	0,44	4528,92	9,44

Table 3 presents the data that allows comparing the results of actual input required for application processing with the calculated data.

The absolute error of labour input required for application processing is calculated by the formula:

$$\Delta WDi = | WDi \text{ actual.} - WDi \text{ calc.}|$$

The relative error of labour input: $\varepsilon (WDi) = \Delta WDi / WDi$ actual.

The error between actual WDi and calculated WDi is insignificant as shown in Table 3.

Table 3. The comparison of actual and calculated data of labour input required for applications processing by the developer

S/n	Name of application	Module	WDi (per.-day) fact.	WDi (per.-day) calc.	Δ WDi (per.-day)	ε (WDi) (%)
1	Unblock	Credits	11	11,72	0,72	6,55
2	Stepped rate	Credits	15	15,38	0,38	2,53
3	Calculation of the duration	Credits	5	4,41	-0,59	11,8
4	Cancellation of deposit	Credits	13	12,89	-0,11	0,85
5	Changes mortgage	Credits	4	4,82	0,82	20,5
6	Delivery of documents	Credits	4	4,61	0,61	15,25
7	Calculation of the homogeneity	Credits	9	9,44	0,44	4,89

The results of using the technique based on LFC metrics show that the error of the results of input estimation compared to actual data is relatively small (at least for one module).

Let's note that the attempts of using the specified approach for labour input estimation required for applications processing that affect multiple modules have not been successful. Therefore, the described technique can be applied only in case of severe restrictions on the subject area and in the presence of reliable data about actual labour input of software development.

4. Conclusions

To estimate the labour input of software development, an adaptive system of input estimation based on formalized specification, a model of which includes corresponding correctors that ensures system configuration for improvement of calculation accuracy, was proposed.

The analysis based on the actual data was conducted in order to evaluate principal applicability of formal specification. At the same time, the quantity of words and symbols were used as the metrics of formal specification (LFC).

The results of using the method based on LFC metrics show that the error of results of labour input estimation compared to the actual data is relatively small (at least for one module). The maximum value of the error is 20%; the medium is about 9%.

The attempts of using the specified approach for labour input estimation required for applications processing that affect multiple modules have not been successful. Therefore, the described technique can be applied only in case of severe restrictions on the subject area and in the presence of reliable data about actual labour input of software development.

Let's note that although the proposed metrics is formal, it can be recalled that the structure of formal specification developed by an expert gives necessary substantial sense to the whole technique.

Further development of the approach can be a system that computes the correction factor p by the actual results of design and self-defining type of function fwc. The possible approaches can be the factor analysis, clustering and pattern recognition algorithms, and also algorithms for semantic analysis.

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DEVELOPMENT OF DATABASE FOR EXPERT SYSTEMS OF INFORMATION SECURITY AUDITING

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In this era of high technology, the information is involved in almost every aspect of human lives. Due to rapid growth of information technologies, came the need for increasing the security of information. Information security auditing plays key role in providing any organization's good security level. But, the security of information technologies is one of the difficult and comprehensive systems. The main problem lies in the data organization, collection and its processing methods. One of the solutions could be development of expert system that will reduce cost, speed up and facilitate the process of Information Security auditing. The valuable item in developing such system could be database development.

This paper presents the study of information security at international and national standards and guidelines for the management of IT, audit and IT-security (such as ISO 27001, COBIT 4.1 and ITIL V3) and the structure of database for expert systems of information security auditing.

Keywords: *information security, information security auditing, standards for auditing information security, expert systems, database, UML, Transact-SQL*

1. Introduction

The main goal of this study is based on the development of database of expert system, which will be fully audited information security and will be guided by the information that underlies the international standards ISO 27001, COBIT 4.1 and ITIL V3 [1].

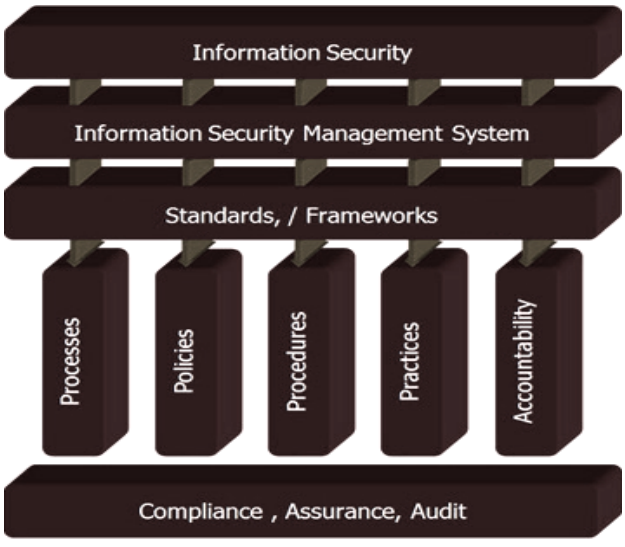

Figure 1. The structure of providing information security via standards/frameworks

The best global practices in the field of information security management are described in international standards that ensure compliance, assurance and audit of information security (see Fig. 1). We have also developed software implementation of database for expert systems of information security auditing in the language of queries Transact-SQL with the use of tool for developing relational database Microsoft SQL Server 2005 Management Studio Express.

2. Information Security Auditing

Firstly, let us focus your attention on the main concepts of information security.

Information security is defined by the absence of unacceptable risk of information leakage via technical channels, unauthorized and unintended effects on the data and other resources used in information systems (IS) [8].

Secondly, we should define the main characteristics of the audit of information security.

An audit is an independent examination of specific areas of organizational functioning. The objectives of the safety audit are [5]:

- The risk analysis;
- The assess the current level of protection of IS;
- The IS assessment of conformity with existing standards of Information Security;
- To develop recommendations for security mechanisms for IS.

For a professional approach to the issues of information security we should be guided by the regulating documents, such as standards. During the development of database for Expert Systems of information security auditing (ESISA) addressed the following international information security standards, such as ISO 27001, ITIL V3 and COBIT 4.1.

ISO 27001 was developed by the International Organization for Standardization (ISO) and International Electrotechnical Commission (IEC). ISO 27001 consists of 11 targets and monitoring mechanisms, which organize the protection of their information resources by establishing requirements for information security management system (ISMS).

On the basis of ITIL V3 laid process approach, consisting of seven volumes. It focuses on achieving business goals, analysing key performance indicators, as well as the resources expended to achieve those goals.

COBIT 4.1 consists of 34 high-level processes, which are aimed at business managers, IT managers and owners of business processes [7]. This approach is designed to extract maximum benefit from the use of information technology in organizations.

3. The Structure of the Expert Systems of Information Security Auditing

Expert System (ES) is an intellectual computer program that can give advice, counsel and analysis. The use of ES in the control and security management IS, and in the information security audit can facilitate the process of auditing [2]. The developed ES generates a report and recommendations based on the standards of information security and experts opinions. Go to the dignity of the ES also attribute to the possibility to describe the experience of information security professionals in a form accessible to the analysis of the rules If (condition) – Then (Corollary).

The structure ESISA consists of: a user interface, subsystem explanations, inference systems, the knowledge base and database. Structural elements of the expert system perform the following functions:

The user interface exists for direct interaction between ESISA and user, such as data entry and displays the results of the processed data.

The subsystem of explanations exists to clarify for the users the actions of the expert systems logic. The data from subsystem of explanations stored in database table – Recommendation.

The system of logical inference (SLI) carries a substitution of values from the database in the field of parcel If (condition) of the rules knowledge base and in the case of filling in all the parcels are ready to activate the processing rules, forming a conclusion in accordance with part Then (Investigation) regulations [6]. In the developing system SLI executes an application that created the language of logic programming Fril.

Knowledge Base (KB) is the core of the expert system. In the developing ES knowledge base is the main decision-making tool, the basic structure, which takes into account international experience and documents on the safety audit of IS, such as ISO 27001, ITIL V3 and the COBIT 4.1.

The relationship between the standards shown in Table 1, a fragment of which is shown below. Table1 is the source of the work [3].

Table 1.

ISO/IEC 27002 Classifications (Supporting Information)	Key ISO/IEC 27002 Areas	CobiT 4.1 Control Objectives	CobiT IT Processes	ITIL V3 Reference
4.1 Assessing security risks	**4.0 Risk assessment and treatment**	• P09.4 Risk assessment	• P09 Manage IT risks	
4.2 Treating security risks			• P09 Manage IT risks	
5.1 Information security policy	**5.0 Security policy**			
5.1.1 Information security policy document		• P06.1 IT policy and control environment • P06.2 Enterprise IT risk and control framework • P06.3 IT policies management • P06.5 Communication of IT objectives and direction • DS5.2 IT security plan • DS5.3 Identity management • ME2.1 Monitoring of internal control framework	• P06 Communicate management aims and direction • DS5 Ensure systems security • ME2 Monitor and evaluate internal control	• SS 6.4 Organisational culture • ST 5.1 Managing communications and commitment • SO 3.6 Communications • SO 4.5 Access management • SD 4.6.4 Policies, principles, basic concepts • SD 4.6.5.1 Security controls (high-level coverage, not in detail)

There are a few questions from the established knowledge base, which is focused on the three categories of users: Govern – G, Admin – A, User – U (Table 2).

Table 2.

№	Question	Category
	Security Policy	
1	How often do changes/additions to the security policy in your company?	A
2	Have an occasion to inform outside parties documented information security policy of your company?	G
	Resource management	
3	Is there an inventory of all the important resources in your company?	G,A,U
4	Does your company support an inventory of all critical resources?	G,A

4. Development of Database

The database is a collection of organized data, stored in a computer memory. For creating, maintaining and sharing databases between many users used the set language and software tools, called a database management system (DBMS).

DBMS supports various methods of logical organization of data. The best-known data models are hierarchical, network and relational models. To develop ESISA database has been used a relational model. The basic concepts of relational databases are the normalization, keys, entities and relationships. The principles of normalization [4]:

- Each database table must not include repeated fields;
- Each table must have a unique identifier (primary key);
- Each primary key value must match the sufficient information about the type or nature of the object table;
- Change the values in the table should not affect the information in other fields.

Keys:

The key is a column or multiple columns to be added to the table and allow establishing a connection with the records in another table. There are two types of keys: primary and secondary. The primary key is used to relate a table to foreign keys in other tables. A foreign key indicates how to join with other tables. There are many types of relation, such as of “one-to-one,” “one-to-many” and “many-to-many”.

In the design process of ESISA determined the structure of a relational database, which contains 14 tables. Each table in DB consists of columns, data types, sizes and keys of table:

- ISO,
- ITIL,
- COBIT,
- Category,
- Questionnaire,
- Test,
- Report,
- Recommendation,
- TesterReport,
- Tester,
- Expert,
- Govern,
- Admin,
- Users.

For creating a database used development tools such as the Star UML and MS SQL 2005.

StarUML is a software modelling tool that supports the Unified Modelling Language (UML). Below are given the relationships between data tables in a database of association, direct association, generalization and composition in the development environment StarUML (Fig. 2).

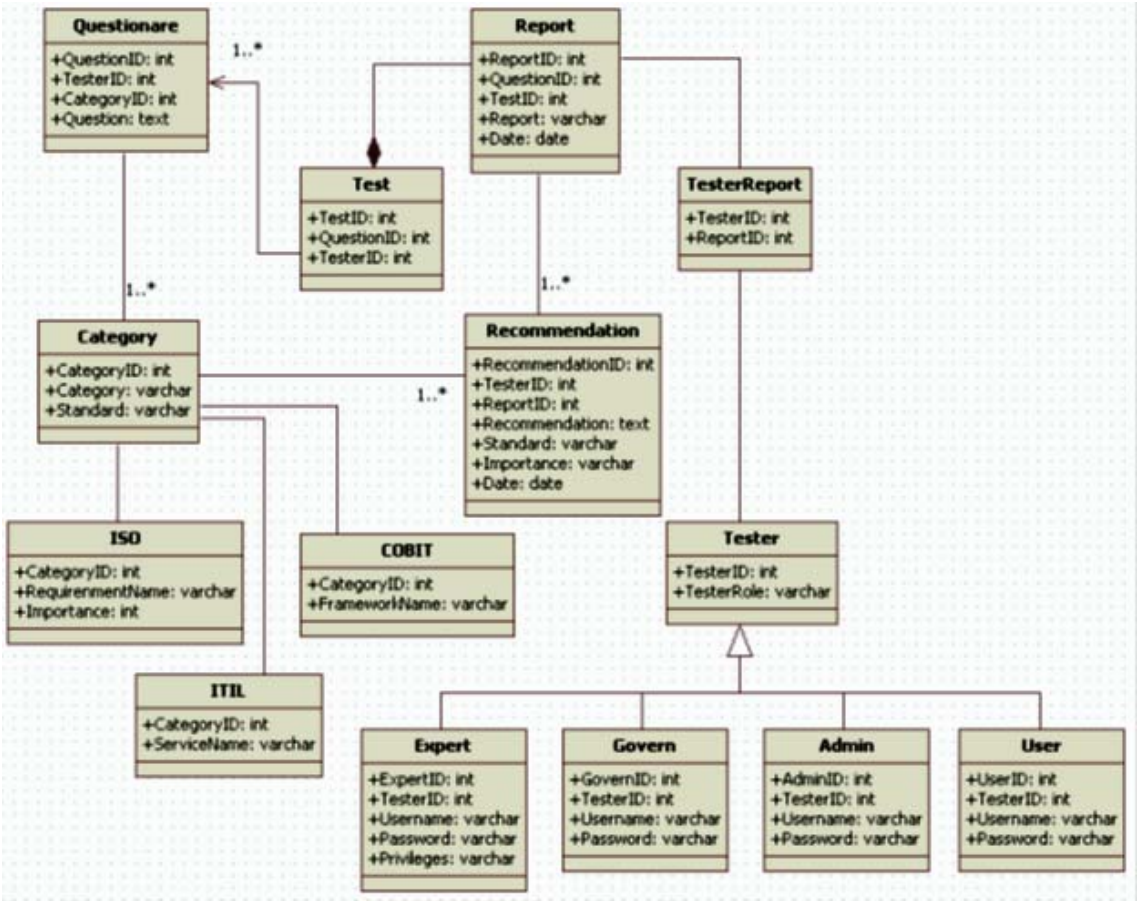

Figure 2. Model DB for ESISA in StarUML

Microsoft SQL Server is a DBMS developed by Microsoft. The primary query language used here is Transact-SQL. The advantage of SQL Server 2005 is the manageability, availability, scalability and security [4].

Let's consider the main points of application and work environment in MS SQL Server 2005.

First of all, for creating a database in MS SQL we use the operator to create a database: CREATE DATABASE databasename;

Then, the following queries are executed for creating tables and primary keys, which are defined for each table (queries for some tables are illustrated in the work area MS SQL Server 2005) (Fig. 3):

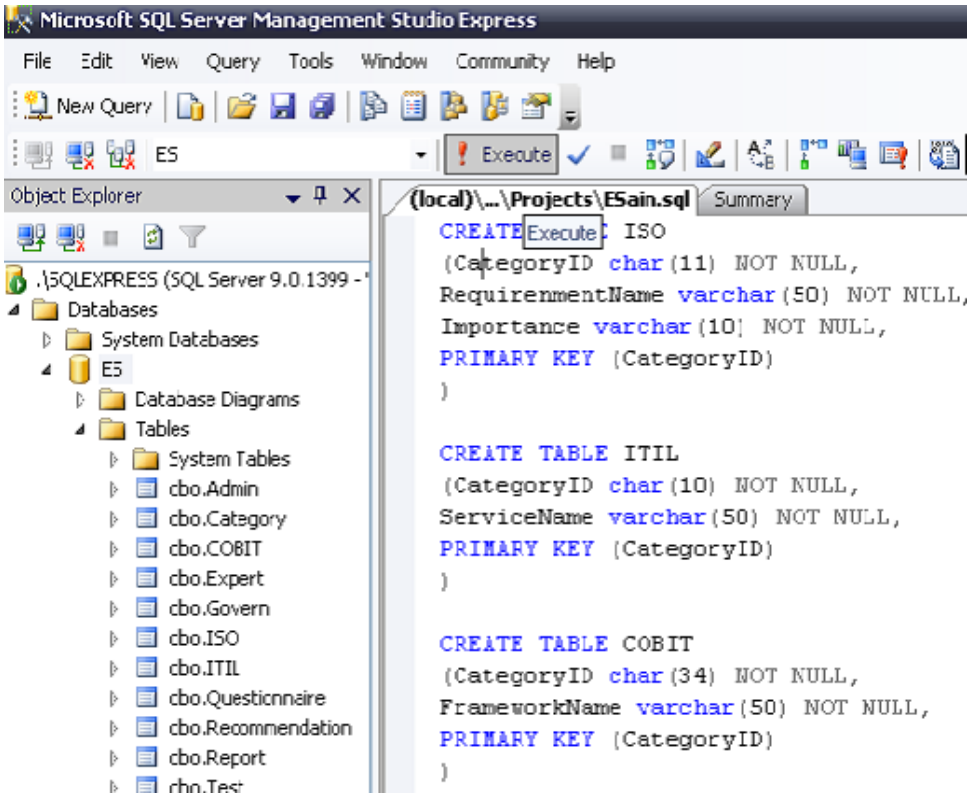

Figure 3. Queries for some DB tables in MS SQL Server 2005

The last step is filling tables with user's data. In MS SQL Server 2005 data filling is made through queries or manual entry of information.

5. Conclusions

This article focuses on the development of database for expert systems of information security auditing. The result of research is developed review and analysis of information security in accordance with international standards and guidelines for the management of IT, audit and IT-security, such as ISO27001, COBIT 4.1 and ITIL V3. Together, these standards contain requirements for information security for the creation, development and maintenance of information security management system.

The knowledge base for ESISA was created on the basis of the best international practices in the management of information security. It includes questions about the security of information and presented in the form of a questionnaire, the relevant standards of ISO27001, COBIT 4.1 and ITIL V3.

Structure of the database was designed on the Unified Modeling Language in the development environment StarUML. Software implementation is made in the queries language Transact-SQL with the use of Relational Database Management MS SQL Server 2005. Database tables have been designed according to knowledge base for ESISA.

Let us note that nowadays in Kazakhstan the research is conducted towards the development and implementation of expert system in security auditing. This framework of project named as "Development of intelligent systems for management and auditing of information security" is being financed by Ministry of education and science of Republic of Kazakhstan for 2012-2014 years.

In conclusion, we would like to note that the research results can be used in conjunction with the developing expert system in the auditing companies and any organizations interested in the proper functioning of safety systems.

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BUILDING LINUX VIRTUAL SERVER BY NETWORK ADDRESS TRANSLATION TECHNOLOGY

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Linux virtual server is a technology of building failover architecture server systems which will automatically balance the load from requests. This technology works on Linux based servers especially on Debian and Red Hat operating systems because they have patched kernel. This technology is used for the web servers of Wikipedia project.

The main goal is to create load balancing server system based on Linux Virtual Server technology (Figure 1) and network address translation system. Load balancing servers will be based on Red Hat Linux while real servers can run mostly any operating system. Linux virtual server based systems can operate with great efficiency. The main idea of this architecture is – when one load balancer will be broken down second load balancer will be able to connect virtual IP address to the real IP address and work instead of the first load balancer.

Keywords: *Linux, Linux virtual server, LVS, network address translation, NAT, failover architecture, load balancing, real server, virtualisation*

1. Introduction

Every load balancer during the work will balance the load between three real servers. The amount of transferred packets varies due to the special relative number which will show the operating efficiency of each real server. For example, if real server will have operating efficiency 10, the second server 34 and the third server will have operating efficiency 75, then at one moment of time they will receive amount of packets proportionally to each number.

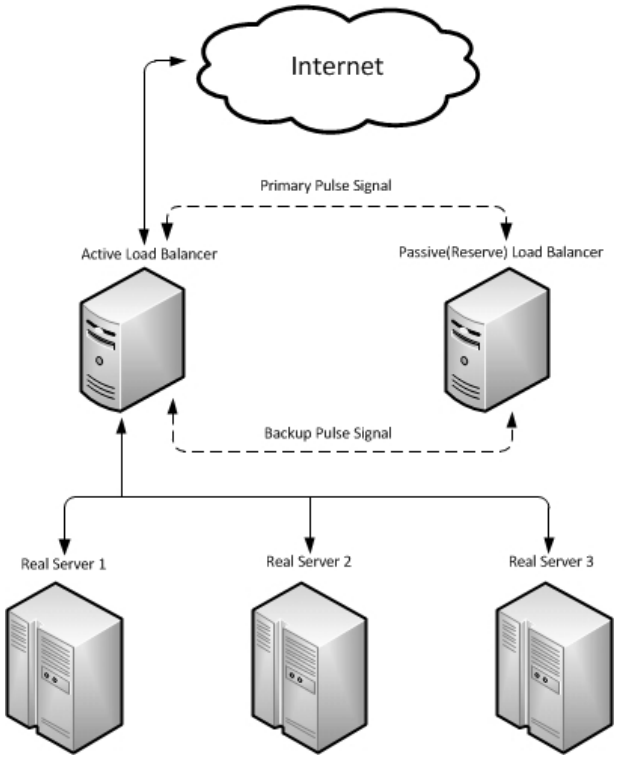

Figure 1. Linux Virtual Server

An LVS cluster consists of one or more virtual services each may have zero or more real servers. The IP address of a virtual service is what end-users connect to and is typically advertised over DNS. When a connection is made to a virtual service, it is allocated a real server, and all packets for this connection are forwarded to this real server. Piranha is a daemon to monitor and administer servers in a LVS cluster of load balanced virtual servers. Piranha monitors the health of the real servers by periodically requesting a known script and checking that the response contains an expected output. If a real server fails then the server is removed and will be reactivated once it comes back on line.

Here is an example of load balancing system, which will contain 2 load balancer and 3 real servers built on network address translation technology.

2. Configuration of Load Balancer 1

First of all we need to configure the services, which will be started during the boot:

```
/sbin/chkconfig  --level 35 piranha-gui on
/sbin/chkconfig  --level 35 pulse on
/sbin/chkconfig  --level 35 sshd on
```

To see the list of services type:

```
/sbin/chkconfig –list
```

Then we need to create a password for piranha user:

```
/usr/sbin/piranha-passwd
```

Also we need to turn on the packet forwarding by editing information in the text file /etc/sysctl.conf , the line “net.ipv4.ip_forward = 0” should be changed to “net.ipv4.ip_forward=1”.

To check the state of ipforwarding we need to type:

```
/sbin/sysctl net.ipv4.ip_forward
```

To turn on ipforwarding manually type:

```
/sbin/sysctl –w net.ipv4.ip_forward=1
```

Configuration of network interfaces:

Edit the file /etc/sysconfig/network-scripts/ifcfg-eth2 to look as follows:

```
DEVICE=”eth2”
BOOTPROTO=”static”
ONBOOT=”yes”
IPADDR=”192.168.26.9”
NETMASK=”255.255.255.0”
GATEWAY=”192.168.26.254”
```

Edit the file /etc/sysconfig/network-scripts/ifcfg-eth3 to look as follows:

```
DEVICE=”eth3”
BOOTPROTO=”static”
ONBOOT=”yes”
IPADDR=”10.11.12.9”
NETMASK=”255.255.255.0”
```

Network interfaces should look as follows (Figure 2):

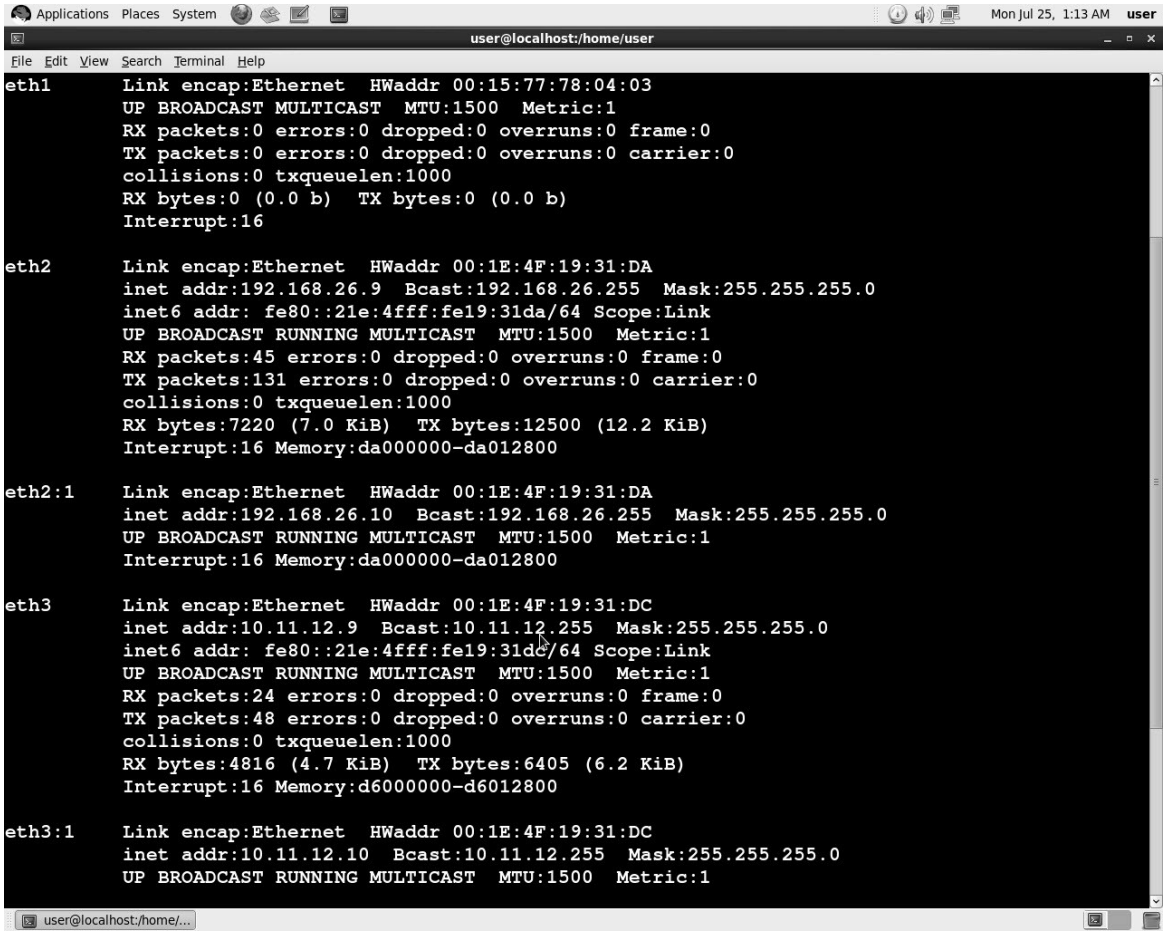

Figure 2. Network interfaces

3. Configuration of Load Balancer 2

First of all we need to configure the services, which will be started during the boot:

/sbin/chkconfig --level 35 pulse on
/sbin/chkconfig --level 35 sshd on

Also we need to turn on the packet forwarding by editing information in the text file /etc/sysctl.conf, the line “net.ipv4.ip_forward = 0” should be changed to “net.ipv4.ip_forward=1”.

To check the state of ipforwarding we need to type:

/sbin/sysctl net.ipv4.ip_forward

To turn on ipforwarding manually type:

/sbin/sysctl –w net.ipv4.ip_forward=1

Configuration of network interfaces.

Edit the file /etc/sysconfig/network-scripts/ifcfg-eth2 to look as follows:

```
DEVICE=”eth2”
BOOTPROTO=”static”
ONBOOT=”yes”
IPADDR=”192.168.26.19”
NETMASK=”255.255.255.0”
GATEWAY=”192.168.26.254”
```

Edit the file /etc/sysconfig/network-scripts/ifcfg-eth3 to look as follows:

```
DEVICE=”eth3”
BOOTPROTO=”static”
ONBOOT=”yes”
IPADDR=”10.11.12.19”
NETMASK=”255.255.255.0”
```

4. Configuration of Real Servers 1, 2, 3

Edit the file /etc/sysconfig/network-scripts/ifcfg-eth0 to look as follows:

```
DEVICE=”eth0”
BOOTPROTO=”static”
ONBOOT=”yes”
IPADDR=”10.11.12.1” (10.11.12.2 10.11.12.3)
NETMASK=”255.255.255.0”
GATEWAY=”10.11.12.10”
```

Also we need to turn on these services:

```
/sbin/chkconfig  --level 235 httpd on
/sbin/chkconfig  --level 35 sshd on
```

And we need to create an index.html file in /var/www/html folder with such content:

```
<html>
    <head>
                <title>Hello Page</title>
        </head>

        <body bgcolor=”white” text=”blue”>
        <h1>This is RealServer #1<h1> (RealServer#2 RealServer#3 )
        </body>
</html>
```

We need to open /etc/httpd/conf/http.conf file and uncomment line "Linsten 12.34.56.78:80" and change it to "Linsten 10.11.12.1:80" (10.11.12.2. and 10.11.12.3), then comment the line "Listen 80"
The status of httpd need to be checked by command:

```
/etc/init.d/httpd status
```

If httpd is not running then we need to start it by command:

```
/etc/init.d/httpd start
```

Now let’s enter the Piranha program on the LoadBalancer1 by opening a browser and typing:

```
localhost:3636
Login: piranha
Password: (the password that we set up previously)
```

Now check every page of Piranha and type the settings from the pictures (Figure 3–9).

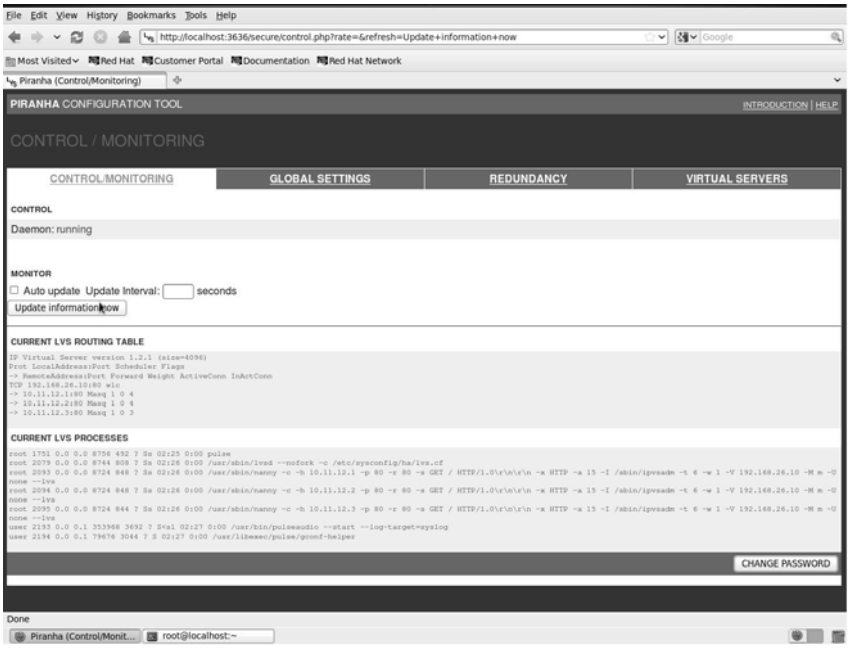

Figure 3. Control monitoring panel of Piranha daemon tool

Figure 4. Global settings panel of Piranha daemon tool

Figure 5. Redundancy panel of Piranha daemon tool

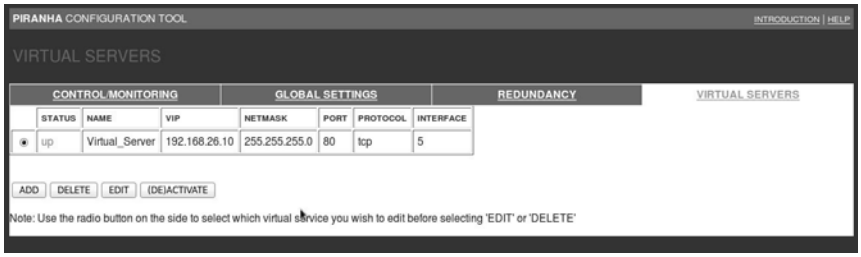

Figure 6. Virtual servers panel of Piranha daemon tool

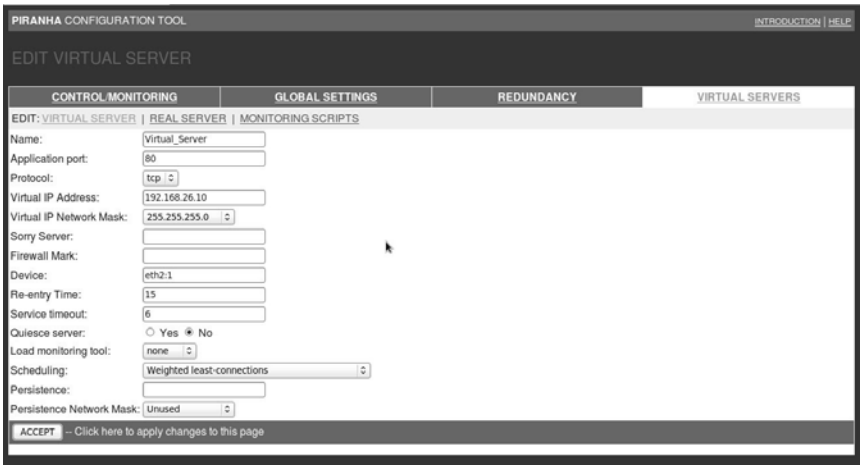

Figure 7. Virtual servers panel of Piranha daemon tool

Figure 8. Virtual servers panel of Piranha daemon tool

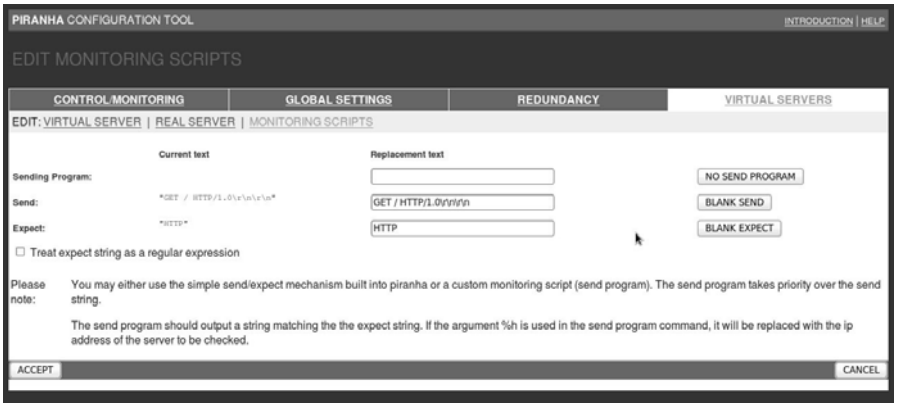

Figure 9. Virtual servers panel of Piranha daemon tool

All configurations will be stored in /etc/sysconfig/ha/lvs.cf

Also we need to synchronize lvs.cf files between LoadBalancer1 and LoadBalancer2 by running next command on the LoadBalancer1:

scp /etc/sysconfig/ha/lvs.cf 192.168.26.19:/etc/sysconfig/ha/lvs.cf

Check script:

```
#!/bin/sh
TEST= dig -t soa example.com @$1 | grep -c dns.example.com
if [$TEST !=1 "1" ]; then
        echo "OK"
else
        echo "FAIL"
fi
```

At the next step we will configure iptables on LoadBalancer1, LoadBalancer2, RealServer1, RealServer2 and RealServer3.

For the first check we can just turn off iptables on every server by commands:

```
/etc/init.d/iptables save
/etc/init.d/iptables stop
```

To check the state of iptables use the following command:

```
/sbin/iptables  -L –n
```

If we need to edit iptables we can use such commands as:

```
Iptables –A FORWARD -s 192.168.26.10 -d 10.11.12.1 -p tcp --dport 80 -j ACCEPT
```

INPUT, OUTPUT, FORWARD – parameters for different traffic
-s means ip address for incoming packages
-d means ip address for outcoming packages
-p means port
-dport means destination port

ACCEPT means accept
REJECT send the package back
DROP just send the package to /dev/null
iptables –D INPUT 4 (here –D means delete, INPUT the option, witch can take such values as INPUT,OUPUT, FORWARD, and 4 is the number of the line in INPUT, OUTPUT or FORWARD list)

Conclusions

To check the system we need open browser from the computer with ip 192.168.26.11 and type into the browser 192.168.26.10 and we will see the HTML page. Now we can check the redundancy of the system by unplugging load balancing servers or any real server.

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CUMULATIVE INDEX

COMPUTER MODELLING and NEW TECHNOLOGIES, volume 15, No. 4, 2011

(Abstracts)

Lobanova-Shunina, T., Shunin, Yu. N. Quality Control System as a Tool for Competitiveness Enhancement in Private Higher Education Management: The Systemic Criteria Assessment, *Computer Modelling and New Technologies*, vol. 15, No 4, 2011, pp. 7–15.

Strategies to deal with competitiveness enhancement in private higher education should start with its performance assessment. The importance to carry out such an evaluation is determined by a vast array of factors. The major ones include the requirement to develop innovative approaches to competitiveness increase, to compile new programs to capture the customer perception and to enter new education marketplaces, to construct effective and flexible assortment and education fee policies. All the aforementioned measures are directed to define the place of a higher education institution on the market. The possibility to attain this goal gains grounds in integration of operational and objective methods implemented for competitiveness assessment that will allow evaluating institutional performance and outcomes as well as offering particular ways to improve competitiveness.

Keywords: system approach, intelligent system structure, quality system, higher education management

Kiruta, N. V., D'yachkov, E. P., D'yachkov, P. N. Supramolecular Complexes of Carbon Nanotubes with Doxorubicin and Poly (Ethylene Glycol) Studied Using the Molecular Docking and Dynamic Methods, *Computer Modelling and New Technologies*, vol. 15, No 4, 2011, pp. 16–22.

Using the molecular dynamic and docking techniques, the binary and ternary complexes of antitumour drug doxorubicin, carbon nanotubes, and poly (ethylene glycol) are studied. On this basis, we determine the hydrophilic/lipophilic behaviour, the structures and stabilities of supramolecular complexes in water and organic (octanol) solutions and give recommendations on what type of nanotubes should form the most perspective compositions for delivery of the doxorubicin. It is shown that coupling between the nanotube and solvent molecules results in a regular approximately circular alignment of both water and octanol molecules in the outer region and in the inner cavity of the nanomaterial. Both solvents influence the doxorubicin conformation. In water, the conjugated core of doxorubicin is orientated almost parallel to the nanotube surface favouring a surface complexation of the drug and tubule. In organic solvent, the core and the nanotube surface are orientated virtually perpendicular, pointing on the absence of π-π-stacking coupling. In the case of water, increase of distance between the tubule and drug results in energy increase, but in the organic solvent, the lager distance between tubule and doxorubicin the smaller is energy. The stable nanotube-doxorubicin supramolecular complexes being formed in water solutions are to be destroyed in biological tissues resulting in drug release. For nanotubes of small diameters $d < 12.5$ Å of any chirality (armchair or zigzag), the doxorubicin molecule is located on the outside of the nanotube, but for nanotubes of larger diameters it is to be located inside the tube. The tubule diameter dependence of the doxorubicin bond energy is nonmonotonic: the complexes with nanotubes having $d \sim 13.5$ Å are the most stable, the doxorubicin molecule being located inside the nanotube. The external or internal location of poly (ethylene glycol) in the complexes with nanotubes is dictated by the tube diameter too; however, the boundary diameter is different ($d \sim 11$ Å). This fact makes it possible to predict that in the ternary supramolecular complexes of (8, 8) and (14, 0) nanotubes the poly (ethylene glycol) molecule is to be located inside and the doxorubicin molecule outside the nanotube. These complexes should be the best water soluble doxorubicin carriers on the basis of the water soluble nanotubes.

Keywords: Molecular dynamic; molecular docking; nanotube; doxorubicin

Sedov, Ye., Borisyuk, A,. Pasechnik, I. E-Learning in the Environment of the University Uniform Information Space, *Computer Modelling and New Technologies*, vol. 15, No 4, 2011, pp. 23–27.

The results of application of the modern approaches of e-learning (EL) in the university teaching process are discussed. EL is considered in the university uniform information space. It is concluded that today the optimal variant of application of EL is a realization of "mixed learning" that unites EL with a traditional teaching.

Keywords: uniform information space, e – learning, mixed learning

Mykytenko, N., Sedov, Ye. Some Particular Cases of Multi-Layer Feed-Forward Networks Modelling, *Computer Modelling and New Technologies*, vol. 15, No 4, 2011, pp. 28–34.

The paper considers an input data representation of the sequence for time series forecasting using the multi-layer feed-forward (MLFF) neural network with supervised learning. The values of input sequence are chosen in three different ways: using standardization in some interval, transferring to binary code and transferring to Gray code. To form the training set for the network learning the sliding window method was applied.

Each representation variant determines a rightness and speed of network learning with some network configuration using different values of window width. As a result it is possible to compare the rightness degree of forecasting for each variant of data presentation and to define the most preferable variant for this sequence.

Keywords: multi-layer feed-forward neural network, time series forecasting, input data representation

Kuchin, Y. I., Muhamedyev, R. I., Muhamedyeva, E. L., Gricenko, P., Nurushev, Zh., Yakunin, K. The Analysis of the Data of Geophysical Research of Boreholes by Means of Artificial Neural Networks, *Computer Modelling and New Technologies,* vol. 15, No 4, 2011, pp. 35–40.

The analysis of geophysical research of boreholes in uranium fields is an important phase of deposits searching, exploration and mining. The method of pre-processing of data and training of artificial neural network is described. This method gives stable results. About 2000 calculation experiments have been made; software and templates for pre-processing of data and results interpretation have been developed. Different methods of normalization, smoothing, excluding shifting data, preparing of training samples were researched. These experiments showed the perspective of neural network approach to solving the problem of rock recognition on stratum-infiltration uranium deposits. Problems of the further experiments which will allow raising the degree of automation of recognition process and its accuracy have been formulated.

Keywords: geophysical research of boreholes, artificial neural network, pre-processing data, normalization, smoothing

Askarov, N., Kozhakhmet, K., Atymtayeva, L. Analysis of Web-Based Applications for Expert System, *Computer Modelling and New Technologies,* vol. 15, No 4, 2011, pp. 41–45.

Convergence of technologies in the Internet and the field of expert systems have offered new ways of sharing and distributing knowledge. However, there has been a general lack of research in the area of creating web-based application for expert systems (ES). Our work will address the issues associated with the analysis of design, development, and use of web-based ES from a standpoint of the benefits and challenges of developing and using them. As a case study, the architecture of a Web site/application will be presented. The benefits and challenges in developing and using web-based application for Expert System will be mentioned by comparing them with traditional and existent web-based ES. Based on the gained experience, useful tips will be given on the construction of such Web sites applications.

Keywords: WEB-based applications, expert system

Muhamedyev, R. I., Kupensheyeva, A. I. Early Estimation Method of Software Development, *Computer Modelling and New Technologies,* vol. 15, No 4, 2011, pp. 46–51.

In order to estimate the effort put into software development various models are used, which are basically based on some form of analysis specification of customer requirements or technical project. In particular, FP metrics that allow to estimate the effort based on the numbers of the function points is widely known [1, 2].

In our opinion, adaptive evaluation system based on formalized specifications of a customer can be used in established system of development (elaboration). This evaluation system can be named as “early”, since it does not include the in-depth analysis methods of the projected system. This system of effort estimation should be based on some important parameters of formalized specifications and additional parameters, which include, for example, qualification of software developer, type of module, etc. For an assessment of basic applicability of formalized specification the analysis based on actual data was performed. The quantity of words and characters were used as the metrics of formalized specification (LFC).

The results of the technique based on the LFC metrics show that error of evaluation results compared with the actual data is relatively small (at least for one module). The maximum error value is 20%, the average is around 9% as compared to the actual data.

Keywords: software engineering, labour effort estimation, formal specification, labour input estimation metrics, estimation methods

Bekezhanova, A., Atymtayeva, L. Development of Database for Expert Systems of Information Security Auditing, *Computer Modelling and New Technologies,* vol. 15, No 4, 2011, pp. 52–57.

In this era of high technology, the information is involved in almost every aspect of human lives. Due to rapid growth of information technologies, came the need for increasing the security of information. Information security auditing plays key role in providing any organization's good security level. But, the security of information technologies is one of the difficult and comprehensive systems. The main problem lies in the data organization, collection and its processing methods. One of the solutions could be development of expert system that will reduce cost, speed up and facilitate the process of Information Security auditing. The valuable item in developing such system could be database development.

This paper presents the study of information security at international and national standards and guidelines for the management of IT, audit and IT-security (such as ISO 27001, COBIT 4.1 and ITIL V3) and the structure of database for expert systems of information security auditing.

Keywords: information security, information security auditing, standards for auditing information security, expert systems, database, UML, Transact-SQL

Amandossov, A. Building Linux Virtual Server by Network Address Translation Technology, *Computer Modelling and New Technologies,* vol. 15, No 4, 2011, pp. 58–65.

Linux virtual server is a technology of building failover architecture server systems which will automatically balance the load from requests. This technology works on Linux based servers especially on Debian and Red Hat operating systems because they have patched kernel. This technology is used for the web servers of Wikipedia project.

The main goal is to create load balancing server system based on Linux Virtual Server technology (Figure 1) and network address translation system. Load balancing servers will be based on Red Hat Linux while real servers can run mostly any operating system. Linux virtual server based systems can operate with great efficiency. The main idea of this architecture is – when one load balancer will be broken down second load balancer will be able to connect virtual IP address to the real IP address and work instead of the first load balancer.

Keywords: Linux, Linux virtual server, LVS, network address translation, NAT, failover architecture, load balancing, real server, virtualisation

COMPUTER MODELLING and NEW TECHNOLOGIES, 15.sējums, Nr. 4, 2011

(Anotācijas)

Lobanova-Šuņina, T., Šuņins, J. N. Kvalitātes kontroles sistēma kā instruments konkurētspējas veicināšanai privāto augstskolu menedžmentā: *sistēmisko kritēriju vērtējums, Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 7.–15. lpp.

Stratēģijām, lai tās risinātu konkurētspējas uzlabošanu privātās augstskolās, ir jāsākas ar šo augstskolu darbības novērtējumu. Svarīgums, lai veiktu šādu novērtējumu, tiek noteikts ar plašu faktoru loku. Lielākie iekļauj prasības inovatīvu pieeju attīstībai, lai palielinātu konkurētspēju, jaunas programmas klientu izpratnes uztveres apkopošanai, kā arī jaunu tirgus apguvei, lai veidotu efektīvu un elastīgu sortimentu un izglītības maksas politiku. Visi minētie pasākumi ir virzīti, lai noteiktu augstākās izglītības institūcijas vietu tirgū. Iespējas, lai sasniegtu šo mērķi, gūst pamatu operacionālo un objektīvo metožu integrācijā, kas ieviestas konkurētspējas novērtēšanai, kas, savukārt, atļaus novērtēt institucionālo darbību un rezultātu, piedāvājot īpašus ceļus konkurētspējas uzlabošanai.

Atslēgvārdi: sistēmas pieeja, inteliģentā sistēmas uzbūve, kvalitātes sistēma, augstākās izglītības menedžments

Kiruta, N. V., Djačkov, E. P., Djačkov, P. N. Oglekļa nanocaurulīšu ar doksorubicīnu un poli (etilēnglikola) supramolekulāro kompleksu pētījums, pielietojot molekulārās novietošanas un dinamikas metodes, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 16.–22. lpp.

Izmantojot molekulārās dinamikas un novietošanas metodes, tiek pētīti binārais un trīskāršais kompleksa pretaudzēju zāļu doksorubicīns, oglekļa nanocaurules un poli (etilēnglikols). Pamatojoties uz minēto, mēs nosakām hidrofīlisko/lipofilo uzvedību, supramolekulāro kompleksu struktūras un stabilitātes ūdenī un organiskos (oktanola) šķīdumos, kā arī sniedzam ieteikumus par to, kāda veida nanocaurules būtu jāveido visperspektīvākām kompozīcijām, lai piegādātu doksorubicīnu. Ir pierādīts, ka savienojums starp nanocauruli un šķīdinātāja molekulu rezultējas aptuvenā apļveida saskaņojumā kā ūdens, tā arī oktanola molekulās nanomateriālu ārējā reģionā un iekšējā dobumā.

Pētījumā aprakstītie kompleksi būtu labākie ūdenī šķīstošie doksorubicīna pārvadātāji, pamatojoties uz ūdenī šķīstošām nanocaurulēm.

Atslēgvārdi: molekulārā dinamika, molekulārā novietošana, nanocaurules, doksorubicīns

Sedovs, J., Borisjuk, A., Pasečnik, I. E-mācīšanās universitātes vienotā informācijas vidē, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 23.–27. lpp.

Rakstā tiek apskatīti mūsdienu e-mācīšanās pieejas pielietošanas rezultāti universitātes mācību procesā. E-mācīšanās tiek ņemta vērā vienotā universitātes telpā. Tiek secināts, ka šodien e-mācīšanās pielietošanas optimālais variants ir 'jauktā mācīšanās', kas apvieno sevī e-mācīšanās un tradicionālās mācības.

Atslēgvārdi: vienota informācijas telpa, e-mācīšanās, jauktā mācīšanās

Mikitenko, N., Sedovs, J. Daži īpaši gadījumi tīklu daudzslāņu tiešo sakaru modelēšanā, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 28.–34. lpp.

Rakstā tiek apskatīts laikrindu prognozēšanas secības ieejas datu attēlojums, pielietojot daudzslāņu tiešo sakaru (angl. *multi-layer feed-forward (MLFF))* neironu tīklu ar uzraudzītu apmācību. Ieejas secības vērtības tiek izvēlētas trīs dažādos veidos: pielietojot standartizāciju dažos intervālos, pārsūtot binārajam kodam un pārsūtot *Gray* kodam. Bīdāmo logu metode tika pielietota, lai izveidotu apmācību rindu tīkla mācībām.

Katrs reprezentācijas variants nosaka pareizību un ātrumu tīkla mācībām ar kādu tīkla konfigurāciju, pielietojot logu platumu dažādas vērtības. Rezultātā ir iespējams salīdzināt prognozēšanas pareizības pakāpi datu prezentācijas katram variantam un definēt visvairāk vēlamo variantu šai secībai.

Atslēgvārdi: neironu tīkla daudzslāņu tiešie sakari, laikrindu prognozēšana, ieejas datu attēlojums

Kučins, J. I., Muhamedjevs, R. I., Muhamedjeva, E. I., Gricenko, P., Nuruševs, Ž., Jukumins, K. Datu analīze par urbumu ģeofizikālo izpēti ar mākslīgajiem neironu tīkliem, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 35.–40. lpp.

Urbumu, kas veikti urānu laukos, ģeofizisko pētījumu analīze ir depozītu meklēšanas, izpētes un ieguves svarīga fāze. Tiek aprakstīta datu pirms apstrādes un mākslīgo neironu tīklu apmācības metode. Šī metode dod stabilus rezultātus. Tika veikti ap 2000 aprēķinu eksperimentu; programmatūras un veidņu datu pirms apstrādei un rezultātu interpretēšana tika izstrādāta. Šie eksperimenti parādīja perspektīvu neironu tīkla pieejai, lai risinātu iežu atzīšanas problēmu slāņa infiltrācijai urāna depozītos. Turpmāko eksperimentu problēmas, kuras ļaus paaugstināt atzīšanas procesa automatizācijas pakāpi, un to pareizība ir formulēta dotajā pētījumā.

Atslēgvārdi: ģeofizisko pētījumu urbumi, mākslīgie neironu tīkli, datu pirms apstrāde, normalizācija, nolīdzināšana

Askarovs, N., Kožahmets, K., Atimtajeva, L. Tīmekļa lietojumprogrammas ekspertu sistēmām un to analīze, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 41.–45. lpp.

Interneta tehnoloģiju un ekspertu sistēmu jomas konverģence ir piedāvājusi jaunus veidus, kā dalīties un izplatīt zināšanas. Tomēr pastāv vispārējs pētījumu trūkums tīmekļa bāzētu lietojumprogrammu radīšanā ekspertu sistēmām (ES). Šis pētījums risinās jautājumus, kas saistīti ar projekta analīzi, izstrādi un tīmekļa bāzētu lietojumprogrammu izmantošanu no labumu gūšanas un izaicinājumu redzes viedokļa. Ieguvumi un izaicinājumi, izstrādājot un lietojot tīmekļa bāzētas lietojumprogrammas ekspertu sistēmām, tiks sastatītas ar tradicionālajām, pašreizējā lietošanā esošām lietojumprogrammām ekspertu sistēmām. Pamatojoties uz iegūto pieredzi, noderīgi padomi tiks sniegti, lai uzbūvētu šādas tīmekļa vietnes lietojumprogrammas.

Atslēgvārdi: tīmekļa bāzētas lietojumprogrammas, ekspertu sistēma

Muhamedjevs, R. I., Kupenšejeva, A. I. Agrīnā novērtējuma metode programmatūras izstrādei, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 46.–51. lpp.

Lai novērtētu pūles, kas ir ieliktas programmatūras izstrādē, tiek pielietoti dažādi modeļi, kas pamatā ir balstīti uz kādu analīzes specifikācijas veidu, kas atbilst klienta prasībām, vai tehnisko projektu. Jo īpaši, *FP* rādītāji, kas ļauj novērtēt pūles, kas balstās uz funkciju punktu numuriem, ir plaši pazīstami [1, 2].

Pēc mūsu domām, adaptīvā vērtēšanas sistēma, balstīta uz klienta formālām specifikācijām, var tikt pielietota izstrādes izveidotajā sistēmā. Šī novērtējuma sistēma var tikt saukta kā 'agrīnā', tā kā tā neiekļauj projektētās sistēmas padziļināto analīzes metodi. Šai piepūles novērtējuma sistēmai ir jābūt balstītai uz dažiem veidoto specifikāciju svarīgiem parametriem un papildu parametriem, kuri iekļauj, piemēram, programmatūras izstrādātāja kvalifikāciju, moduļa veidu u.c.

Atslēgvārdi: programmatūras inženierija, darba intensifikācijas novērtējums, formāla specifikācija, darbaspēka resursu aplēšu metrika, novērtēšanas metodes

Bekežanova, A., Atimtajeva, L. Datu bāzes attīstība informācijas drošības auditēšanas ekspertu sistēmām, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 52.–57. lpp.

Šajā augsto tehnoloģiju ērā, informācija ir iespiedusies gandrīz katrā cilvēka dzīves aspektā. Līdz ar informācijas tehnoloģiju strauju izaugsmi, ir radusies nepieciešamība pēc informācijas drošības. Informācijas sistēmas auditēšana spēlē galveno lomu, nodrošinot ikviena uzņēmuma labu drošības līmeni. Informācijas tehnoloģiju drošība ir ļoti sarežģīts un grūti veicams uzdevums, kas prasa kā zināšanas, tā arī izmaksas. Ekspertu sistēmas izveide ir viens no risinājumiem.

Rakstā autori pēta informācijas drošību pēc starptautiskajiem un nacionālajiem standartiem (tādiem kā ISO 27001, COBIT 4.1 un ITIL V3) un datu bāzu struktūras informācijas drošības auditēšanas ekspertu sistēmām.

Atslēgvārdi: informācijas drošība, informācijas drošības auditēšana, informācijas drošības auditēšanas standarti, ekspertu sistēmas, datu bāze

Amandossovs, A., Linux virtual servera veidošana ar tīkla adreses tulkošanas tehnoloģijas palīdzību, *Computer Modelling and New Technologies,* 15.sēj., Nr.4, 2011, 58.–65. lpp.

Linux virtuālais serveris ir arhitektūras serveru sistēmas kļūmjpārlēces novēršanas tehnoloģijas izveide. Šī tehnoloģija strādā, balstīta uz *Linux* severiem, it īpaši, uz *Debian* un *Red Hat* operātājsistēmām, tāpēc ka tām ir salabots kodols. Šī tehnoloģija tiek izmantota web-serveriem no Wikipedia projekta.

Pētījuma galvenais mērķis ir radīt slodzes līdzsvarošanas servera sistēmu, balstītu uz *Linux Virtual Server* tehnoloģiju (skat. 1. zīm.) tīkla adreses tulkojuma sistēmu. Slodzes līdzsvarošanas serveri tiks balstīti uz *Red Hat Linux*, kamēr reālie serveri var izmantot lielākoties jebkuru operētājsistēmu. Sistēmas, kas balstītas uz *Linux Virtual Server* var strādāt ar lielu efektivitāti.

Atslēgvārdi*: Linux Virtual Server*, tīkla adreses tulkošana, kļūmjpārlēces arhitektūra, reālais serveris, virtualizācija

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