

**INNOVATIVE INFOTECHNOLOGIES  
FOR SCIENCE, BUSINESS AND EDUCATION  
Vol. 2(9) 2010**

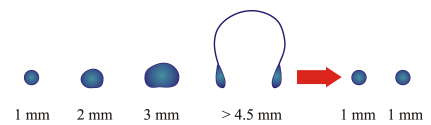
# CONTENTS

IITSBE, Vol. 2(9) 2010

## Section: IT - applied solutions

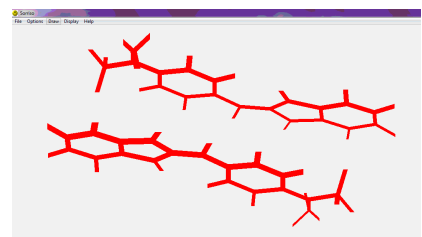
- 3-10 PREDICTION OF ELECTROMAGNETIC WAVE  
ATTENUATION DUE TO WATER IN  
ATMOSPHERE. 1. ATTENUATION DUE TO RAIN

Milda Tamošiūnaitė, Milda Tamošiūnienė, Alytis  
Gruodis, Stasys Tamošiūnas



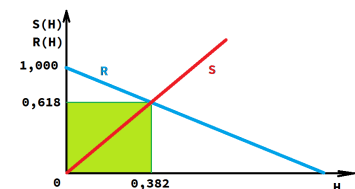
- 11-16 *SORRISO*: QUANTUM CHEMISTRY TOOL FOR  
VISUALIZATION OF ELECTRON TRANSFER  
PROCESSES

Ildar Galikov, Alytis Gruodis



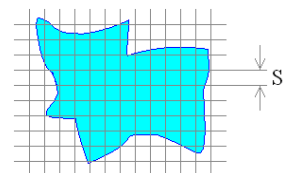
- 17-22 SPATIAL SELF-ARRANGEMENT OF EXPANDING  
STRUCTURES. 1. OVERVIEW OF ASSESSMENT  
CONCEPTS

Jelena Nesterova



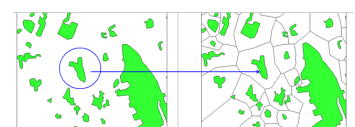
- 23-29 SPATIAL SELF-ARRANGEMENT OF EXPANDING  
STRUCTURES. 2. STRUCTURE MODEL  
CONSTRUCTION

Jelena Nesterova



- 30-36 SPATIAL SELF-ARRANGEMENT OF EXPANDING  
STRUCTURES. 3. NOVEL MODELING ROUTINE

Jelena Nesterova



## Prediction of electromagnetic wave attenuation due to water in atmosphere. 1. Attenuation due to rain

Milda Tamošiūnaitė<sup>1,2</sup>, Milda Tamošiūnienė<sup>3</sup>, Alytis Gruodis<sup>1</sup>, Stasys Tamošiūnas<sup>1,2 a</sup>

<sup>1</sup> Faculty of Physics, Vilnius University, Saulėtekio 9, korp. 3, Vilnius, Lithuania

<sup>2</sup> Institute of Applied Research, Saulėtekio 9, korp. 3, Vilnius, Lithuania

<sup>3</sup> Semiconductor Physics Institute, Center for Physical Sciences and Technology,  
A.Goštauto 11, Vilnius, Lithuania

*Received 27 September 2010, accepted 27 October 2010*

**Abstract.** The prediction of the electromagnetic wave (EW) power losses is a very important step in the design of radio systems. It is especially important for high operating frequencies. Accurate prediction of losses can ensure a reliability of the radio system, decrease in equipment cost, and maybe the system can become less injurious to health of people. Rainfall is one of the factors causing the attenuation of the electromagnetic waves while they are propagating through the atmosphere. In this paper, difficulties in prediction of electromagnetic waves attenuation due to rain are analyzed. According to the climatic peculiarities of Lithuania, appropriate model for calculation of electromagnetic waves attenuation due to rain (rain attenuation) was chosen. Applying this model a large quantity of precipitation data was computed and the specific rain attenuation considering the peculiarities of localities of Lithuania was determined.

**Citations:** Milda Tamošiūnaitė, Milda Tamošiūnienė, Alytis Gruodis, Stasys Tamošiūnas. Prediction of electromagnetic wave attenuation due to water in atmosphere. 1. Attenuation due to rain – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 3-10.

**Keywords:** Electromagnetic wave propagation; Rain attenuation; Rain rate.

**PACS:** 92.60.Ta; 92.40.Ea.

**Short title:** Prediction of EW attenuation due to rain.

### Introduction

In a design of the radio links the most desirable operating electromagnetic wave (EW) frequencies are below 10 GHz. The reasons causing such demand are listed in the Ref. [1]: “Galactic noise and man – made noise are minimum; atmospheric absorption and rainfall loss may generally be neglected; finally, there is a mature technology with competitive pricing of equipment”.

However, the frequency–band below 10 GHz is congested in most of the countries. In addition, the use of high frequency provides larger bandwidth, narrower beam width, good resolution and smaller component size [2]. Therefore, the operating frequencies of 10 GHz and above are often used in the design of the radio systems. However, in the cases of higher frequencies, the losses of energy of the electromagnetic waves (EW) propagating through the atmosphere are more noticeable.

One of the reasons is attenuation due to *hydrometeors* [1]. Hydrometeors are any particles of water or ice that have formed in the atmosphere or at the Earth’s surface as a result of condensation or sublimation. With increasing the EW frequency, the influence of the attenuation due to hydrometeors increases. Water or ice particles blown from the ground into the atmosphere are also classified as some sort of hydrometeors. Some well-known hydrometeors are clouds, fog,

rain, snow, hail, dew, rime, glaze, blowing snow, and blowing spray [3].

In the Ref. [4], it is noted that hydrometeors may be classified in a number of different ways, the following one is an example of one of them:

- 1) liquid or solid water particles formed and remaining suspended in the air (damp (high relative humidity) haze, cloud, fog, ice fog, and mist);
- 2) liquid precipitation (drizzle and rain);
- 3) freezing precipitation (freezing drizzle and freezing rain);
- 4) solid (frozen) precipitation (snow, hail, ice pellets, snow pellets (soft hail, graupel), snow grains, and ice crystals);
- 5) falling particles that evaporate before reaching the ground (*virga*);
- 6) liquid or solid water particles lifted by the wind from the earth’s surface (drifting snow, blowing snow, and blowing spray) [4].

The principal interactions between electromagnetic radiation and hydrometeors are scattering and absorption by the individual particles. Rainfall is one of the hydrometeors affecting electromagnetic waves path loss.

This work is devoted: i) to analyze the Lithuanian climate conditions; and ii) to determine the distribution of specific rain attenuation.

<sup>a</sup>Corresponding author, email: [stasys.tamosiunas@ff.vu.lt](mailto:stasys.tamosiunas@ff.vu.lt)

## 1. EW attenuation due to water

Water is in the atmosphere even during bright days. If we would pour on the Earth surface all the atmospheric water vapors, drops, and ice crystals, the layer as thick as 10 m would be formed around the all Earth [5].

Water of all three states can be found naturally in the atmosphere: the liquid (rain, fog, and clouds), the solid (snowflakes, ice crystals), and gas (water vapor). Attenuation due to water in the atmosphere varies with the density of the rainfall cell or cloud and the size of the rainfall drops or water particles such as fog or mist [1]. Hence, the atmosphere is not homogeneous. The raindrop is an obstacle in the link of the electromagnetic wave (EW). Water is a lossy dielectric medium. The dielectric properties of a raindrop differ from ones of the surrounding medium.

A part of an electromagnetic wave energy is absorbed and a part is scattered when the electromagnetic wave passes over the raindrops. The absorbed energy heats the absorbing raindrop. The molecules of water are polarized, because the centers of charges in the molecules of water are not in one line. Those molecules rotate in such way that positive part of one molecule would be as near as possible to the negative part of another molecule. Therefore, the molecules are rotating, hammering one on another and heating. The water molecule also rotates when a negative charge is brought near to it. Electromagnetic waves consist of electric force fields. As time goes on they vary and force water molecules to rotate subsequently [6]. The energy, which is scattered, is quasi-isotropic and relates to the wavelength of the incident wave [1].

The attenuation due to absorption is larger than attenuation due to scatter for wavelengths that are small compared with the drop size; for wavelengths that are long compared to drop size, the attenuation due to scatter is larger than attenuation due to absorption [7]. Scattering is most significant when the wavelength of the electromagnetic radiation is comparable to the dimension of the scattering particles (the diameters of the raindrops typically varied in the range  $0.2 \div 6$  mm) [8]. The absorption and scattering by raindrops depends on the size, shape and complex dielectric constant of the drops, and also on polarization and wavelength of the electromagnetic wave. Rain is highly non-uniform and this fact complicates the determination of rain attenuation of electromagnetic waves. It exhibits considerable variation in number density, size and shape. For any given rainfall rate, there is no unique distribution of drop sizes, and it varies in time and space.

The density of the water depends on its temperature. Water is the densest at temperatures up to  $+4^{\circ}\text{C}$ . The water relative dielectric constant is high in the contrast to the one of the surrounding air. The dielectric constant and the refractive index of the water depend on the temperature and on the operating frequency of the radio system. The specific heat of the water is high. Therefore, the water absorbs a large amount of warmth, while warms itself.

The dielectric constant of water also depends on the temperature. Therefore, the liquid water and ice are attenuating the electromagnetic waves in different degree. For example, one can ignore the microwave attenuation due to the dry snow, but the attenuation due to the rainfall or due to wet

snow is more noticeable and must be predicted in the radio system design. The attenuation due to the wet snow is near the attenuation due to the big raindrops in case of shower rain with the thunderstorm.

The surface tension of water is large. This is the reason why the molecules of water hold together. One of the problems in predicting power losses in electromagnetic waves is the description of the shape of the raindrops. The shape of a raindrop depends on drop's size. It is known, that only very small drops are like spheres. Such droplets form in clouds when water vapours condense on the nuclei of condensation. Further, these droplets grow by coalescence and shape of the raindrops is no more spherical. Larger raindrops are not tear-shaped, as it is commonly presented in pictures. The shape of the larger falling raindrops is like a hamburger (see Fig.1) [9].

Both the shape of the drops' size distribution and its parameters are related from the first principles to the dynamics of a single drop deforming as it falls in the air, ultimately breaking into a dispersion of smaller fragments containing the whole spectrum of sizes observed in the rain [10].

The large surface tension of water holds out the airflows pressure on the top of the drop and this is why the drop's shape is still spherical at the top of it. But the airflows are stronger at the bottom of the raindrop and for this reason the bottom of it is flattened [9].

Phillip Lenard (Nobel Prize Laureate 1905) concluded that a velocity of the falling drop depends on its size and grows with it [11]. But he also noticed that the velocity of a falling drop could not exceed  $8 \text{ m} \cdot \text{s}^{-1}$ . A change in the shape of the drop is a reason for the change in the velocity of the drop. The velocity of the falling drop decreases when the bigger drop takes the shape of a hamburger. The surface area and air resistance increase. However, the increases of raindrop size are limited by the value of the surface tension, which still can compensate the airflows pressure. The hollow in the bottom of the drop increases so greatly that the drops' surface tension can not hold any more pressure of the air and the drop divides nearly into two parts when its size increases to  $4 \div 4.5$  mm. Briefly those parts are still together connected by water bail. But eventually the drop divides into two smaller droplets (diameter about 1 mm).

However, in Ref. [12], raindrops diameters of even  $0.5 \div 10$  mm were presented. In Ref. [13], was concluded that in thunderstorms raindrops vary in sizes from about 0.5 mm to as much as 8 mm.

Wilson A. Bentley [14] presented data of size distribution of the raindrops. The data shows, that quantities of very small drops (in diameters  $\leq 0.85$  mm) and very large drops (in diameters  $3.6 \div 5.1$  mm) are nearly equal (17% and 16% correspondingly). The parts of small drops with a diameter  $0.84 \div 1.4$  mm and moderate ones with diameters  $1.4 \div 3.2$  mm are the largest of all (34% and 29% correspondingly). The part of very large drops with diameters  $>5.1$  mm is very small (only 4%) [14].

Many researchers have been studying the *drop sizes distribution* (DSD). The DSD derived by Laws and Parson [15] is the DSD most commonly used in the prediction of rain attenuation of the electromagnetic waves (EW).

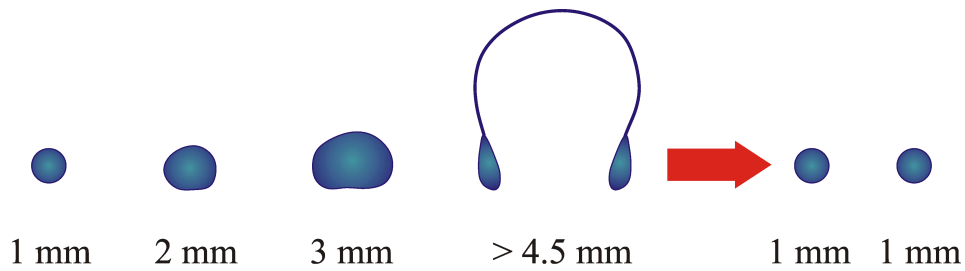


Fig. 1. The variation of the raindrop shape depending on its size (diameter of the drop). Modified according to Ref. [9].

Specific rain attenuation model in prediction methods presented in Ref. [1] and ITU-R's recommendation [16] is based on DSD proposed by Laws and Parson.

The analysis of the rainfall data has assumed traditionally that the raindrop size distribution (DSD) has an exponential form; that is, with  $N(D)$  [ $\text{m}^{-3} \cdot \text{cm}^{-1}$ ] equal to the number of raindrops per unit volume per unit size interval having equivalent spherical diameter  $D$  [cm], then

$$N(D) = N_0 \cdot \exp[-\Lambda \cdot D], \quad (1)$$

$$0 < D < D_{max}. \quad (2)$$

$N_0$  [ $\text{m}^{-3} \cdot \text{cm}^{-1}$ ] and  $\Lambda$  [ $\text{cm}^{-1}$ ] are parameters of the distribution and  $D_{max}$  is the maximum drop diameter [17]. Constant value  $N_0$  is equal to  $80\,000 \text{ m}^{-3} \cdot \text{cm}^{-1}$ . This form was originally found by Marshall and Palmer (1948) [18] who also suggested that  $\Lambda$  varied with rainfall rate  $R$  [ $\text{mm} \cdot \text{h}^{-1}$ ]:

$$\Lambda = 41 \cdot R^{-0.21}. \quad (3)$$

A similar analysis of the drop size spectra of Laws and Parsons (1943) [15] reveals that their data can also be represented closely by an exponential form  $\Lambda=f(R)$  and  $N_0$  weakly dependent on rainfall rate through expression (5):

$$\Lambda = 38 \cdot R^{-0.20}, \quad (4)$$

$$N_0 = 51000 \cdot R^{-0.03}. \quad (5)$$

The shape of the larger raindrops determines that fact that the horizontally polarized waves suffer greater attenuation than vertically polarized waves. The reason is that large raindrops are generally shaped as oblate spheroids and are aligned with the vertical rotation axis [1].

## 2. Calculation of EW attenuation due to the rain

The rain attenuation prediction methods can be grouped into two classes: i) the physical method which makes an attempt to reproduce the physical behavior involved in the attenuation process, and ii) the empirical method which is based on the analysis of databases of the physical measurements. It is necessary to point out that mentioned measurements were done in the stations placed in different climatic zones within a given region [19-20]. When the physical rain attenuation

prediction method is being used, one of the difficulties is the description of the shape of raindrops. In most cases the shape of a drop is described as spherical. For example, presented in Ref. [21], a simple spherical model was used for the calculation of the effect of temperature and multiple scattering on rain attenuation of electromagnetic waves. As mentioned above, this description of a raindrop shape in most cases is wrong. Empirical method for prediction of electromagnetic waves attenuation is used more often and more successfully than the physical one.

Commonly, the electromagnetic wave losses are expressed as a function of the rain rate  $R$ . In prediction of the radio waves attenuation due to the rainfall (rain attenuation), the well known semi-empirical model according to Ref. [1], [16] is being used. Specific rain attenuation is obtained from the rain rate  $R$  using the relationship:

$$\alpha = a \cdot R^b, \quad (6)$$

where  $\alpha$  represents a specific rain attenuation - dimension in [ $\text{dB} \cdot \text{km}^{-1}$ ];  $R$  - rain rate [ $\text{mm} \cdot \text{h}^{-1}$ ];  $a$  and  $b$  are functions of the rain temperature and operating frequency  $f$ .

The values of  $a$  and  $b$  from Ref. [1] (see Table 1) are presented for vertical and horizontal polarization. For frequencies other than presented in Table 1, the values of coefficients  $a$  and  $b$  can be obtained by interpolation.

The rain rate  $R$  can be described as the thickness of the layer of the precipitation which fell down over the time period of one hour in the case when the precipitation is not evaporated, not soaked into the soil, and is not draught by the wind.  $R$  depends on liquid water content and the fall velocity of the drop. The velocity, in turn, depends on the size of a raindrop [1].

$R$ -value must be determined for some percentage of time of the year and it must be in correlation with the reliability of the system. In most cases, the  $R$ -value for 0.01% of time ( $R_{0.01\%}$ ) is desirable in the design of radio systems. It means that  $R_{0.01\%}$ -value can be exceeded only about 52.56 min. in a year. In this case the reliability of the radio system would be 99.99%.

Despite that  $R_{0.01\%}$ -value is expressed in [ $\text{mm} \cdot \text{h}^{-1}$ ], the rainfall amount data for the calculations of the  $R$ -value must be measured in one-minute intervals.

Table 1. Specific rain attenuation coefficients  $a$ ,  $b$  for horizontal (h) and vertical (v) polarized waves, respectively. According to Ref. [1].

$f$ , GHz	$a_h$	$a_v$	$b_h$	$b_v$
1	0.0000387	0.0000352	0.912	0.88
2	0.000154	0.000138	0.963	0.923
4	0.00065	0.000591	1.121	1.075
6	0.00175	0.00155	1.308	1.265
7	0.00301	0.00265	1.332	1.312
8	0.00454	0.00395	1.327	1.31
10	0.0101	0.00887	1.276	1.264
12	0.0188	0.0168	1.217	1.2
15	0.0367	0.0335	1.154	1.128
20	0.0751	0.0691	1.099	1.065
25	0.124	0.113	1.061	1.03
30	0.187	0.167	1.021	1
35	0.263	0.233	0.979	0.963
40	0.35	0.31	0.939	0.929
45	0.442	0.393	0.903	0.897
50	0.536	0.479	0.873	0.868
60	0.707	0.642	0.826	0.824
70	0.851	0.784	0.793	0.793
80	0.975	0.906	0.769	0.769
90	1.06	0.999	0.753	0.754
100	1.12	1.06	0.743	0.744

The time interval between the measurements of the rainfall amount is called integration time  $\tau$ . In the mentioned case the integration time  $\tau=1$  min. is required.

One-minute  $R_{0.01\%}$ -value  $R_{1min.}$  is commonly referred as “instantaneous” value and has been recognized as the most practical for calculation of signal loss [22]. One-minute rain rate statistics also have applications in other areas, such as the design and operation of aerospace vehicles and radar systems [22].

Though there can be some difficulties while predicting the  $R_{1min.}$  -value. In Lithuania, usually the rainfall amount data is measured with the integration time  $\tau=10$  min. or more. Consequently in most cases we can calculate only  $>1$  min. rain rate values  $R_{\tau min.}$ . Therefore in cases when one-minute rainfall amount data is unavailable, the models converting  $R_{\tau min.}$  values into  $R_{1min.}$  values can be used. One-minute rainfall rate models are presented in Ref. [20] and Ref. [23]. One of the models mentioned above is Moupfouma model [24], where  $R_{1min.}$  represents one-minute rain rate value and  $R_{\tau min.}$  - rain rate value, when integration time is equal to  $\tau$  min.

$$R_{1min.} = R_{\tau min.}^d \quad (7)$$

$$d = 0.987 \cdot \tau^{0.061} \quad (8)$$

### 3. The peculiarities of Lithuanian climate

Lithuania, being in the transition geography zone from the Baltic Sea Region to Atlantic and continental east Europe

climate, may be distinguished for its variable climate [25]. In Lithuania, humid weathers predominate all over the year; the annual precipitation in a rainy wet year is almost twice higher than in a dry year [26]. The climate of the continental part of Lithuania is definable as middling cold and climate of the west part of Lithuania is specified as the moderate warm climate.

The climate of the continental part of Lithuania is a typical climate of the middle part of the East Europe. The type of the climate of the west part of Lithuania is dominating in the West Europe. Therefore, the conditions of the electromagnetic waves propagation can be different in the East and in the West of Lithuania.

There are many contrasts in Lithuanian climate conditions. For example, the maximum and minimum of annual rainfall amounts - both were registered in Laukuva ( $>900$  mm and  $0.0$  mm correspondingly) [27]. Thereby, the average annual rainfall amount can be a very informative and at the same time a very deceptive parameter.

In Ref. [26] it was concluded, that the hypothesis about the only value of  $R$  for all the territory of Lithuania must be rejected. In average, there are 51.4 events of rain in Žemaitija and 40.4 rain events in the other part of Lithuanian territory. In Vilnius, the maximum rain intensity of rain event with duration of 20 min. (integration time  $\tau = 20$  min.) is  $69 \text{ mm} \cdot \text{h}^{-1}$ . The rain rate value determined by using rainfall data measured with one-minute integration time may be higher. Such rain rates are observed once per 5 years [26].

### 4. Thunderstorms in Lithuania

The number of the thunderstorms per year is an important parameter in determining the rain rate. The strong vertical air streams are forming in the thunderstorms clouds. The speed of the air streams is  $15 \div 20 \text{ m} \cdot \text{s}^{-1}$  [28]. The rain rate depends on the convection strangeness and the cloud thickness. The stronger convection and the thicker the cloud the higher the rain rate value. The rain rate depends also on the cloud electrification. Therefore, the stronger showers put down in the thunderstorms.

There are  $19 \div 30$  days per year with the thunderstorms in Lithuania. However, the number of days of thunderstorms can be even  $40 \div 45$  (according to Ref. [28]). In the South part of Lithuania, the thunderstorms have been observed frequently, because the rough surface of the earth stops the air streams and stimulates the convective processes. 96% of the events of thunderstorms happen in May  $\div$  September period [28]. Thunderstorms have a local character. They do not occur in large territories because the convection is the local phenomenon. However, during the summer, the convection is very intense and thunderstorms can occur in more than half of the territory of Lithuania.

The maximum number of days,  $N_{max}$  in the year with thunderstorms was registered in the year 2001 in Vilnius.

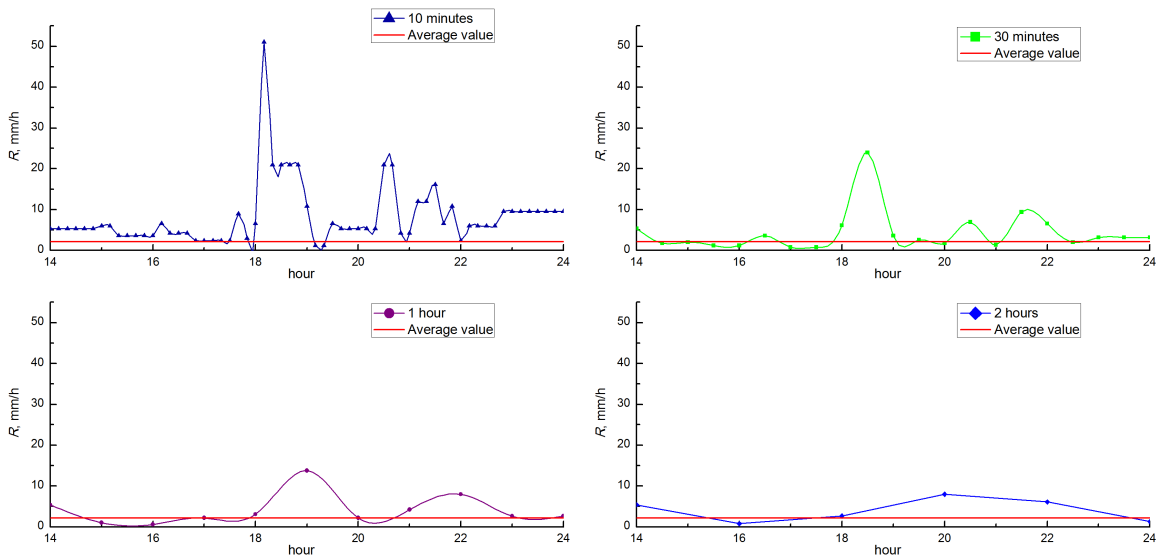


Fig. 2. The variation of rain rate  $R$  depending on the integration time  $\tau$ . Rain event on 17 July 2000.

The duration of all thunderstorms events (in Vilnius, 2001) was  $N_{max}=77$  h 18 min. [29]. It is worth to mention, that Vilnius is one of the cloudiest localities in Lithuania. There are about 100 overcast days in the year in this location. The minimum yearly duration (4 hours 30 min) of thunderstorms events was registered in Palanga in the year 1998 [29].

The distribution of the thunderstorm duration in Vilnius Airport is presented in Table 2. The data shows that 55% of the duration of thunderstorm in Vilnius is longer than 1 hour (longer than 0.01% of time of year). In most cases, strong showers are in the correlation with thunderstorms.

Rice-Holmberg model presented in Ref. [30] requires thunderstorm data. It also requires certain parameters like: highest monthly rainfall accumulation observed in a set of 30-year period, the average annual accumulation, and the ratio of thunderstorms precipitation amount with the annual precipitation amount. However, it has been acknowledged that the Rice-Holmberg method overestimates rain rates in the high-availability range (0.01% of time) and underestimates in the range between 0.1% and 1% [23].

Our model (9) was derived in Ref. [25] and [31] on the basis of Rice-Holmberg model [30] in accordance with the peculiarities of Lithuanian climate. They are events of heavy rain and showers happen frequently in the months of May – September; during the warm period, the part of the convection precipitation is 0.48 [32]:

$$R_{1min.} = \frac{1}{0.03} \ln \left( 0.0144 \cdot \frac{M_{V-IX}}{t_p} \right). \quad (9)$$

$R_{1min.}$  represents 1 minute rain rate value,  $M_{V-IX}$  - 30 years average rainfall amount during period from May to September,  $t_p$  - the percent of time in a year, when  $R_{1min.}$  may be exceeded (when reliability of the radio system should

be 99.99%,  $t_p = 52.56$  min. = 0.876 hours).

## 5. Results and discussion

### 5.1. Integration time influence on the $R$ value

We examined the influence of the integration time to the values of the rain rate. One rain event occurs 17 July 2000. We evaluated the rain rate  $R$  [ $\text{mm} \cdot \text{h}^{-1}$ ] values imagining that rain amount data of this rain event was collected with intervals (integration time  $\tau$  is equal to 10 min., 30 min., 1 hour, and 2 hours, see Fig. 2). The smallest integration time of 10 minutes was chosen because it is the minimal time interval in Lithuanian rain amount data.

Mentioned interval is 10 times bigger than the recommended one. Despite that, comparison of  $R$ -values calculated using bigger integration time also reveals how the  $R$ -values depend on the integration time - see Fig. 2.

The same rain event was shown in four dependences. Each graph represents different integration time: 10 min., 30 min., 1 hour, and 2 hours. Also, in each graph the line representing the average rain rate value is shown. This value is calculated only from two values of rain amount data: the value measured at the start of the rain event and the value measured at the end of the rain event.

Table 2. The distribution of the thunderstorm duration in Vilnius. Data according to Ref. [29].

Duration, h	Events, %
< 1	45
1 ÷ 2	37
2 ÷ 3	12
> 3	6

Table 3. Distribution of rain rate values  $R_{1min.}$  in the localities of Lithuania.

City	$M_V$ mm	$M_{VI}$ mm	$M_{VII}$ mm	$M_{VIII}$ mm	$M_{IX}$ mm	$M_{V-IX}$ mm	$t_p$ h	$R_{1min.}$ mm · h <sup>-1</sup>
Skuodas	52	54	82	97	88	373	0.876	60.45
Mažeikiai	47	55	78	78	69	327	0.876	56.06
N.Akmenė	48	54	77	77	68	324	0.876	55.75
Joniškis	50	67	81	70	63	331	0.876	56.47
Pasvalys	58	71	87	86	64	366	0.876	59.82
Biržai	59	74	90	87	68	378	0.876	60.89
Rokiškis	64	84	98	89	72	407	0.876	63.36
Kretinga	49	56	81	96	92	374	0.876	60.54
Plungė	53	61	90	96	83	383	0.876	61.33
Telšiai	58	60	93	96	85	392	0.876	62.10
Šiauliai	50	63	79	78	63	333	0.876	56.67
Pakruojis	44	58	71	73	58	304	0.876	53.63
Klaipėda	46	52	72	88	82	340	0.876	57.36
Šilalė	61	73	103	102	89	428	0.876	65.03
Kelmė	51	68	90	89	72	370	0.876	60.18
Radviliškis	47	59	74	73	59	312	0.876	54.50
Panevėžys	54	71	76	87	57	345	0.876	57.85
Kupiškis	57	73	86	79	63	358	0.876	59.08
Anykščiai	63	82	95	91	70	401	0.876	62.86
Utena	61	79	89	88	63	380	0.876	61.07
Zarasai	64	83	89	88	71	395	0.876	62.36
Ignalina	62	82	92	89	69	394	0.876	62.27
Šilutė	57	63	86	96	88	390	0.876	61.93
Tauragė	57	74	93	93	75	392	0.876	62.10
Jurbarkas	61	73	94	101	74	403	0.876	63.03
Raseiniai	57	64	88	93	72	374	0.876	60.54
Kėdainiai	63	72	86	96	61	378	0.876	60.89
Ukmergė	61	75	86	90	61	373	0.876	60.45
Molėtai	64	83	97	96	63	403	0.876	63.03
Švenčionys	62	84	87	91	70	394	0.876	62.27
Šakiai	54	64	83	86	56	343	0.876	57.65
Kaunas	66	80	100	104	64	414	0.876	63.92
Jonava	61	72	89	98	60	380	0.876	61.07
Širvintos	68	76	88	87	58	377	0.876	60.80
Vilkaviškis	53	71	90	96	60	370	0.876	60.18
Marijampolė	56	67	89	93	61	366	0.876	59.82
Prienai	57	74	87	87	57	362	0.876	59.45
Kaišiadorys	61	79	92	91	61	384	0.876	61.42
Trakai	57	77	90	89	60	373	0.876	60.45
Vilnius	56	74	87	85	56	358	0.876	59.08
Lazdijai	58	73	91	91	58	371	0.876	60.27
Alytus	58	75	88	87	58	366	0.876	59.82
Varėna	63	83	98	82	59	385	0.876	61.50
Šalčininkai	57	81	91	91	56	376	0.876	60.72
AVERAGE								60.23

As can be seen in Fig. 2, the lesser the integration time the higher the values of rain rates. As integration time decreases the pikes of rain rate becomes lower, wider and late. This means that when integration time is more than 10 minutes, the largest rain rate values “hide”.

For example, the rain rate value at 18 hour 15 min. with

the integration time of 10 min. is double the value with the integration time of 30 min. That means that data for the calculation of electromagnetic wave (EW) attenuation in Lithuania should be collected with as small as possible integration time (10 min. or less). This assumption is similar to recommendation according tropical environment.



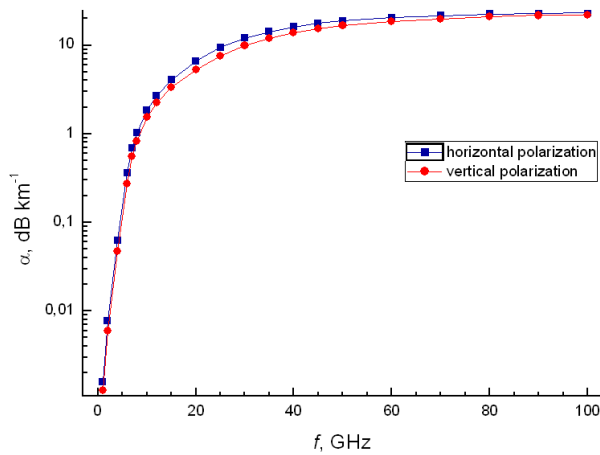


Fig. 3. Dependence of averaged specific rain attenuation for horizontally and vertically polarized EW,  $\alpha_h$  and  $\alpha_v$ , respectively, on frequency  $f$ .

## 5.2. $R_{1min.}$ values in the localities of Lithuania

Secondly, we calculated  $R_{1min.}$  values for different localities in Lithuania. (8) method has been used. The results are given in Table 3.

The  $R_{1min.}$  values in different localities in Lithuania vary from  $53.63 \text{ mm} \cdot \text{h}^{-1}$  in Pakruojis to  $65.03 \text{ mm} \cdot \text{h}^{-1}$  in Šilalė. Average value in Lithuania is equal to  $R_{1min.} = 60.23 \text{ mm} \cdot \text{h}^{-1}$ . This rain rate value is double the recommended rain rate value for Lithuania (for recommended  $R$ -value see Ref. [16]).

## 5.3. The specific electromagnetic waves attenuation due to the rainfall

Finally, having  $R_{1min.}$  value, we are able to compute the average specific EW attenuation due to the rainfall  $\alpha$  [ $\text{dB} \cdot \text{km}^{-1}$ ]. Eq. (6) was used. We used the average value in Lithuania  $R_{1min.} = 60.23 \text{ mm} \cdot \text{h}^{-1}$  as  $R$ . The values of  $a$  and  $b$  were taken from Table 1. The  $\alpha$  values for the operating frequencies  $1 \div 100$  GHz were calculated. Values of horizontal and vertical polarization were calculated separately. The results are shown in Fig. 3. There can be seen, that horizontally polarized electromagnetic waves are attenuated more than the vertically polarized ones. Furthermore, the relation between the operating frequency and the electromagnetic waves attenuation starting from about 4 GHz starts to grow and grows exponentially, but this growth slows down at frequency about 60 GHz and almost stops at 100 GHz.

The purpose to distinguish the  $\alpha$  values for horizontal polarization and vertical polarization at operating frequencies smaller than 15 GHz the rate  $p$  was introduced. The  $p$  value

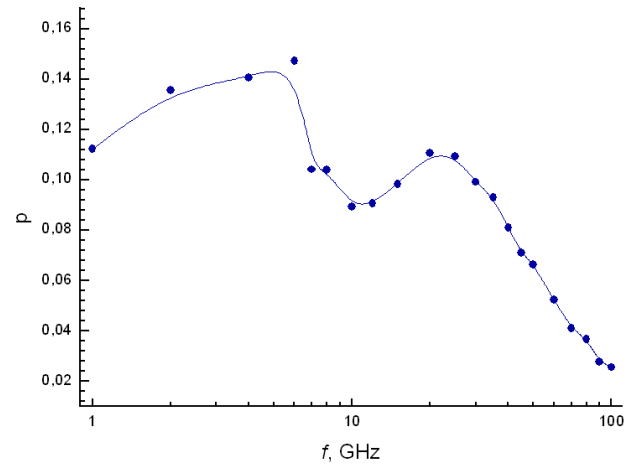


Fig. 4. Dependence of  $p$  value on frequency  $f$ .

is a normalized difference of  $\alpha$  for horizontal polarization and vertical polarization, and it is expressed as follows:

$$p = \frac{\alpha_h - \alpha_v}{\alpha_h + \alpha_v}, \quad (10)$$

where  $\alpha_h$  and  $\alpha_v$  are average specific attenuation for horizontally and vertically polarized EW, respectively.

The dependency of  $p$  value to the operating frequency  $f$  is shown in Fig. 4. There can be seen that the  $p$  value fluctuates at operating frequencies below about 20 GHz, and at operating frequencies above 20 GHz starts to constantly decline from about  $p = 0.11$  at  $f = 20$  GHz to about  $p = 0.02$  at  $f = 100$  GHz. Hence for higher frequencies the  $\alpha$  value (both for horizontally and vertically polarized electromagnetic waves) increases, but the normalized difference of the  $\alpha$  value for horizontally and vertically polarized electromagnetic waves decreases.

## 6. Conclusions

The values of one-minute rain rate  $R$  and average specific electromagnetic waves attenuation due to the rain  $\alpha$  were obtained. The average value of the rainfall rate in Lithuania is  $60.23 \text{ mm} \cdot \text{h}^{-1}$ . It is double the recommended value. The values of average specific electromagnetic waves attenuation due to the rain differs for different operating frequencies and depends on polarization of the electromagnetic wave. The relation between operating frequency and electromagnetic waves attenuation starting from about 4 GHz starts to grow and grows exponentially, but this growth slows down at frequency about 60 GHz and almost stops at 100 GHz. Horizontally polarized electromagnetic waves are attenuated more than the vertically polarized ones.

## References

1. R. L. Freeman. Radio System Design for Telecommunications – Hoboken, New Jersey: JOHNWiley&SONS, INC, 2007.
2. S. Bhattacharyya, M. Dan, A. K. Sen. Modelling of drip size distribution of rain from rain rate and attenuation measurements at millimeter and optical wavelengths – *International Journal of Infrared and Millimeter Waves* Vol. 21, No. 12 (2000) 2065 – 2075.
3. Encyclopædia Britannica. <<http://www.britannica.com/EBchecked/topic/278940/hydrometeor>>, retrieved 2010 09 17.
4. Glossary of Meteorology American Meteorological Society. <<http://ams.glossary.allenpress.com/glossary>>, retrieved 2010 09 17.
5. J. Guralnikas. Meteorologija. <<http://www.studijoms.lt/meteorologiniai-tyrinėjimai.htm>>, retrieved 2010 09 17.
6. <[http://www.colorado.edu/physics/2000/microwaves/water\\_rotates2.html](http://www.colorado.edu/physics/2000/microwaves/water_rotates2.html)>, retrieved 2010 09 17.
7. G. Ivanovs and D. Serdega. Rain Intensity Influence on to Microwave Line Payback Terms – *Electronics and Electrical Engineering* N.6(70) (2006) 60–64.
8. A. Maitra, C. J. Gibbins. Interference of raindrop size distribution from measurements of rainfall rate and attenuation at infrared wavelengths – *Radio Science* Vol.30, N.4 (1995) 931–941.
9. <<http://weather.about.com/od/cloudsandprecipitation/a/rainburgers.htm>>, retrieved 2010 09 17.
10. E. Villermaux, B. Bossa. Single-drop fragmentation determines size distribution of raindrops – *Nature Physics* Vol.5 (2009) 697 – 702.
11. Heidorn, Keith C. Philipp Lenard: Brushing the Teardrops from Rain – *The Weather Doctor* 1 July 2000.
12. Characteristics of Particles and Particle Dispersoids. In: Handbook of Chemistry and Physics. 62 nd Edition. – New York: CRC, 1981.
13. Formation of Raindrops. <[www.encyclopedia.com](http://www.encyclopedia.com)>, retrieved 2010 08 10.
14. Heidorn Keith C., Wilson A. Bentley. The Raindrop Man Too. – *The Weather Doctor*, 1 July 2000.
15. J. O. Laws and D. A. Parsons. The relation of raindrop size to intensity. – *Trans. Amer. Geophys. Un.* Vol.24 (1943) 452–460.
16. Characteristics of precipitation for propagation modeling. In: RECOMMENDATION ITU–R P.837–4 (Question ITU–R 201/3). – 1992–1994–1999–2001–2003. – P. 1–8.
17. C. W. Ulbrich. Natural variations in the analytical form of the raindrop size distribution. – *Journal of Climate and Applied Meteorology*, Vol. 22 (October 1983) 1764–1775.
18. J. S. Marshall and W. McK. Palmer. The distribution of raindrops with size – *Journal of Meteorology* Vol.5 (1948) 165 – 166.
19. L. D. Emiliani, J. Agudelo, E. Gutierrez, J. Restrepo, and C. Fradique–Mendez. Development of Rain–attenuation and Rain–Rate Maps for Satellite System Design in the Ku and Ka Bands in Colombia – *IEEE Trans. Antennas and Propagation Magazine* Vol.46. N.6 (2004) 54–68.
20. E. Setjadi, A. Matsushima, N. Tanaka, G. Hendrantoro. Effect of temperature and multiple scattering on rain attenuation of electromagnetic waves by a simple spherical model – *Progress in Electromagnetics Research*, PIER 99 (2009) 339–354.
21. P. Tattelman, K. Scharr. A model for estimating one – minute rainfall rates – *Journal of Climate and Applied Meteorology* Vol.22 (September 1983) 1575 – 1580.
22. P. Tattelman and D. D. Grantham. A review of models for estimating 1 min rainfall rates for microwave attenuation calculations – *IEEE Trans. on communications* Vol. Com-33, No.4 (1984).
23. J.S. Ojo, M. O. Ajewole. Rain rate and rain attenuation prediction for satellite communication in Ku and Ka bands over Nigeria – *Progress in Electromagnetics Research B* Vol. 5 (2008) 207– 223.
24. F. Moupfouma, L. Martin. Modelling of the rainfall rate cumulative distribution for the design of satellite and terrestrial communications systems – *International J. Of Satellite Comm.*, Vol.13, No.2, 105 – 115 (1995).
25. M. Zilinskas, M. Tamosiunaite, S. Tamosiunas, and M. Tamosiuniene. The influence of the climatic peculiarities on the electromagnetic waves attenuation in the Baltic Sea Region – *PIERS ONLINE* Vol.4, No.3 (2008) 321 –325.
26. A. Rimeika, Lietaus charakteristikos Lietuvoje: intensyvumas, trukmė, pasikartojimas (in lith.) – *Geografijos metraštis* Vol.33 (2000) 41–49.
27. [[http://lt.wikipedia.org/wiki/Lietuvos\\_klimatas](http://lt.wikipedia.org/wiki/Lietuvos_klimatas)], retrieved 2010 09 01.
28. A. Bukantis. The Unusual Natural Phenomenon in the Territory of Lithuania in the 11th – 20th Centuries (in lith.). – Vilnius, 1998.
29. R. Čepaitytė, M. Masaitytė. Perkūnijų pasiskirstymas ir trukmė tarptautiniuose Lietuvos aerodromuose (in lith.) – Respublikinė mokslinė konferencija *Meteorologija ir hidrologija Lietuvoje: raida ir perspektyvos* 2005.03.23, Vilnius university (2005) 45–46.
30. L. Rise and N.R. Holmberg. Cumulative time of surface – point rainfall rates – *IEEE Trans. Commun.* Vol COM – 21(10) (1973) 1131 – 1136 .
31. V. Daukšas, M. Tamošiūnaitė, S. Tamošiūnas. Elektromagnetinių bangų silpninimo dėl lietaus įvertinimas (in lith.) – 51-oji mokslinė konferencija *LAISVIEJI SKAITYMAI 2008*, Vilnius, 2008 m. balandžio 4 d. – 23 – 25.
32. M. Pankauskas and A. Bukantis. The dynamics of the Baltic Sea region climate humidity in 1950 – 2004 – *Annales Geographicae* Vol. 39, No.1 (2006) 5 –14 [in Lithuanian].

## *SORRISO*: Quantum chemistry tool for visualization of electron transfer processes

Ildar Galikov <sup>a</sup>, Alytis Gruodis  
Department of General Physics & Spectroscopy, Vilnius University  
Saulėtekio 9, korp. 3, Vilnius, Lithuania

Received 3 September 2010, accepted 3 November 2010

**Abstract.** User friendly program *SORRISO* was created for two-dimensional (2D) viewing of molecular system. Created „from zero“ using object-oriented programming (OOP) paradigm, *SORRISO* is able to visualize the positions of nuclei of the molecular system, presented in different formats such as XYZ (cartesian), YES (hexadecimal record), ENT (Brookhaven pdb). Additional possibilities of *SORRISO* include the visualization of the dynamic process – intermolecular electron transfer (IET) presented in the framework of molecular orbitals (MO) through atomic orbitals (AO). Rate of IET for each intermolecular transition between one-particle states is presented in typical spectral form, and increasing / decreasing of charge density in the surrounding of nuclei is presented dynamically - by blinking of balls.

**Citations:** Ildar Galikov, Alytis Gruodis. *SORRISO*: Quantum chemistry tool for visualization of electron transfer processes – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – 2(9) 2010 – Pp. 11-16.

**Keywords:** Sorriso; Charge transfer; Intermolecular electron transfer; Visualization.

**PACS:** 82.30.Fi.

**Short title:** Sorriso - electron transfer.

### Introduction

XXI century could be named as century of information in natural sciences. Big flow of different kind of unsorted information makes life difficult for researchers in many fields of molecular physics, applied mathematics, bioinformatics etc. Unsorted information represents some times the wrong image of phenomenon of due to partial, perfunctory view into the problem. But necessity to sort and summarize the initial information always is related to two significant factors: i) big expenses of computer resources; ii) *know-how* idea - how to present the sophisticated idea in convenient form.

Scientific information represented visually is much easier and quicker to understand in comparison to tabular/row number way. Visualization in chemical physics is always related to the *molecular* model or model of *molecular system*. Distribution of molecular fragments presented in the structural IUPAC form is less easier than in spatial form (see Fig. 1). Both models are equivalent chemically, but spatial distribution allows us to model the electronic charge redistribution by optical excitation. Moreover, presence of additional parameters to atomic spatial distribution presented in user-friendly form allows us to manipulate not by static representation but by dynamic also. This is the reason, why visualisation of digital information of spectral distributions is very important and

difficult problem in physics.

Rapid growth of computer usage in the molecular modelling calls the formation of three essential tool types:

- i) *molecule editors* as application programs or applets - *plug-ins* for creating and modifying three-dimensional (cartesian, Z-matrix, etc) representations of molecular structures. Editing in graphical mode as well as in text mode requires several knowledges and previous run-in;
- ii) *molecular viewers* as application programs or applets - *plug-ins* for imaging of molecular structures;
- iii) many applied tools contain both properties: molecule editors as well as molecular viewers.

Typical examples of molecule editors are follow: ChemDraw [1], BKChem [2], and molecular viewers (usually together with some elements of molecule editors): HyperChem [3], Gausview [4], RasMol [5] etc. These programs are convenient and effective, although sometimes they are not sufficient. In order to fully process data of specific problems, special programs or *plug-ins* must be created.

In the field of many recent problems in chemical physics, intermolecular electron transfer (IET) plays a significant role. Several chemical (Fe corrosion, redox etc) as well as photochemical (light harvesting, exciplex absorption etc) reactions in pigmentary pairs of donor-acceptor molecules can be well modeled using quantum-chemistry approaches.

<sup>a</sup>Corresponding author, email: galikov@gmail.com

The purpose of this work is visualisation of dynamics of IET parameters through data obtained by using quantum-chemistry packages - Gaussian03 [6], GAMESS [7], Dalton 2.0 [8].

Visualization of IET parameters is presented for several molecular forms of chemical compound N-N-dimethylamino benzylidene indan-(1,3)dione (DMABI) which was very extensively studied last decade [9-12].

*SORRISO* [ital. *smile*] - is a new and unique program designated for convenient and quick analysis of large amounts of data. C++ source code was written in *object-oriented programming* (OOP) manner, using *Windows.h* [13] and *OpenGL* [14] libraries. *Visual Studio 8.0* [15] was used as an integrated development environment from *Microsoft* corporation. Executable file was prepared as an *Win32-API*.

The aim of the project *SORRISO* was to create a convenient tool for simulation of molecular view (2D projection), that would allow:

- i) static view - representation of positions of atoms (nuclears) using different models: nuclears presented by balls only, by balls with sticks, by sticks only;
- ii) dynamic view - recalculation of recent projection of nuclear position "by the way" according to user request, using left and right button of mouse manipulator (rotation in plane and rotation in space, respectively);
- iii) dynamic view - recalculation of recent projection of nuclear position "by the way" according to user request, using left and right button of mouse manipulator (magnifying and shrinking, respectively);
- iv) "pseudo-perspective" viewing of part of molecular system in order to recognize the distance from viewing point until different atoms; small radius of ball creates the effect of long distance;
- v) spectral representation of the IET rate on the energy of donor state (number of donor MO);
- vi) requesting of the corresponding change of the electron density in donor and acceptor systems and blinking visualization of intermolecular electron transfer.

## 1. Visualization principle

### 1.1. Assumptions for molecular system

Creating the model of molecular system it is necessary to understand which essential factors must be estimated during energetic changes. Under energetic changes, particularly, several processes could occur – decreasing / increasing of electronic cloud density; molecular conformational changes; decomposition of aggregate; etc. In mentioned cases molecular system containing by nuclears as well as electrons must be estimated in different aspects.

First assumption of quantum chemistry claims that nuclear positions predetermine the molecular energetics. This means that spatial distribution of nuclears (but not electrons) is essential for describing energetical interactions.

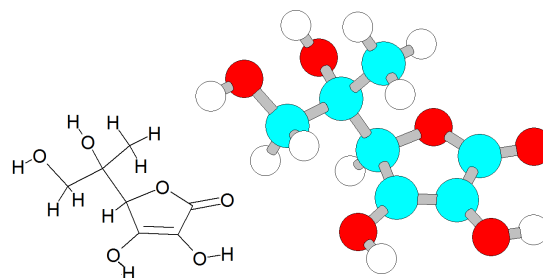


Fig. 1. Different molecular representation of vitamin C: structural IUPAC form (left) and spatial form.

According to this assumptions, electrons always adapt (fit) to the positions of nuclears. This assumption allows us to describe molecular geometry as the spatial distribution of nuclears (in 3D coordinates).

Second assumption of quantum chemistry claims that geometries of molecular system in the ground and excited states must be closed to each other. This means that only slightly perturbed molecules (for example, by optical excitation) could be described using quantum chemistry approaches.

According to such two main assumptions, many molecular visualization models operate. Positions of nuclears in 3D space represents molecular geometry, and this factor is basic and fundamental. Main task of nuclear visualization could be titled as an *projection calculation task*. Additionally, electronic density related to each atom (in the nearest nuclear surrounding) could be presented in some ways, for example, using molecular orbital (MO) methods and so on.

### 1.2. Calculation of projections

Molecular geometry or three-dimensional (3D) distribution of atoms (nucleus) is traditionally performed by matrix of different type: cartesian form as well as *Z*-matrix form, as shown in Fig. 2. Cartesian matrix represents an record of three real numbers representing  $\{x,y,z\}$  coordinates for each atom. *Z*-matrix represents an record of three real numbers representing distance, plane angle and dihedral angle  $\{r, \psi, \phi\}$  as spherical coordinates for each atom.

Project *SORRISO* was prepared as tool of molecular viewer. No *plug-ins* for structure editing was inserted, only tools of rotating and zooming are present.

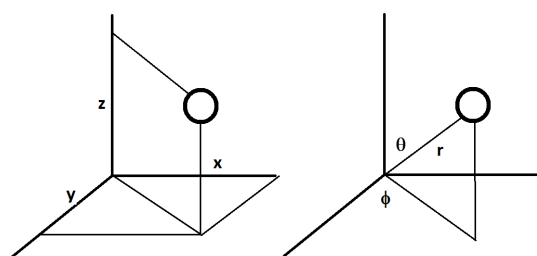


Fig. 2. Cartesian and *Z*-matrix (spherical) coordinates.

In order to realize smooth 3D rotation and zooming, several mathematical operations were required [16]:

- i) transformation of cartesian coordinates to spherical;
- ii) factoring of  $r$  (zooming operation);
- iii) transformation of spherical coordinates to cartesian;
- iv) routine calculation of 2D projections from cartesian  $\{x, y, z\}$  coordinates (3D rotation operation).

In order to prevent distortion of coordinates, zooming was realized by using spherical coordinates. In order to calculate the zooming, it is sufficient to change the radius  $r$  and transform the coordinates back to cartesian. The transformation from spherical to cartesian is performed according following formulae:

$$x = r \cdot \sin \psi \cdot \cos \phi \quad (1)$$

$$y = r \cdot \sin \psi \cdot \sin \phi \quad (2)$$

$$z = r \cdot \cos \psi \quad (3)$$

where variables  $r$ ,  $\psi$ ,  $\phi$  are prelimited in presented intervals:

$$r \in [0, \infty), \psi \in [0, \pi), \phi \in [0, 2\pi), \quad (4)$$

Mathematically, the problem is solved as following. Lets assume the existing of two coordinate system: usual  $\{XYZ\}$  and transformed  $\{X'Y'Z'\}$ . If the spatial rotation of molecular system is performed (by angle  $\alpha$  in  $XY$  plane and angle  $\beta$  in  $Y'Z'$  plane) the new projections in previous coordinate system have to be recalculated. Vector  $\mathbf{r}$ , describing place of an atom is introduced for that cause in two different coordinate systems:

$$\mathbf{r} = x_1 \cdot \mathbf{n}_1 + x_2 \cdot \mathbf{n}_2 + x_3 \cdot \mathbf{n}_3 \quad (5)$$

$$\mathbf{r} = x'_1 \cdot \mathbf{n}'_1 + x'_2 \cdot \mathbf{n}'_2 + x'_3 \cdot \mathbf{n}'_3 \quad (6)$$

where  $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}'_1, \mathbf{n}'_2, \mathbf{n}'_3$  are unit vectors in two different cartesian systems, respectively. Since vector did not change, the equations are equal:

$$x_1 \cdot \mathbf{n}_1 + x_2 \cdot \mathbf{n}_2 + x_3 \cdot \mathbf{n}_3 = x'_1 \cdot \mathbf{n}'_1 + x'_2 \cdot \mathbf{n}'_2 + x'_3 \cdot \mathbf{n}'_3 \quad (7)$$

We then multiply everything by  $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ , in turn and after applying the orthogonality of vectors, we get a system of equations:

$$x_1 = x'_1(\mathbf{n}_1 \cdot \mathbf{n}'_1) + x'_2(\mathbf{n}_1 \cdot \mathbf{n}'_2) + x'_3(\mathbf{n}_1 \cdot \mathbf{n}'_3) \quad (8)$$

$$x_2 = x'_1(\mathbf{n}_2 \cdot \mathbf{n}'_1) + x'_2(\mathbf{n}_2 \cdot \mathbf{n}'_2) + x'_3(\mathbf{n}_2 \cdot \mathbf{n}'_3) \quad (9)$$

$$x_3 = x'_1(\mathbf{n}_3 \cdot \mathbf{n}'_1) + x'_2(\mathbf{n}_3 \cdot \mathbf{n}'_2) + x'_3(\mathbf{n}_3 \cdot \mathbf{n}'_3) \quad (10)$$

This is the expression of old projections over new ones. Analogically, we may express them vice versa where  $\alpha_{ik}$  is an coefficient of transformation:

$$\alpha_{ik} = \mathbf{n}_i \cdot \mathbf{n}'_k = \cos(\mathbf{i} \cdot \mathbf{k}) \quad (11)$$

We now calculate the coefficient matrix  $\alpha_{ik}$ :

$$\alpha_{ik} = \begin{vmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{vmatrix} \quad (12)$$

In our case we need to solve nine stereometry tasks in order to obtain coefficients:

$$\alpha_{ik} = \begin{vmatrix} \cos(\alpha) & \sin(\alpha) * \sin(\beta) & -\sin(\alpha) * \cos(\beta) \\ 0 & \cos(\beta) & \sin(\beta) \\ \sin(\alpha) & -\cos(\alpha) * \sin(\beta) & \cos(\alpha) * \cos(\beta) \end{vmatrix} \quad (13)$$

## 2. Routine scheme

Libraries used in *SORRISO* are shown in Table 1.

The main file of the program *sorriso.cpp* consists of several fragments. Description of standard libraries (see Table 1) constitute the first fragment. Following it is the main method of program *WinMain* and auxiliary *CallBack* method. *WinMain* is responsible for creation of dialogue window. All objects are initialized in this method during the execution process. An action listener loop is performed in *WinMain*. The purpose of it is to analyse system messages for specific actions, such as mouse click and selection of menu. *CallBack* methods describe the execution upon specific user-requested actions.

### 2.1. Organisation of data input

Input of data is realised *via* an easy to access menu, which is written in *sorriso.rc* file. After selection of an adequate menu item, dialog window with option to select a file of a specific type, appears. The selection of file type is filtered, so users will not be able to choose files of other types. According to well-known information storage rule, it is recommended to read data from file only once, especially large ones.

Fig. 3 shows main window part of *SORRISO* as menu item opened for file input. After selection of the file, all it's contents are copied to a container of vector type object in order to process it and create a neat structure. Vector instead of and ordinary array was chosen because molecules have different number of atoms. Reading of file is performed in two phases:

- a) insertion of all contents in file to a vector and calculation of atoms;
- b) analysis of vector and creation of a structure consisting of required data.

Table 1. Standard libraries used in *SORRISO*.

OpenGL	glu.h	Advanced graphics
C++	string	Container for character string
	fstream	File input-output operation
	iomanip	Description of stream formats
	vector	Container of universal type
	math	Standard mathematics
C	windows.h	windows tools
	stdio.h	File input-output operation

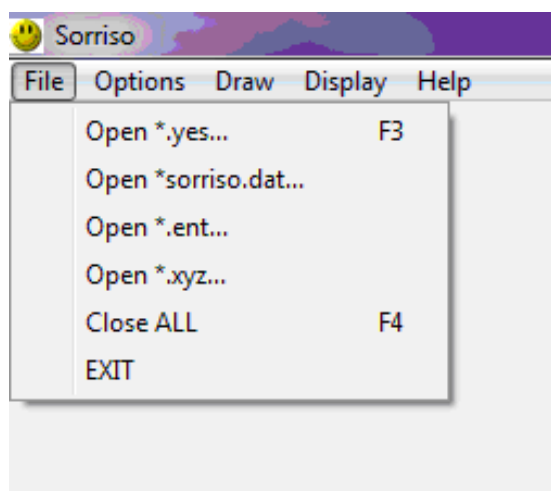


Fig. 3. Main window part of *SORRISO*: menu item for input.

Once the number of atoms is known, fixed-size arrays may be created. Since arrays are processed faster, they are preferred over vectors.

## 2.2. Possible formats of input data

**XYZ file format.** This file format (file extension - \*.xyz) is known as a so called *chemical file format* [17]. Formal standard is absent, and many IT companies use several variations. Typical XYZ format (presented in Table 2) is devoted for determination of molecule geometry by giving requested lines of records containing atom name (IUPAC standard) and atomic cartesian coordinates separated by space. The units are generally in Ångströms. Precision must be presented as three or more quantities after comma.

**YES file format.** YES file format (file extension - \*.yes) is used for practical purposes as high-precision format. Precision of number is defined as standard *double precision* for real numbers with floating point coded by four byte (4B) coding system. Formal YES standard was created originally for project *NUVOLA* [18] in order to keep the same precision of real numbers by information exchanging between operating modules through file reading/writing operation. Typical YES format (presented in Table 2) is devoted for determination of molecule geometry by giving requested lines of records containing atom name (IUPAC standard) and atomic cartesian coordinates separated by space (the same like in XYZ format). Additional string of 16 characters (ASCII only) represents the coded real number (8 bytes). Each byte (1B=8b) is presented in form of two hexadecimal characters (4 bits into 1 char).

**ENT-matrix file format.** ENT file format (file extension - \*.yes) belongs to the group of the chemical file format. Textual file format for describing the three dimensional structures of molecules is very useful for exchanging purposes [19].

Table 2. Acetylene. XYZ, YES, ENT, Z-matrix data formats.

### XYZ data format

```
C      -1.869  -0.737  0.000
C      -0.957  0.027  -0.000
H      -2.686  -1.420  -0.000
H      -0.140   0.710   0.000
```

### YES data format

```
        6      C      1
        6      C      2
        1      H      3
        1      H      4
BFFDE76C8B439581  -1.869000000000  1 1
BFE795810624DD2F  -0.737000000000  1 2
0000000000000000  0.000000000000  1 3
BFEE9FBE76C8B439  -0.957000000000  2 1
3F9BA5E353F7CED9  0.027000000000  2 2
8000000000000000  -0.000000000000  2 3
C0057CED916872B0  -2.686000000000  3 1
BFF6B851EB851EB8  -1.420000000000  3 2
8000000000000000  -0.000000000000  3 3
BFC1EB851EB851EC  -0.140000000000  4 1
3FE6B851EB851EB8  0.710000000000  4 2
0000000000000000  0.000000000000  4 3
402805B573EAB368  12.011150000000  1
402805B573EAB368  12.011150000000  2
3FF020A5269595FF  1.007970000000  3
3FF020A5269595FF  1.007970000000  4
```

### ENT data format

```
HETATM  1  H  1  -2.686  -1.420  -0.000
HETATM  2  H  2  -0.140   0.710   0.000
HETATM  3  C  3  -1.869  -0.737   0.000
HETATM  4  C  4  -0.957   0.027  -0.000
CONNECT  1  3
CONNECT  2  4
CONNECT  3  4  1
CONNECT  4  3  2
END
```

### Z-MATRIX data format

```
X1
X2  1  1.8
X3  2  1.8  1  90.0
X4  3  1.8  2  90.0  1  180.0
C5  2  0.665  3  90.0  4  -90.0
C6  2  0.665  3  90.0  4  90.0
H7  5  1.03  2  180.0  3  -90.0
H8  6  1.03  2  180.0  3  90.0
```

ENT format (represented in Table 2) as a variation of Protein Data Bank (pdb) file format is devoted for determination of molecule geometry similar like in XYZ format.

**Z-matrix file format.** Z-matrix file format (file extension - \*.zmt) belongs to the group of the chemical file format. [16] as an internal coordinate representation. Due to the modeling purposes, it is convenient to prepare Z-matrix in structure prelimited terms such as bond length, plane angle, dihedral angle. In that case bonding characteristics will be presented easier in comparison to XYZ. Additional elements of geometry (symmetry plane, axis etc) could be included using dummy atom formalism - see example in Table 2. Fig. 4 represents the spatial distribution of mentioned Z-matrix containing real C,H as well as dummy X atoms.

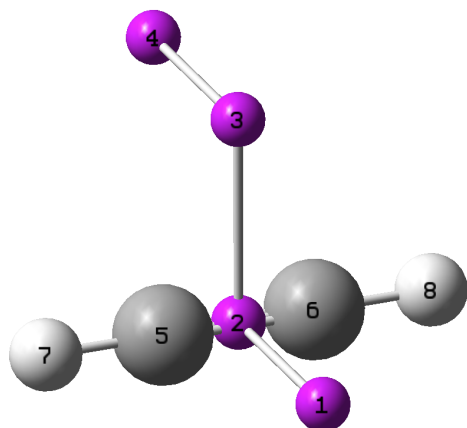


Fig. 4. 3D-distribution of acetylene atoms; dummy atoms X represent the symmetry plane.

### 2.3. Problems of visualisation

The visualisation task of molecule projection needs an enormous amounts of computer resources. The main problem is the calculation of trigonometrical functions. Mathematical calculation of them is expansion of Taylor's sequence until desired accuracy is achieved. This routine is resource dependent in very high degree, since every new projection of an atom requires at least 6 functions. Graphical function for drawing of a sphere requires at least 720 calls of function. In total, one atom requires 726 expansions of Taylor's sequence. Using of *windows.h* methods that depend only on processor power, even on very powerful workstations was too slow. This circumstance forcing to rewrite all functions using *OpenGL* library, which uses the graphics accelerator as well.

Projection on z axis seems unnecessary, but it is essential to realization of 3D perspective - closer atoms may block ones further away. Mathematically this condition is realised over projective selection of an atom diameter. Atoms further away seem smaller, thus making the view more realistic.

Fig.5-7 represent the DMABI dimmer using *Balls and sticks*, *Balls only*, *Sticks only* methods, respectively. User can decided according his own meaning which type of visualization is the best. Reswitching between three different regimes - *Balls and sticks*, *Balls only*, *Sticks only* - is allowed by standard windows bottoms on the program window.

### 3. Intermolecular electron transfer.

Calculation of IET parameters was provided using *NUVOLA* [18]. After opening YES file and selecting menu option "Open sorriso.dat" in "File" menu, *SORRISO* extracts information of spectrum which is represented in the main window. For user convenience, required peak of spectrum is selected by a mouse click. The selected peak changes colour to blue, and the selected spectrum is displayed in red (see Fig. 8).

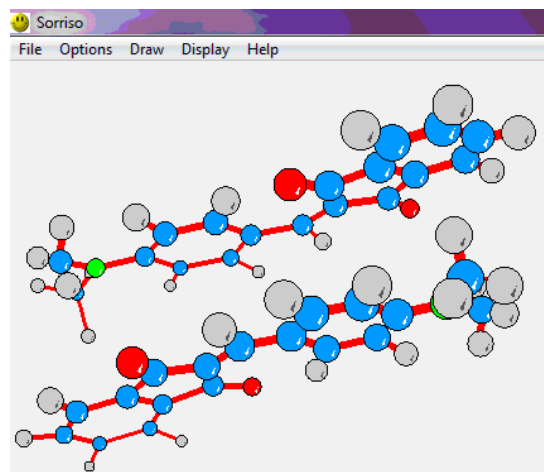


Fig. 5. DMABI dimmer represented in *Balls and sticks* method.

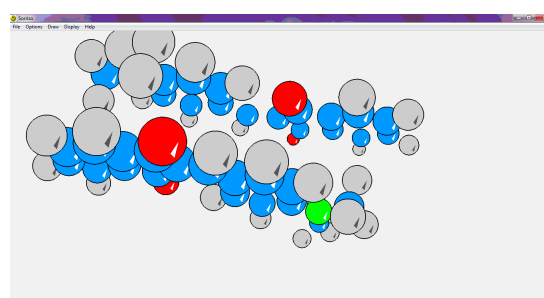


Fig. 6. DMABI dimmer represented in *Balls only* method.

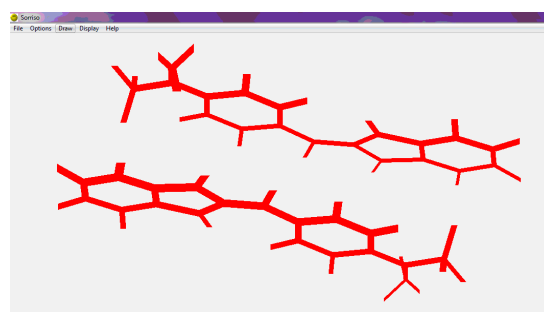


Fig. 7. DMABI dimmer represented in *Sticks only* method.

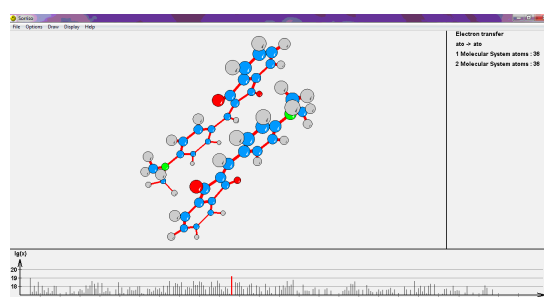


Fig. 8. Molecule and its IET spectrum.

Every peak of spectrum represents information of intermolecular electron transfer, thus by manipulating mouse on the expansion of spectrum on the bottom of the window it is possible to gain visual information of IET in real time - if, for example, user wants to find out the exact atoms participating in the electron transfer (see Fig. 9).

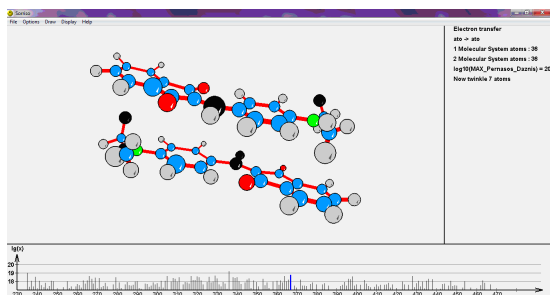


Fig. 9. DMABI dimer and its spectrum with selected peak. At initial time moment, 7 atoms of the highest frequency are displayed in black.

In order to display this, fourth dimension - time is taken into consideration. Program reads required data and sorts

the array in bubble sort method. Since only the most active transfers are required, the program displays only seven, most active atoms. These atoms increase twice in size and start blinking. The higher the frequency - the higher probability of a jump the electron has.

## Conclusions

Convenient tool *SORRISO* for simulation of molecular view in 3D space was created. *SORRISO* as molecular viewer could be useful for estimating of molecular 2D projections when molecular derivatives are represented in XYZ, YES, ENT data formats. Also *SORRISO* allows simultaneously visualise the parameter of intermolecular electron transfer through local charge redistribution.

## References

1. Mills, N. ChemDraw Ultra 10.0. – *J. Am. Chem. Soc.* 128 (41) (2006) 13649–13650.
2. <<http://bkchem.zirael.org/index.html>>, accessed 2010-01-05.
3. HyperChem™, Hypercube, Inc., <<http://www.hallogram.com/science/hyperchem/>>, accessed 2010-01-19.
4. Gausview™, Gaussian Inc., <<http://www.gaussian.com/>>, accessed 2010-01-05.
5. RasMol <<http://en.bio-soft.net/3d/rasmol.html>>, accessed 2010-01-24.1
6. Gaussian03, Gaussian Inc., <<http://www.gaussian.com/>>, accessed 2010-01-05.
7. GAMESS, <<http://www.msg.ameslab.gov/gamess/index.html>>, accessed 2010-01-05.
8. DALTON, a molecular electronic structure program, Release 2.0 (2005), <<http://www.kjemi.uio.no/software/dalton/dalton.html>>, accessed 2010-01-05.
9. M. Balevicius, E. Stumbrys, B. Sorokolit, A. Gruodis. Theoretical studies of electronic absorption spectra of dimethylaminobenzylidene 1,3-indandione (DMABI) by means of semiempirical quantum chemical calculations. – *Lithuanian Journal of Physics* Vol.35 N.1 (1995) 20–26.
10. V.Gulbinas, G. Kodis, S. Jursenas, L. Valkunas, A. Gruodis, J. C. Mialocq, S. Pommeret, T. Gustavsson. Charge transfer induced excited state twisting of N,N-dimethylaminobenzylidene-1,3-indandione in solution. – *Journal of Physical Chemistry A* 103 (1999) 3969–3980.
11. N. Galikova, M. Kelminskas, A. Gruodis, L. M. Balevičius. Tyrosine – tryptophan complex: intermolecular electron transfer using quantum chemistry approach. – *Computer Modelling and New Technologies* Vol.15 N.1 (2011) 19–23.
12. Nuriya Galikova, Mantas Kelminskas, Alytis Gruodis, Leonas Mindaugas Balevičius. Modelling of electron transfer in DMABI dimer by quantum chemistry approach. – *Chemija* 22(2) (2011) 73–79.
13. OPENGL, <<http://www.opengl.com>>, accessed 2010-04-02.
14. <<http://edu.ioffe.ru/register/?doc=physica/lect.ch4.tex>>, accessed 2010-01-20.
15. Microsoft Visual Studio 2008. Version 9.0.21022.8 RTM – 2007 Microsoft corporation.
16. Jerod Parsons, J. Bradley Holmes, J. Maurice Rojas, Jerry Tsai, Charlie E. M. Strauss. Practical conversion from torsion space to Cartesian space for in silico protein synthesis – *Journal of Computational Chemistry* 26(10)(2005) 1063–1068.
17. XYZ format specification, <[http://openbabel.org/wiki/XYZ\\_%28format%29](http://openbabel.org/wiki/XYZ_%28format%29)>, accessed 2010-04-20.
18. Nuriya Galikova, Alytis Gruodis. *NUVOLA*: intermolecular electron transfer properties using quantum chemistry approach. – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – N2(3) (2008) 12.1–12.9.
19. <<http://www.wwpdb.org/documentation/format33/v3.3.html>>, accessed 2010-04-09.



# Spatial self-arrangement of expanding structures.

## 1. Overview of assessment concepts

Jelena Nesterova <sup>a</sup>

Department of Geophysical Sciences, Faculty of Mathematics and Natural Sciences,  
Klaipėda University, H. Manto st. 84, LT-92294 Klaipėda, Lithuania

*Received 14 April 2010, in revised form 2 September 2010, accepted 5 November 2010*

**Abstract.** Vital systems distinguish in some typical features making them resistant to disturbing action. Their ability to take advantage of interactions with surrounding is called *self-organization* (pointing the functional aspects) or *self-arrangement* (considering the spatial traits). The research of such organized systems (due to of their affinity to life and human race) has outspread globally. Theories of non-linear and non-equilibrium dynamics, of chaos and dissipative structures, the fractal geometry and other branches of modern science have been induced by organization problems. Present work is but a small touch to this great topic. The spatial features typical for most organized structures and the quantification problem of this property have been discussed here. Two measures of spatial organization dissimilar essentially in their nature have been studied more detailed. One of them comes from the perception of information; other is deduced from dynamical equations. Review of organization assessment concepts is reported in this study. Main paradigms - system, structure, information - and corresponding parameters - entropy, negentropy - are described for characterization two different - metric as well as information system.

**Citations:** Jelena Nesterova. Spatial self-arrangement of expanding structures. 1. Overview of assessment concepts – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 17-22.

**Keywords:** Spatial organization; Expanding Structures; Organized structures; Indices of organization; Informational organization; Self-arrangement; Metrical organization; Cartographic structures; Entropy; Negentropy.

**PACS:** 91.10.Da

**Short title:** Overview of assessment concepts - 1.

## Introduction

Generally, populations, settlements and other developing structures are possessed by features sustaining their existence, survival or prevalence. It is significant to study these features – to learn to recognize and measure them as promising new ways of indirect (simpler and more effective) management of development phenomena. The main attention of this paper is focused on the spatial organization – to (geo)metrical and topological features giving the functional advantages to the structure.

## 1. Task formulation

The informational measure  $R$  of spatial organization is grounded on the Shannon entropy  $H$ . This function can be defined as the distribution of spatial features of the individuals at fixed moment of time (i.e. making untold assumption of ergodicity of phenomenon). Similarly the metrical measure of spatial organization  $M$  can be defined on the statis-

tical features of spatial units. It is derived from dynamical equations and therefore it is carrying terms imperative for development [1]. One may note some links between these measures. Really, probabilities of spatial states  $\pi_i$ , governing values of entropy  $H$  and values of measure  $R$ , depend on distribution of metrics  $(x, y, \dots)$ . Statistical features of individuals (comprising the given distribution) determine values of the metrical measure  $M$ . So it is reasonable to expect that values  $R_i$  and  $S_i$  (calculated for the same structures) should be significantly correlated. Otherwise, each of them reflects different properties of spatial organization. In order to test this assumption, comparative study of both measures should be performed using the common and real data.

## 2. Historical overview

The term *cybernetics* is known from Ancient times in the context of “the study of self-governance”. Science about the ruling of environment or nation was called cybernetics

<sup>a</sup>email: [jelena.nesterova@gmail.com](mailto:jelena.nesterova@gmail.com)

by Pluto (428-347 B.C.) [greek *kybernētēs* - steersman, governor]. According to scientific notation of the end of XX century, interdisciplinary study of the structure of regulatory systems was defined by Norbert Wiener.

French physicist A. M. Amper (1775 - 1836) also observed cybernetics as a form of science. A famous russian medic, philosopher and scientist A. A. Bogdanov - Malinovskij (1873 - 1928) published an original philosophical treatise [2] that represents the general idea of cybernetics - theory of organized systems. Unfortunately, the science and culture were not ready for publications of Pluto, A. M. Amper and A. A. Bogdanov at that time.

Clause Shenon (1948) in pioneering work [3] proposed the measurement of something new - *information*. His work was treated as a fundamental work for the theory of information that constituted science of cybernetics. The new concept of information was a standpoint of mathematical communication theory [4,5]. The main difference between cybernetics and physics or chemistry is the way the system works - opposed to the way of physics and chemistry, it does not move along the path of the highest probability. According to notation of the founder of modern cybernetics - Ross Ashby, cybernetic system selects the reaction pathway on direction not related to the highest probability. Cybernetic system performs the different actions using the information received. These systems were called *cybernetic* as well as *organized*.

Physicists, as well as various analysers of system describe their object of focus - *system* - as a function of cause-consequence and describe it as a mathematical - logical bond. In physics and chemistry, this is put together as a conversion between energy and material, characterised by transformation laws, while it is described as transfer functions that obey to general material laws, such as conservation law in the theory of systems and signals. It is known that tangible systems naturally move along the direction of the highest energy state. That is the second law of thermodynamics, also known as principle of Carnot that could be described as follows: "as time passes everything collapses, dissipates and all the differences and gradients become void". It is a parameter of unorganized physical-chemical structures [6].

Live forms of organisms, social-economical and even some of human-made technical systems that comply with law of energy conservation while do not comply with the second law of thermodynamics - they tend to move along the directions of even the smallest energetic states, thus causing the growth of gradients. Characteristic example is well known as the growth of embryo. Sniadecky [7] proposed the term *organized form* or *organic life form* in 1804. Nowadays, they are known as *organized systems*.

While observing various systems, we obtain data about that system (areas and numbers of our observed objects) information about them. When observing any system - whether it is organized or not, we can obtain generated sequences of data, making the system a source of information. Predic-

tion of that kind enables observing the system from theoretical point of view. Information theory statistically describes properties of a signal instead of the ways the signal is transmitted. In other words, it describes the source of a signal.

Shannon introduced some interesting ideas and techniques to analyze sequences of discrete (binary) numbers generated by various systems. The main purpose of information theory was to analyze electrical signals but in a matter of several years it became indistinctable part of statistics, applied statistics, computer sciences, cryptography, biology and physics.

### 3. Description of system and structure

**System.** System [greek *systema* – composition] is a set of interacting or interdependent components forming an integrated whole. It is not required that an element would be bond with every other element of the system, but an element has to have a bond with at least one element in the system. The properties of a system are described as a form of integrity between bonds of elements in the system.

**Structure.** Structure [lot. *structura* – framework, constitution] is a fundamental description that describes location and bonds of elements that make up any object. Structure is the essential property that describes the stability and quality of a system. Every structure has its own conditions of appearance (causes), and it interacts with other structures (consequences / effects), also affecting the first structure. Nevertheless, it should be considered that every structure is independent. Only then observing of structures becomes possible.

Entropy is a thermodynamic property that can be used to determine the energy of certain system available for useful work in a thermodynamic process. The term *entropy* was compiled in 1865 by Rudolf Clausius [greek *entropía*, *en* + *tropē* - in conversion.] There are two related definitions: thermodynamic and statistical mechanics. Thermodynamic entropy is a non-conserved state function. Increases in entropy correspond to irreversible changes in a system, because some energy is expended as waste heat. In statistical mechanics, entropy is a measure of the number of ways in which a system may be arranged, often taken to be a measure of "disorder".

**Boltzmann entropy.** The expression of entropy  $S$  used in thermodynamics and statistical mechanics [6] is Boltzmann entropy (initiators are Ludwig Boltzmann and J. Willard Gibbs, 1870):

$$S = -k_B \cdot \sum_{i=1}^N P_i \cdot \log_e(P_i) \quad (1)$$

The summation is to be provided over all the possible states  $N$  of the system, and  $P_i$  is the probability that the system is in the  $i$ -th state.

Entropy in physics is a state function of a thermodynamical system that describes irreversibility of processes in an isolated system:

$$dS \geq \frac{dQ}{T} \quad (2)$$

where  $T$  - absolute temperature of a system,  $dQ$  - heat. For isolated systems  $dS=0$ .

Although this law does not apply to open systems, so, entropy describes very important class of processes - development processes (from physical to social).

Apparently, both sides of equation are equal for reversible processes and unequal for irreversible processes. The second law of thermodynamics is an expression of the system tendency that over time, differences in temperature equilibrate in an *isolated* physical system. In classical thermodynamics, the second law is a basic postulate applicable to any system involving measurable heat transfer and defines the concept of thermodynamic entropy  $dS$ .

#### 4. Information

The term *information* means the knowledge that reduces or cancels uncertainty of occurrence of an event from possible events sequence [8-9]. Information theory describes the meaning of *event* in the same way as does the theory of probability:

- i) event is appearance of specific element in specific array of elements;
- ii) occurrence of an indicated word or sign in a specific message or a specific place of a message;
- iii) any of different results of an experiment.

The purpose of a connection between two objects belonging to the same system is the transfer of information from source to its user. The measurement of information may be described as follows. The amount of transferred data depends on the surprise factor (the probability of receiving a message) the lesser the probability, the more information it transfers. The amount of information  $I_j$  transferred by the  $j$ -th message sent from digital source of information is described as follows, where  $P_j$  is the probability of the  $j$ -th message. The unit of measure of information is bit.

$$I_j = \log_2 \left( \frac{1}{P_j} \right) \quad (3)$$

Since the probability of different messages is different, there is a difference in transferred data. It is more convenient to call the digital source of information as an *average amount of information* transferred by a single message. By using the definition of an average and the expression of amount of information on a single message, we can write down an expression of average amount of information:

$$H = \sum_{j=1}^m P_j I_j = \sum_{j=1}^m P_j \log_2 \left( \frac{1}{P_j} \right) \quad (4)$$

where  $m$  is the number of possible messages. The average amount of information on a single message is called as an entropy  $H$  of source of information.

**Amount of information.** The amount of information is a measurement of occurrence of an event when the probability is known. It is equal to a logarithm of a unit that is inversely proportional to the probability:

$$I(x) = \log \frac{1}{p(x)} = -\log p(x) \quad (5)$$

where  $p(x)$  is the probability of an event  $x$ . If probability of every event is equal, then the amount of information is equal to the amount of solutions of this set.

**General amount of information.** The general amount of information is a measure of appearance of two events,  $x$  and  $y$ . It is equal to a logarithm of a unit inversely proportional to the probability  $p(x, y)$  of occurrence of both events simultaneously:

$$I(x, y) = \log \frac{1}{p(x, y)} \quad (6)$$

**Relative amount of information.** Relative amount of information  $I(x|y)$  - is a measurement of information about the appearance of an event  $x$  when another event  $y$  occurred. It is equal to a logarithm of a unit that is inversely proportional to relative probability of an event  $x$ :

$$I(x|y) = \log \frac{1}{p(x|y)} \quad (7)$$

Relative amount of information is equal to the difference between general amount of information of two events and an amount of information of second event.

$$I(x|y) = I(x, y) - I(y) \quad (8)$$

**Shannon entropy.** Shannon entropy  $H$  (see Refs. [3-5]) describes the unpredictability of information content. For variable  $X$ :

$$H(X) = - \sum P(x) \cdot \log_2(P(x)) \quad (9)$$

where  $P(x)$  is the probability that variable  $X$  occupies the state  $x$ . In case if  $P=0$  (no events)

$$\lim_{P \rightarrow 0} (P \cdot \log_2 P(x)) = 0 \quad (10)$$

Shannon entropy allows measurement of the minimal amount of bits required to decode a sequence of symbols based on the frequency of symbols.

Let us assume that probability is the same for every state:

$$P_i = \frac{1}{N} \quad (11)$$

then

$$H(X) = \log_2(N) \tag{12}$$

Entropy is equal to 1 only if the number of all possible states of system is equal to 2.

**Rényi entropy, Hartley entropy.** Rényi entropy (named in honour of Alfred Rényi) is more general form of Shannon entropy in information theory [10] and it belongs to a branch of functions that evaluate variety, uncertainty and coincidence. Rényi entropy is known as a indexed power function (where index  $\alpha \geq 0$ )

$$H_\alpha(X) = \frac{1}{1-\alpha} \log_2 \left( \sum_{i=1}^n p_i^\alpha \right) \tag{13}$$

where  $p_i$  is probability of  $x_i$  from a set  $\{x_1, x_2, \dots, x_n\}$ . If all probabilities are equal, Rényi entropy is equal to:

$$H_\alpha(X) = \log_2 n \tag{14}$$

Otherwise entropy is defined as slowly descending functions of  $\alpha$ . When  $\alpha = 0$ , there is a singular point:

$$H_0(X) = \log_2 n = \log_2 |X| \tag{15}$$

where  $H_0(X)$  - is called as Hartley entropy of variable  $X$ . This is the case when probabilities of receiving a signal are equal. When  $\alpha \rightarrow 1$ ,  $H_\alpha(X)$  converges to:

$$H_1(X) = \sum_{i=1}^N p_i \log_2(p_i) \tag{16}$$

that is Shannon entropy. Rényi entropies are applied in ecology and statistics as a index of diversity.

**Information entropy.** Entropy in information theory is a value indicating the information gained from the result of an experiment. Information entropy for a system with a finite amount  $r$  of states  $\xi = \{C_1 \dots C_n\}$  is expressed by equation:

$$H(\xi) = - \sum_{i=1}^r p_i \log_2(p_i) \tag{17}$$

$H(\xi)$  is called as information entropy, where  $p_i$  is the probability of  $i$ -th state,  $r$  - number of states. Information entropy has these features as following.

1.  $H=0$  if and only if all probabilities  $P_i$  except one equal zero.
2. For a given number of results  $n$ ,  $H$  is max and equals to  $\log_e(n)$ , when all probabilities are equal. This is the most uncertain situation.
3. Information entropy is additive: overall entropy of two independent experiments is equal to the sum of separate entropies of these experiments.

Entropy of random results of an experiment that consists of possible results is expressed as follows:

$$H = \log_e(N) \tag{18}$$

Lets assume that the set  $X = \{x_1, \dots, x_n\}$  is a set of events  $x_i$  ( $i=1, \dots, n$ ). Expressions  $I(x_i)$  are amounts of information of events  $x_i$ ,  $p(x_i)$  as a probabilities of appearance of these events. Also:

$$\sum_{i=1}^n p(x_i) = 1 \tag{19}$$

Entropy is the average of information bits that are incompatible between themselves and constituting a full system of events.

$$H(X) = \sum_{i=1}^n p(x_i) I(x_i) = \sum_{i=1}^n p(x_i) \log \frac{1}{p(x_i)} \tag{20}$$

When there are two mutually exclusive systems of finite sets consisting of mutually exclusive elements and an event occurs in one of those systems, it is an average value of conditional information values, also known as relative entropy:

Lets assume  $X = \{x_1, \dots, x_n\}$  as a set of events  $x_i$  ( $i=1, \dots, n$ ). Lets assume  $Y = \{y_1, \dots, y_m\}$  as a set of events  $y_j$  ( $j=1, \dots, m$ ). Expression  $I(x_i|y_j)$  is a conditional amount of information of  $x_i$  (if  $y_j$  is fulfilled), and if  $p(x_i, y_j)$  is overall probability of  $x_i$  and  $y_j$ .

$$H(X | Y) = \sum_{i=1}^n \sum_{j=1}^m p(x_i, y_j) I(x_i|y_j) \tag{21}$$

Average entropy of a sign:

$$H' = \lim_{m \rightarrow \infty} \left( \frac{H_m}{m} \right) \tag{22}$$

there is an overall entropy of  $m$ -signs. This limit may be void if signs differ. Average entropy of a sign may be measured by shannons per one sign (1 shannon - unit of information named in honor of Shannon).

**S-function and R-function.** In order to calculate the proportion between order and chaos, we implement the so-called *S-function*:

$$S = \frac{H}{H_{\max} - H} \tag{23}$$

where  $H$  is Shannon entropy,  $H_{\max}$  is the maximum entropy of a system. When probability of every condition is equal (marginal chaos) - it is a continuous function and its values vary from 0 to infinity (see Fig. 1), although this function is not limited. Then we introduce another function with a limit and name it as an *redundancy* or *R-function*:

$$R = \frac{H_{\max} - H}{H_{\max}} = 1 - \frac{H}{H_{\max}} \tag{24}$$

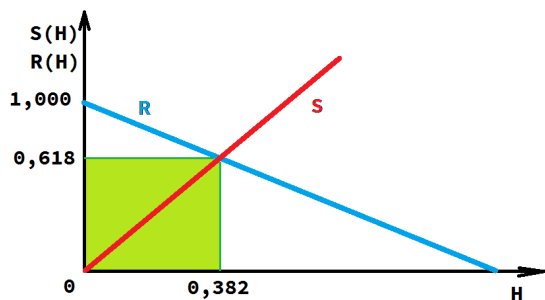


Fig. 1. S and R functions. Adapted according to Ref. [11].

It is easy that this R-function, unlike an S-function varies from 0 to 1 in an interval  $0 \div H_{max}$ . We may assume, that when these functions cross each other, system is in a harmonic (balanced) state. After solving the equation, we get the result:

$$H = 0.382 * H_{max} \tag{25}$$

This expression is called a *golden crossection*. According to Kolkov [11] it is an universal unit of chaos and order. In other words, there has to be 0.382 of chaos and 0.618 of order in total to maintain a harmonic state in a system. System in such state is stable enough, while on the other hand, the level of scatter and uncertainty is high enough to allow changes or further stable evolution.

Shannon and Kolmogorov established that such examples may be found: the limit entropy of any language reaches number of 1.91 bit/character. Furthermore, if we divide the limit value of entropy by maximum, we get the number 0.382 that we have already seen. There were researches in music, poetry and arts, aswell. The relative entropy of top art works is close to the golden crossection.

**Antientropy.** Antientropy is the cause of appearance of information as well as it's unit of measurement or an expression of organization (grading) of a system. According to the law of Nernst, entropy by itself always increases and may never disappear.

Shannon entropy is compared to a phenomenon called *negentropy*. In the pioneering work [12] Leon Brillouin described the principle of information negentropy saying that obtaining information of micro-aggregate states of a system leads to a decrease in entropy:

- i) work has to be done to obtain the information;
- ii) deletion leads to increase in thermodynamic entropy.

It complies with the 2nd law of thermodynamics, because, according to Brillouin, reduction in thermodynamic entropy on a local system, causes an increase in entropy elsewhere. Negentropy is a contradictory conception, because effective value of Carnot cycle may be higher than 1. Negentropy is a measurement of both - information and organization of a system.

There is a lot of information considering the informational organization because there are a lot of different entropy

forms. Therefore, our focus is placed on the aspects of metrical organization in order to recognise the favourable geometrical properties for development of an observed structure. Following section is devoted for metrical organization

### 5. Spatial Organization

It is known that some spatial features are imperative for a population to function and to survive in spaces of finite extent [13]. Structures exhibiting such properties have been called as *spatially organized*.

**Recognition problem.** Populations and other similar structures function remaining under constant disturbances of various factors. Some of them (like scarcity of resources or lack of space) distinguish in growing trends. Namely such disturbances are putting inevitably the strain on population dynamics. A critical situation (crisis) frequently leads to the extinction of a population. However some of them manage to survive learning to exploit more effectively habitats they occupy (specialization). Finally, just very small part of growing populations contrives (sometimes in virtue of lucky mutation) to function and survive outside habitats they upstart. It was deduced [13] that a population to overcome repeating crises should meet the inequality:

$$M(f(x_1, x_2, \dots, x_k)) \leq f(M(x_1), (x_2), \dots, (x_k)); \tag{26}$$

where  $f(\dots)$  – function describing a spatial unit;  
 $(x_1, \dots, x_k)$  – (geo)metrical features used to describe a unit;  
 $M(\dots)$  – symbol of a mean value.

Ineq.(26) is a case of Jensen's inequality [14]. A common structure does not satisfy it (because of the function  $f(x_i)$  which as the rule is of convex type). Hence, a structure to survive must change itself insomuch to change this type of inter-relationship  $f(x_i)$ . It was obtained by modeling [15-16] that the negative correlations among some spatial features  $(x_1, \dots, x_k)$  are able to resolve this contradiction (note that a *functional* feature causes the *spatial* transformation). Expanding structure may not survive ignoring this term. Accordingly to Ineq.(26) can be raised to the status of distinctive sign (or criterion) of spatial organization.

**Measuring the organization.** The criterion to find the certain structure of population (expressed using Ineq.(26)) often differs in values of ratio  $r_i$ :

$$r_i = \frac{M(f(x_1, x_2, \dots, x_k))}{f(M(x_1), (x_2), \dots, (x_k))} \tag{27}$$

(meaning of variables as in Ineq.(26). It is reasonable to expect (see Ref. [1]) that the smaller is this ratio, the higher is the organization of a given structure. Consequently in order to assess the spatial organization degree  $M$  of a structure, the measure can be used [1]:

$$M = 1 - \left[ \frac{M(f(x_1, x_2, \dots, x_k))}{f(M(x_1), M(x_2), \dots, M(x_k))} \right]; \tag{28}$$

(meaning of variables as in Ineq.(26).

Only positive values of this measure from the range  $[0 \div 1]$  are pointing the organization. While the negative values show the structure states, when some part of structure is forced to leave the space suitable for its existence. In this sense the measure  $M$  is indicating the capability of a structure to compress itself, sustaining (even increasing) the diversity achieved before the later spatial crisis.

## Discussion

Each of measures can be revised by condition associated with the different features (functional, dynamical, etc.). Again, the function  $f(x_i)$  is able to represent a spatial unit of any compound structure (population, community, etc.) There is no logical contradiction against such interpretation. Concerning this freedom the questions arise: which of these *virtual* measures would be better revealing the essence of organization? Which of them would be more preferable for assessment of the spatial organization in particular? Or would be more effective for examination of community structure? What sense would have a composition of both measures (say the expression

$$R = 1 - \left[ \frac{H(p(r_i))}{H_{max}} \right], \quad (29)$$

## References

1. A. Tiknius. Territorial Aspects of Development. Monograph (in lith.). – Klaipėda: Klaipėdos universiteto leidykla, 2002.
2. A. A. Bogdanov - Malinovskij. Essays in Tektology: The General Science of Organization. – Seaside, CA: Intersystems Publications, 1980.
3. C. E. Shannon. A Mathematical Theory of Communication. – *The Bell System Technical Journal* 27 (1948) 379–423.
4. R Price. A conversation with Claude Shannon: one man's approach to problem solving. – *Cryptologia* 9(2) (1985) 167-175.
5. Shannon C. E. Prediction and Entropy of Printed English. – *Bell System Technical Journal* 30(1) (1951) 50–64.
6. See textbooks of general physics, such as: Richard Feynman. The Feynman lectures on Physics (3 vols); David Chandler. Introduction to Modern Statistical Mechanics, 1987.
7. A. Sniadecki. Teorya Jestestw Organiczných. - Warszawa, 1804.
8. Fazlollah M. Reza. An Introduction to Information Theory. – New York: Dover Publications Inc., 1994.
9. Robert B. Ash. Information Theory. – New York: Dover Publications, 1990. – 339 p.
10. Jizba P., Arimitsu T. The world according to Rényi: Thermodynamics of multifractal systems. – *Annals of Physics* (Elsevier) 312 (2004) 17–59.
11. Anatolij Kolkov. Only in our illusory freedom ... (in rus.) – *Chimija i zhizn* 9 (1990) 51-53. – <<http://www.veinik.ru/science/biolog/article/158.html>>, accessed 2010 04 01.
12. Leon Brillouin. Science and Information Theory. – New York: Dover, 2004.
13. Algimantas Tiknius, Kęstutis Dučinskas, Benediktas Jankauskas. Deriving the spatial traits of organized land structures, in I. Petrosillo et al.: Use of landscape sciences for the assessment of environment security. – Springer, 2008. – 121-130. – <<http://www.springerlink.com/content/q6u8m2m545582162/>>, accessed 2010 04 01.
14. Lohwater A. Introduction to Inequalities. – 1982. – <<http://www.mediafire.com/?1mw1tkgozzu>>, accessed 2010 04 01.
15. Tiknius A. Features of the spatial relations in the upgrowing structures. – *Science and art in Lithuania* 18 (1988) 188-208.
16. Tiknius A., Jankauskas B. and Juška V. A method for Quality Assessment of Environment at the Landscape Level. – In: F. Muller, W. Kepner & K. Caesar (eds.). EcoSys, Landscape Sciences for Environmental Assessment, Proceedings from a CCMS Pilot Study Meeting at Salzau Castle, Kiel, Germany, 2003. ISSN:0940-7782 – 56-70.

where  $p(r_i)$  are the probabilities of ratio values - Eq.(27). There are no as yet compelling answers to these questions significant for understanding of organization as well required for practice. The rather relevant seem has to be any comparative study of these measures.

## Conclusions

1. There is no clear motivation how to select the preferable measure for the assessment of spatial arrangement of compound structure.
2. It is unknown yet any direct relation between the functional advantages of a real compound structure and the organization measure  $R$  based on the entropy of spatial features.
3. It is reasonable first to get up a comparative study of different measures using the data of real populations or other constituent structures.

## Acknowledgments

This work was prepared as a part of the Master Thesis. Author would like to thank Assoc. Prof. Algimantas Tiknius (Klaipėda university) for suggestions and comments.

## Spatial self-arrangement of expanding structures.

### 2. Structure model construction

Jelena Nesterova <sup>a</sup>

Department of Geophysical Sciences, Faculty of Mathematics and Natural Sciences,  
Klaipėda University, H. Manto st. 84, LT-92294 Klaipėda, Lithuania

*Received 14 April 2010, in revised form 2 September 2010, accepted 5 November 2010*

**Abstract.** Vital systems distinguish in some typical features making them resistant to disturbing action. Their ability to take advantage from interaction with surrounding is called *self-organization* (pointing the functions) or *self-arrangement* (considering the spatial traits). Research of such organized systems (because of their affinity to life and human race) outspread globally. Theories of non-linear and non-equilibrium dynamics, of chaos and dissipative structures, the fractal geometry and other branches of modern science have been induced by organization problems. Spatial features typical for most of organized structures and the quantification problem of this property are discussed here. Two measures of spatial organization dissimilar essentially in their nature have been studied more in detail. One of them arises from the perception of information; other is deduced from dynamical equations. Review of structure model construction is reported in this study.

**Citations:** Jelena Nesterova. Spatial self-arrangement of expanding structures. 2. Structure model construction – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 23-29.

**Keywords:** Spatial organization; Expanding Structures; Organized structures; Indices of organization; Informational organization; Self-arrangement; Metrical organization; Cartographic structures; Areal; Genome; Morphome; Binome.

**PACS:** 91.10.Da

**Short title:** Structure model construction - 2.

## Introduction

Populations, settlements and other real structures are too complex for research of their organizational features. Best what is possible here is to try to exploit some assorted models of these structures. So the modeling is the stage from which depend the success of guiding research. The robust model should meet some requirements of quality. First, it should be as simple as possible (since the simplicity conditions the efficiency of mathematical analysis). Second, it should keep the essential features of reality (it must be *complete*). In order to identify these properties (simplicity and completeness) it is necessary to extend the viewpoint from a structure of research to the whole reality (herewith entering the philosophy sphere) [1]. Such a generalization helps to stay within bound of reasonable simplification of a model sustaining herewith its minimal similarity to the reality.

Organized structures may be described as a type of spatial order, also known as *negentropy*. Previous publication represents an overview of paradigms [2] used for so complicated modeling. One type of indicators of the organization

are derived from the models of general dynamic processes, while others show specifications of a single process, thus making them either too general (reflecting rather theoretical than practical point of view) or too narrow.

Purpose of this work is to look more comprehensively at this construction with aim to employ a model suitable for the prospective study of cartographical images which allows to describe two-dimensional distribution of real structures - forest areas using several modern assumptions such as fractal tools.

## 1. Model description

As it was pointed above, the simplicity and similarity to reality are two greatest advantages of a model. The amount of meaning kept in the simplicity would be proportional to knowledge and understanding of reality applied to a model. The requirement of simplicity is also valid for axioms, for example, a model gets better when the amount of axioms and principles used to describe it is lesser. According to objectives and the object itself, other properties also may be signi-

<sup>a</sup>email: [jelena.nesterova@gmail.com](mailto:jelena.nesterova@gmail.com)

ficant. The most significant principle for studying organized structures is the systemic principle that requires to model every structure with properties of structures of adjacent higher and lower scale (note the *ternary* composition by means of the principle: given-higher-lower). Let's consider a territorial view of population and its cartographic layer. It would be impossible to analyse such a model using effective (mathematical) methods. To overcome this limitation, a graphical structure model has to be transformed to some quantitative expression called a *mathematical analogue* of given model.

Study of systems by a logical scheme “*what would happen, if...*”, that is, implication, is barely applied at all. Known logical models are based either on the uniqueness of an original territory, or on general traits of many territories, such as the arid region, but there are no models that would be based on both types. Ordinary notions of *simulation* and *modeling* are pointing difference of these approaches.

For example, territorial objects, such as Lithuania (state), Scandinavia (geographic peninsula), Raigardas (valley in south Lithuania), Curonian Spit (peninsula in west Lithuania) are unique in their spatial organization and history. Though one may find among them many similarities in renewal, reproduction, irreversibility, critical modes, conversions and (or) other dynamical properties. Consequently in order to study how such system manages to select the features suitable for its survival and development, it would be reasonable to apply the *simulation* procedure (relying on the individual properties). Respectively the *modeling* (vs *simulation*) would be kind of the preferable procedure (perhaps...) for research of their dynamics (relying on that what is common - emphasizing the similarities).

Now let's assume we face a change of situation, when the structures become different in dynamical, though similar in spatial features. How such a change should be reflected in construction of a structural model? What features should persist in a model when the structure is passing from one to another situation? There are no compelling answers to the later question. Some attempt to approach them is proposed further.

### 1.1. Philosophy of modeling

Theoretical structures are often compared with stained glass, carpet or a puzzle, although, it does not reveal the point and content of landscape. The whole idea of landscape should be

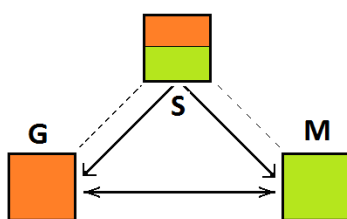


Fig. 1. Structure as an ontological triplet:  
G – genome, M – morphome, S – symphysis.

pervaded with features of dynamics, self-organization, vitality. This requires the specific standpoint, or, to be more exact, return to one of forgotten viewpoint [1].

According to Raicinskis [3], Kant [4], philosophy of Dao [5], every object is triple inside. Each of them is constituted of three inherent origins. Separate compounds could be described as following:

- a) active origin, *genome*,
- b) passive origin, *morphome*,
- c) substance receiving after allowing first two origins act together, *symphysis*.

Genome is usually accounted for cause, morphome – for shape, symphysis – for bonding between genome and morphome (see Fig. 1).

Symphysis may be treated as an informational background of reality. Sometimes it is used to describe the existential potencies of a structure. Several examples are presented below:

- i) energy-information-their junction;
- ii) past-present-future;
- iii) matter-antimatter-vacuum;
- iv) positive unit-negative unit-zero;
- v) something-nothing-anti-something.

There are well known interpretations from physics: from nothing may not appear something, however from nothing may appear and exist something and anti-something. All of them are also the possible interpretations of this general principle. It is natural that a particular basic element is difficult to identify, as the reality appears from “association of three”. And again the structures are composed of different sort of substructures and their boundaries are quite vague (see Fig. 1). So it is more credible for actual model that basic elements will be assumed with some probability to satisfy their definitions than identified certainly. This shortage does not debase the principle itself: a testable mistake is better than the total defiance of the ontological nature of structure [1].

Symphysis describes the bond as well as the possibility, existential potencies of a structure, area of geographical structure. Symphysis is an information model of reality. Active and passive elements of evolving structure may not be defined and constant as well. They are made of difficult inner structure and different origin.

### 1.2. Graphical scheme

Now the structure model may be displayed in geometrical form as a trigram [1] - see Fig. 2. Real structures have geometrical features. The trigram is lacking them, sustaining only the topological mean. The symphysis is represented here by a spatial niche called *areal*. It always stays as a background for other two spatial elements (patches). A patch representing the genome commonly is put in a morphome (representing a functional space) though sometimes both patches can be spatially separated or dislocated in adjacent position (Fig. 3). In some other cases it is reasonable



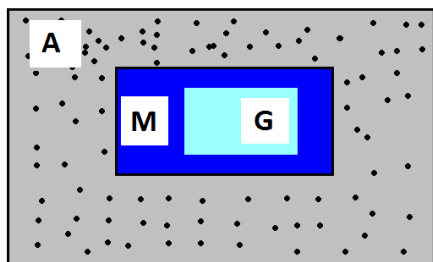


Fig. 2. Structure according to ontological framework. G – genome, M – morphome, A – areal as symphysis.

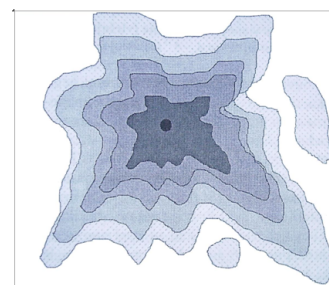


Fig. 3. Map of areal as twodimensional distribution. Each isoline describes the different areal.

to reduce the genomes to points or to represent them as patches coinciding with their functional zones (morphomes).

### 1.3. Areal

Definition and contour of areal returns the axiom to a model graphically in a way where every specific phenomenon of evolution exists in a specific, real and finite spatial area. If evolution of a structure depends only on properties of inner environment, then areal is not a part of a model of discussed structure. If latter condition is fulfilled, areal characteristics are excluded from the equations that describe the structure. Although, if it is excluded, it may miss some hidden parameters, so it is more convenient to use two definitions of areal. Potential areal becomes part of a developing system once it starts interacting with it. The ability of interaction is defined by a probability. Once the interaction between a structure and environment begins, their evolution becomes combined and areal becomes as a part of a structure [1].

The environment of developing structure is made up of interacting elements. Changes that occur at the elements of environment force a change in areal as well - its characteristics, such as size, form, topology, may vary. Although topological dimension of a curve is equal to 1 but otherwise general dimension of a figure is equal to 2. That is a reason for a new type of dimensions - Hausdorff dimension  $D_H$ .

Areal is very difficult and constantly changing structure, although it is usually considered as a constant area or contour as presented in Fig. 3.

It is difficult to determine boundaries of areal while it is almost impossible to forecast the changes of areal because structure observed is only one of many structures and independent factors that affect and force changes in it. In order to obtain more accurate result in geographic studies it is necessary to find solutions that are independent, or depend on characteristics of an areal the least as presented in Fig. 4.

If model parameters of areal are more important than the risk of failure, boundaries of areal are modeled according to a specific procedure, for example methods of Tiessen and Voronj assume that part of areal is proportional to measurements of objects or their distances of interactions. All the area is divided to smaller parts in a way that their boundaries would be of similar distances to nearby binomes.

Such division of areas may look artificial at first sight, but it is not. If there are no visible boundaries in reality, it does not deny their existence. Many of boundaries drawn in cartographic models actually exist in reality. There also are boundaries that exist, but nothing is known about their location, origin and properties. Median boundaries summarize, average past and present, real and imaginary, actual boundaries by reflecting the most common properties. Boundaries of morphomes are modeled alike in cases when genome is an island on morphome. Morphome in such case is like a microareal of genome.

### 1.4. Genome and morphome

Pairs of these elements allow modeling most of the surrounding world. Every element of binome belongs to parts of structure that are essential for the other element, which, in accordance is essential for existence of functioning and development of the structure itself. Every element in binome has its own geometrical and topological properties and changes of it. The proportion between elements is equal to  $(1/N)$ .

For example, if the genome represents rural area (objects of one cartographic layer), morphome represents many layers: land, forests, waters. Sometimes, while creating a model it is unclear which element is active and which is passive - proportion between the elements of observed structure is unclear. In that case, simpler models, such as cartographic views and their graphic schemes may become handy [1]. Usually, *genome* is considered as an element that is capable to develop by itself, while *morphome* is a complimentary

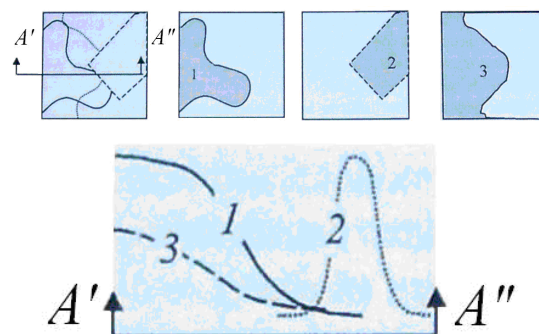


Fig. 4. Area parts of three different areals (top). Density of corresponding components in the cut  $A' - A''$  (bottom)

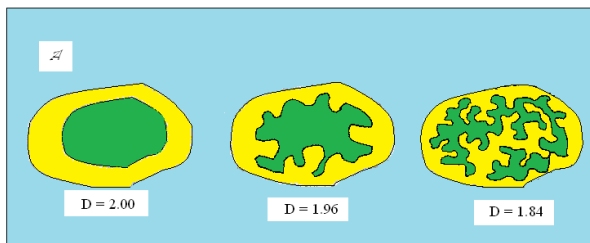


Fig. 5. Different forms of islands after change of fractal dimensionality.  $D$  – fractal dimension.

element for genome. For example, if we would consider population an active element, it would be appropriate to consider its habitat as a passive element of a structure. Interpretation like this is quite frequent, but it is optional. In reality, structures and parts of them vary by their geometrical specifications and change of them. Structures also should differ by their size, form and binome element. Binome may expand to the size of areal ( $A$ ), but may never exceed it. Dots and lines in a model represent small and elongated elements that may never become equal to zero.

In our reality there exist more difficult alterations. In order to model them, islands should be transformed to a background or islands may be formed in other islands, gaps that do not belong to areal may appear on the areal. For example elements of binome may be different by topological proportion: in one case, by removing one of elements, the other element stays the same. In other case, it shrinks and gap appears in its place. Point elements may become linear, while the latter may become an area. That means, that elements may change their dimension - see Fig. 5.

## 1.5. Binome

Territory that is observed may be divided to an infinite number of smaller parts and defined by trinomials. It is obvious that these models will belong to different types because they represent different objects, such as atoms and ecosystems [6].

The same territory may be divided to parts that have analogic meaning or origin, so the amount of them would be significantly smaller. These fragments still have some common properties but may lose them, so it is impossible to further divide them to analogical type as they are themselves. Fragments like these are called elementary, their graphic models are binary, models of binary elements - spots. Elements in such model have geometrical and topological meaning.

Every evolving structure can be modeled according to the fact, that they are open and binary - every structure has an active element, genome, and part of environment that genome interacts with and that is the second side of the same area. Passive element may be referred to a functional area or to the area of interaction. Otherwise, elements form the random crossing.

The difference between traditional and proposed model may be compared to difference between a community and an

ecosystem: landscape acts as a community in a cartographic model. Binary model displays community with its habitat, by highlighting its structure, features and spatial bonds. Binary model is appropriate for modeling of non-reproductive and interacting structures, such as rivers and their basins.

There are two ways to convert traditional single-member model to binary model. That is achieved by converting single-member component as a passive or an active component of binary model. When active component shrinks and becomes a singular point, binary model degenerates and becomes a single-member model, so traditional representation of components on a map is a partial case of a binary model. Every evolving structure may be put together or divided to binary components and their layers. They can be easily transformed to elementary quantitative expressions and studied by using effective mathematical methods. This ability is the most valuable feature of the method. Of course, this method, like any other has its drawbacks, for example, limits of functional space have to be calculated in this method, but these drawbacks do not outshine the merit of this method.

## 2. Indexes of metric organization

Evolution of population of organisms and similar structures depends on their geometric shape. This property (metric organization) is defined by an indicator  $M_i$  - see Refs.[2,7].

### 2.1. Fractal dimension

The indicator of metrical organization is based on mathematical modeling of structures as well as describing the structure itself. One of such properties is fractal dimension. It is now known that it differs from topological which may obtain only integer values (0, 1, 2,...).

The term *fractal* was introduced by mathematician Mandelbrot in 1980's [lot. *fractus* > *fragere* - to break, to create an irregular ornaments].

Fractal structures, such as Cantor set, Pean curve, Koch curve, Sierpinski triangle and carpet, Julia set, also known as so called *mathematical monsters*, had been known before the introduction by Mandelbrot. Although, only Mandelbrot saw something more than mathematician's mind in them and founded new branch of mathematics - *fractal geometry*. In less than 20 years term of fractal found its place in other sciences: physics, biology, chemistry, sociology, urbanistics. As it has already been mentioned - attractors of chaotic systems are fractals. That's why fractal geometry is actually *chaos geometry*.

Fractal is object that has a property of self similarity - object may be divided to small parts that look like shrunken reflection of a structure, for example, branch of a tree looks like a shrunken tree, that's why we can call trees as natural fractals. There are a lot of natural fractals in the nature - from plants and human organs(kidney, lungs) to mountains,

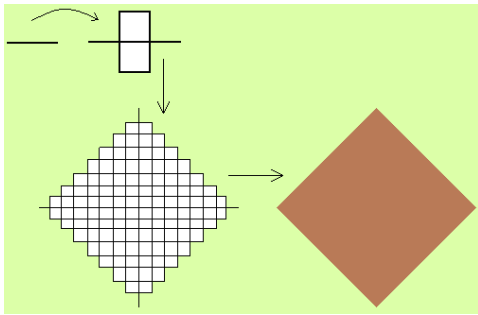


Fig. 6. Pean curve. First three steps of formation and final result - totally filled surface.

clouds and shore lines. Some structures are only partly self similar, for example, trajectory of Brown particle is fractal, but it is only partly self similar. In such case fractal is an object where level of details increases while magnifying it. Mathematically, fractal is a structure whose Hausdorff dimension  $D_H$  is higher than topological dimension  $D_T$ :

$$D_H > D_T \tag{1}$$

Topological dimension  $D_T$  is classical assignment of dimensions of figures - it assigns 0 dimension for a point, 1 to a curve, 2 for a plane, 3 for a cube, etc. There may be no fractional dimensions. Later on appeared geometrical structures that had higher dimension than topological, for example, plane filling curve. Fig. 6. represents Pean curve as a typical example of plane filling curve.

### 2.2. Dimension of self similarity and coverage

The composition of most real structures manifest signs of *self similarity*,  $D_S$ . This feature can be measured by following expression:

$$D_S = \frac{\log a}{\log(s^{-1})} \tag{2}$$

where  $a$  - partition number, amount of parts the figure may be divided to;  $s$  - factor of magnification, the number of times of magnification in order to get a part same sized as a initial figure. As an example, dimension of a square may be calculated: square can be divided to 4 smaller squares.

After mentioned operation half-sized copies of the figure itself occur. As we see - fractal dimension of simple figures is equal to their topological dimension.

Fig. 7 represents the calculation scheme of *coverage* dimension. A figure is covered by squares - in case if it is on a plane. In the case of  $n$ -dimensions, it is covered with  $n$ -dimensional or  $n$ -D cubes. The length of an edge is equal to  $S_k$ . The amount of squares that take up the figure,  $N_k$  is calculated. Computations are compared with length of an edge of another square  $S_{k+1} < S_k$ . Then, the dimension of coverage is presented below:

$$D_b = \frac{\log N_{k+1} - \log N_k}{\log(\frac{1}{S_{k+1}}) - \log(\frac{1}{S_k})} \tag{3}$$

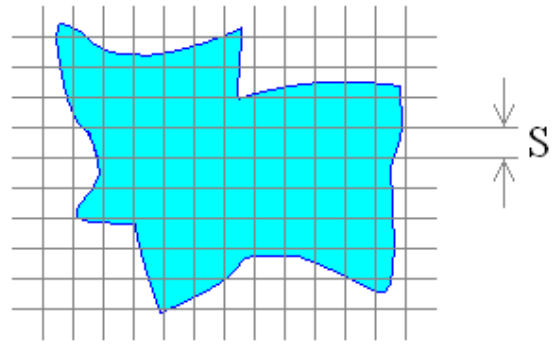


Fig. 7. Calculation of dimension of coverage.

If it is covered with any other elementary  $n$ -dimension units of volume and the radius of those volume units approaches 0, the dimension of coverage  $D_b$  becomes Hausdorff dimension  $D_H$ :

$$D_H = \lim_{s \rightarrow 0} \frac{\log N(s)}{\log \frac{1}{s}} \tag{4}$$

### 2.3. Power law to fractal structure

Another way to describe fractal dimension can be used for practical purposes. Lets suppose our measured unit is  $u$ . If  $s^{-1}$  is the accuracy of measurement, then the power law may be applied to fractal structure:

$$u \approx s^{-d} \tag{5}$$

As we set the logarithm of accuracy  $\log_e 1/s$  on  $x$  axis and the logarithm of measured unit  $\log_e u$  on  $y$  axis, we get a straight line whose slope is  $d$ . Fractal dimension  $D_C = d+1$ .

Using this method, the dimension of Great Britain island shore had been measured:  $D_C = 1.31$ . Actually, as we measure with rulers of different accuracy, we get different length of a shore line. That is the case, because, as we increase our accuracy of measurement, we take even smaller abruptness into consideration.

Table 1 represents the typical fractal objects with the parameters. Fig. 8 represents Koch fractal (left) and Pean fractal (right). Fig. 9 represents Sierpinski triangle (left) and trace of Brown particle (right).

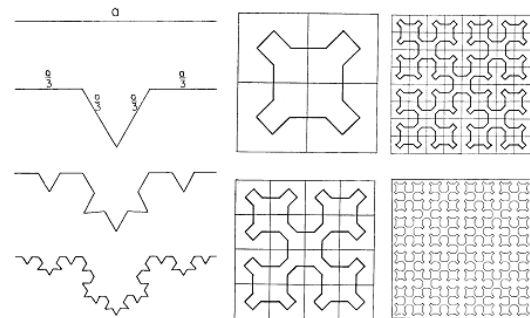


Fig. 8. Koch fractals (left) and Pean fractals (center, right).

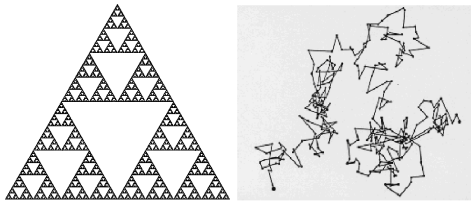


Fig. 9. Sierpinski triangle (left) and trace of Brown particle (right).

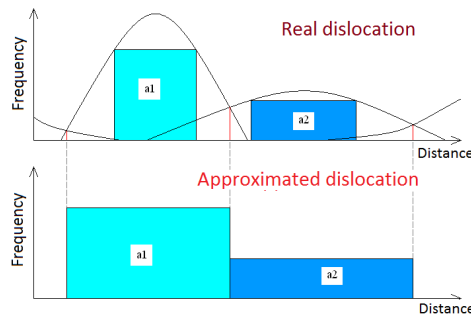


Fig. 10. Scheme of spatial bordering of individs.

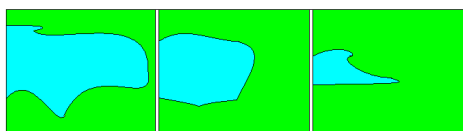


Fig. 11. Surface areas used for modeling.

Besides these three fractal dimensions there are more - information, entropy, etc. Usually, various dimensions on the same object are equal, but sometimes they might differ.

### 3. Possible description of earth surface layers

In order to calculate the indicator of metrical organization, a function of observed objects has to be specified, thus forcing us to specify a model. The calculation of the indicator of metrical organization is based on forms of spatial units in order to determine the difference in organization of a structure after the last crisis [7].

### References

1. Algimantas Tiknius. Territorial Aspects of Development. Monograph (in lith.) - Klaipėdos Universitetas, 2002.
2. Jelena Nesterova. Spatial self-arrangement of expanding structures. 1. Overview of assessment concepts – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – 2(9) 2010 – Pp. 17-22.
3. Raičinskis K. K. Searches and Findings (in lith.) Vol. 1. – Austėja, 1992.
4. Watkins E. The Argumentative Structure of Kant's Metaphysical Foundations of Natural Science. – *Journal of the History of Philosophy* 36(1998) 567-593.
5. See textbooks devoted for Dao philosophy, in particular case: Welch H., Seidel A. Facets of Taoism. – Yale University Press, 1979. – 147 - 151.
6. Ovaskainen O., Hanski I. Spatially structured metapopulation models: global and local assessment of metapopulation capacity. – *Theor. Popul. Biol.* 60(2001) 281–302.

Table 1. Typical fractal objects.

Object	Topological dimension	Fractal dimension
Curve	1	1
Square	2	2
Cube	3	3
Koch fractal	1	1.26
Peano fractal	1	2
Sierpinski carpet	1	1.89
Brown movement trace	1	2

Actually, elements should be displayed as in top of Fig. 10, because forests are live and evolving structures. When creating a model, we have to predict that the structure is likely to grow or shrink. Although, we consider that it will remain constant when making a model - see bottom of Fig. 10.

Also, we need to know that areal may change - grow or shrink, although, it is defined as a  $H=const$  in this model.

The best example of changes of habitat is dynamics of tides. Three states of area of land are represented in Fig. 11: first one defines a high tide - areal is significantly bigger than areal in second state, that is neutral. Third one is low tide - area of areal is significantly reduced [8-9].

### Conclusions

1. The simplest part of a structure sustaining yet the essential properties of reality is the ternary system. Three basic elements at least should present (in recognizable form) in any quantitative model of a real structure.
2. Binary and unitary formalism is incomplete and insufficient to reflect the nature and essence of real developing systems.
3. To recognize the basic elements of a ternary model each of them should be treated as a ternary system.
4. Fractal description is able to reveal and describe the typical features of different structures.

### Acknowledgments

This work was prepared as a part of the Master Thesis. Author would like to thank Assoc. Prof. Algimantas Tiknius (Klaipėda university) for suggestions and comments.

7. Tiknius A., Jankauskas B. and Juška V. A method for Quality Assessment of Environment at the Landscape Level. – In: F. Muller, W. Kepner & K. Caesar (eds.). *EcoSys 2003, Landscape Sciences for Environmental Assessment, Proceedings from a CCMS Pilot Study Meeting at Salzau Castle, Kiel, Germany, 2003*. ISSN:0940-7782 – 56-70.
8. Tiknius A., Jankauskas B., Some effects of population growth on its spatial structure. – In: *EcoSys, Landscape Sciences for Environmental Assessment, Proceedings from a CCMS Pilot Study Meeting at Lecce, Italy, September 6-9, 2004* – pp. 7.
9. Cosma Rohilla Shalizi ir Kristina Lisa Shalizi: Quantifying Self-Organization in Cyclic Cellular Automata. – <<http://www.cscs.umich.edu/crshalizi/research/FN03.pdf>>, accessed 2010 06 12.

## Spatial self-arrangement of expanding structures.

### 3. Novel modeling routine

Jelena Nesterova <sup>a</sup>

Department of Geophysical Sciences, Faculty of Mathematics and Natural Sciences,  
Klaipėda University, H. Manto st. 84, LT-92294 Klaipėda, Lithuania

*Received 14 April 2010, in revised form 9 December 2010, accepted 10 December 2010*

**Abstract.** This work is devoted to the search of correlations - similarities and differences - between indexes of metric and information organization in the complicated cartographic structures. The indicators give the required quality of landscape and represent the quality of residential environment indirectly. Research data are taken from geographical maps and analysed using *geographic information system* (GIS). Analysis of data is based on methods of mathematical statistics. Results of comparative research of two measures are reported in this study.

**Citations:** Jelena Nesterova. Spatial self-arrangement of expanding structures. 3. Novel modeling routine – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 30-36.

**Keywords:** Spatial organization; Expanding Structures; Organized structures; Indices of organization; Informational organization; Self-arrangement; Metrical organization; Cartographic structures; GIS data.

**PACS:** 91.10.Da

**Short title:** Relations in cartographic structures - 3.

## Introduction

Forests of definite size are analyzed in this work so their areal is constant as well. Previous two our publications represent an overview of paradigms [1] and novel model description [2] based on information indicators which are useful for such complicated modelling. The indicators give the required quality of landscape and represent the quality of residential environment indirectly. Research data is taken from geographical maps and analysed using *geographic information system* (GIS).

Purpose of this work is an analysis of data based on methods of mathematical statistics.

## 1. Real forests: methodology of description

Research data is taken from geographical maps and analysed using *geographic information system* (GIS). The analyzed segment of forests is shown in Fig. 1. Area of observation is selected randomly. Then we assign a binome to the functional area according to a model described in Ref. [2]. Fig. 2 represents dividing of layer into binary components.

In order to calculate the indicator of metric organization, we need to take the area of the binome in consideration. To find the area of it, we have to know whole perimeter that consists of outer perimeter of binome and inner perimeter of fo-

rest. Fractal dimension  $D_z$  of binome  $f(z)$  is approaching the value of 2, and for area calculation we use the simplest form:

$$D_z \rightarrow 2 \quad (1)$$

$$f(z) = \left(\frac{P_z}{4}\right)^{D_z} \rightarrow \left(\frac{P_z}{4}\right)^2 \quad (2)$$

$$f(z) = \left(\frac{P_m + P_p}{4}\right)^2 \quad (3)$$

where  $P_m$  - perimeter of the binome - area of forest,  
 $P_p$  - outer perimeter of binome.

It is shown graphically in Fig. 3. This way, by analyzing data from GIS, we may calculate indicators of organization.

## 2. Evaluation of organization in map layers

### 2.1. Metric organization

Index of metric organization  $M_i$  was described in Refs. [2-3]. We use the following routine for current modeling.

**Index of metric organization.**  $f(x)$  - is a function describing a component of a forest layer ( $x_i$  - metrics of forests);  $\bar{f}(x_1, \dots, x_k)$  - function describing average value of a forest layer;  $k$  - amount of components in a layer;

<sup>a</sup>email: [jelena.nesterova@gmail.com](mailto:jelena.nesterova@gmail.com)



Fig. 1. Layer of digital map containing forest arrays.

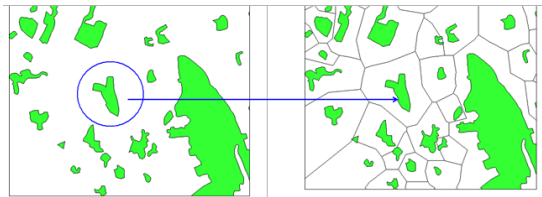


Fig. 2. Dividing of layer (see Fig. 1, center-right) into binary components.

$f(\bar{x}_1, \dots, \bar{x}_k)$  - function of component average values of a layer;

$P_m$  - perimeter of a component;

$P_p$  - outer perimeter of binome;

$D_m$  - fractal dimension of forests;

$S_m$  - area of a component of forest layer.

$$M_i = 1 - \left[ \frac{\bar{f}(x_1, \dots, x_k)}{f(\bar{x}_1, \dots, \bar{x}_k)} \right] \quad (4)$$

$$f(x) = \left\{ \left( \frac{P_m}{4} \right)^{D_m} + \left( \frac{P_z}{4} \right)^2 \right\} \quad (5)$$

$$P_z = P_m + P_p \quad (6)$$

$$D_m = \frac{\ln S_m}{\ln P_m - \ln 4} \quad (7)$$

$$\bar{f}(x) = \frac{1}{n} \sum_{i=1}^n \left\{ \left( \frac{P_m}{4} \right)^{D_m} + \left( \frac{P_z}{4} \right)^2 \right\}_i \quad (8)$$

$$f(\bar{x}) = \left\{ \left( \frac{\bar{P}_m}{4} \right)^{\bar{D}_m} + \left( \frac{\bar{P}_z}{4} \right)^2 \right\} \quad (9)$$

To determine the difference of a structure over the time of evolution, geometrically correct forms of units should be used. Function describing one element of a layer when describing it by metrics  $x$  and  $y$  would look like:

$$f(x) = \bar{x} \cdot \bar{y} + r \cdot s_x \cdot s_y. \quad (10)$$

where  $\bar{x}$  and  $\bar{y}$  are averages of metrics,  $r$  - coefficient of

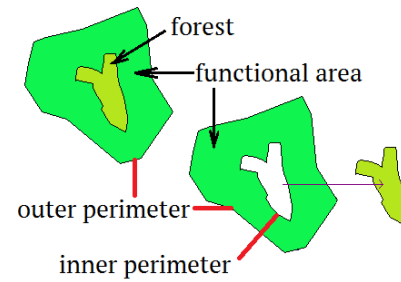


Fig. 3. In order to measure the area of binome, perimeters are calculated, where the perimeter of binome consists of outer and inner perimeters. Inner perimeter is the perimeter of a forest.

correlation of  $x$  and  $y$  values,  $s_x$  and  $s_y$  - standard deviations of metrics.

## 2.2. Informational organization

Three indexes of informational organization were described in Ref. [2]. For current modeling we use the following routine, described in Refs. [4-6].

### First index of informational organization.

$H(X)$  - Shanon entropy;

$H_{\max}$  - value of entropy when all probabilities are the same.

$N_k$  - amount of classes.

$p_i$  - probability of a specific result of experiment.

$n(P_m)$  - amount of elements in a class sorted by a perimeter of forests.

$n(d_m)$  - amount of elements in a class sorted by fractal dimension of forests.

$N$  - total amount of elements.

$S(P_m)$  - area of a class sorted by a perimeter of forests.

$S$  - total area of forests.

$S(d_m)$  - area of a class, sorted by fractal dimension of forests.

$$R = 1 - \frac{H(X)}{H_{\max}} \quad (11)$$

$$H(X) = - \sum_{i=1}^{N_k} p_i \cdot \log(p_i) \quad (12)$$

$$H_{\max} = \ln N_k \quad (13)$$

$$p_i = \frac{n(d_m)}{N} \quad (14)$$

$$p_i = \frac{n(P_m)}{N} \quad (15)$$

$$p_i = \frac{S(d_m)}{S} \quad (16)$$

$$p_i = \frac{S(P_m)}{S} \quad (17)$$

**Second index of informational organization.**

$T(n(P_m), n(d_m))$  - negentropy of experiment;  
 $H(n(P_m))$  - entropy of experiment with parameter  $P_m$ ;  
 $H(n(d_m))$  - entropy of experiment with parameter  $d_m$ ;  
 $n_i$  - number of elements in a class, sorted by perimeter;  
 $N$  - total number of elements;  
 $n_j$  - number of elements in a class, sorted by fractal dimension;  
 $H(n(P_m), n(d_m))$  - entropy of matrix  $n(P_m) \times n(d_m)$ ;  
 $n_{i,j}$  - elements of matrix  $n(P_m) \times n(d_m)$ .

$$R = \frac{T(n(P_m), n(d_m))}{H(n(d_m))} \times 100\% \quad (18)$$

$$R = \frac{T(n(P_m), n(d_m))}{H(n(P_m))} \times 100\% \quad (19)$$

$$T(P_m, d_m) = H(n(P_m)) + H(n(d_m)) - H(n(P_m), n(d_m)) \quad (20)$$

$$H(n(P_m)) = - \sum_i \frac{n_i}{N} \log \frac{n_i}{N} \quad (21)$$

$$H(n(d_m)) = - \sum_j \frac{n_j}{N} \log \frac{n_j}{N} \quad (22)$$

$$H(n(P_m), n(d_m)) = - \sum_i \sum_j \frac{n_{i,j}}{N} \log \frac{n_{i,j}}{N} \quad (23)$$

**Third index of informational organization.**

$T(P_m, d_m)$  - negentropy of experiment;  
 $H(P_m)$  - entropy of experiment with parameter  $P_m$ ;  
 $H(d_m)$  - entropy of experiment with parameter  $d_m$ ;  
 $n_i$  - area of a class, sorted by perimeter;  
 $N$  - total area;  
 $n_j$  - area of a class, sorted by fractal dimension;  
 $H(P_m, d_m)$  - entropy of a matrix  $P_m \times d_m$ ;  
 $n_{ij}$  - elements of matrix  $P_m \times d_m$ .

$$R = \frac{T(P_m, d_m)}{H(d_m)} \times 100\% \quad (24)$$

$$R = \frac{T(P_m, d_m)}{H(P_m)} \times 100\% \quad (25)$$

$$T(P_m, d_m) = H(P_m) + H(d_m) - H(P_m, d_m) \quad (26)$$

$$H(P_m) = - \sum_i \frac{n_i}{N} \log \frac{n_i}{N} \quad (27)$$

$$H(d_m) = - \sum_j \frac{n_j}{N} \log \frac{n_j}{N} \quad (28)$$

$$H(P_m, d_m) = - \sum_i \sum_j \frac{n_{i,j}}{N} \log \frac{n_{i,j}}{N} \quad (29)$$

**2.3. Correlations**

It is very important to know the level of dependence. Various correlations and other measurements of dependence are used according to Ref. [7].

In order to estimate correlation bonds, the coefficient of these bonds (unit of strength in statistical connections between variables) gains significance. It may be applied only when there is a linear dependence in range [-1 ÷ 1]. The connection is very strong if it equals to -1 and very weak when it equals to 1. It is marked as  $\rho$  in theory of probability.

Coefficient of correlation  $\rho_{X,Y}$  of two random values  $X$  and  $Y$  when their averages are  $\mu_X$  and  $\mu_Y$ , and standard deviations  $\sigma_X$  and  $\sigma_Y$  is defined as follows:

$$\rho_{X,Y} = \frac{\text{cov}(X, Y)}{\sigma_X \sigma_Y} = \frac{E((X - \mu_X)(Y - \mu_Y))}{\sigma_X \sigma_Y} \quad (30)$$

Standard deviations  $\sigma_X$  and  $\sigma_Y$  need to be finite and unequal zero for coefficient of correlation to have a defined meaning. In the first part of the equation, we see the covariation of variables  $X$  and  $Y$  that is the average of multiplication of their deviation from average values.

Correlations may be positive or negative, depending on their direction. For example, when there is negative correlation, values of one variable decrease while the values of other variable increase. Pearson's coefficient of correlation is used to measure strength of quantitative connections between variables. Big values of this coefficient, either positive or negative, reflect strong correlation, while small values reflect weak correlation. If correlation is insignificant, coefficient is close to zero. Pearson's coefficient of correlation is calculated by multiplication of pairs of values from two sets, after subtracting the average. The difference is divided by multiplication of standard deviations.

$$r_{xy} = \frac{1}{n-1} \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{s_x s_y} \quad (31)$$

where  $\bar{x}$  and  $\bar{y}$  are average values of observations  $x$  and  $y$ ,  $s_x$  and  $s_y$  - standard deviations of  $x$  and  $y$ . Coefficient of correlation has these properties: when  $r = 1$ , all points  $(x_i, y_i)$  are in a line that has positive coefficient of direction. When  $r = -1$ , all points  $(x_i, y_i)$  are in a line that has negative coefficient of direction. When  $r = 0$ , all variables are linearly independent. Table 1 represents the interpretation of strength of correlation.

In order to prevent very strong correlation between unrelated variables, there is a check of significance in coefficient of correlation:

- i) zero hypothesis  $H_0$  states that coefficient of correlation equals zero;
- ii) alternative,  $H_1$  hypothesis states that coefficient is not equal to zero.



Table 1. Interpretation of strength of correlation.

Negative	Positive	Estimation of correlation
-1.0 ÷ -0.9	0.9 ÷ 1.0	very strong
-0.9 ÷ -0.7	0.7 ÷ 0.9	strong
-0.7 ÷ -0.5	0.5 ÷ 0.7	average
-0.5 ÷ -0.3	0.3 ÷ 0.5	weak
-0.3 ÷ 0.0	0.0 ÷ 0.3	insignificant

In order to prove the  $H_0$  hypothesis, criteria  $t$  is introduced:

$$t = r_S \sqrt{\frac{n-2}{1-r_S^2}} \quad (32)$$

where  $r$  - calculated value of correlation.  $n$  - amount of calculated values. Level of significance is free to choose. Let's assume that the level of significance  $\alpha = 0.05$ . Hypothesis  $H_0$  is rejected if absolute value exceeds the critical value of Student's distribution with  $n-2$  degrees of freedom on  $0.5 \cdot \alpha$  level.

### 3. Data sources

Digital map of Lithuania was chosen as a data source. Layer of forests was chosen as an object of observation. Areas of a map were selected randomly.

**Required amount of data.** Using another form of Student's criteria and selecting the required accuracy, we may determine the required amount of data:

$$t = \frac{(\bar{x} - \hat{x})}{\sigma_n} \quad (33)$$

where  $\bar{x}$  is theoretical average of data,  $\hat{x}$  - mathematical average of data,  $\sigma_n$  - dispersion of data. Switching it for sample parameter, we get:

$$\sigma_n^2 = \frac{\sigma^2}{n} \approx \frac{1}{n(n-1)} \sum_{i=1}^n (\Delta x_i)^2 = s_{\bar{x}}^2 \quad (34)$$

$$s_{\bar{x}} = \frac{s_x}{\sqrt{n}} \quad (35)$$

If there is a need of accuracy of 0.182, we may calculate required amount of data from 2-43:

$$s_{\bar{x}} = 0.182 s_x, \quad (36)$$

$$0.182 s_x = \frac{s_x}{\sqrt{n}}, \quad (37)$$

$$n = \left( \frac{1}{0.182} \right)^2 \approx 30. \quad (38)$$

In order to get accuracy of 0.182, set of amount of 30 values must be used.

## 4. Results and discussion

Starting data represent the primary as well as derived parameters. Several primary parameters such as areas and perimeters of forest elements, areas and perimeters of binomes, amount of elements in classes sorted by perimeter were used. Nine indicators of organization were calculated - see Table 2.

Also derived parameters such as fractal dimensions, values of model function, average values of model function, values of model function of average values; fractal dimension of forests; areas of classes sorted by perimeter and fractal dimension, indicators of probability and informational organization, matrices for calculation of negentropy, values of negentropy were included.

Main task could be formulated as follows: to find the strong correlations as relations between indicators of metrical ( $M$ ) and informational organization ( $R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8$ ). Such type relations could be most interesting. Values of correlations for analyzed indicators are presented in Table 3.

Looking at Table 3, we may conclude that the connection between organizational indicators is weak or insignificant, because correlation does not exceed 0.3.

It is necessary to point out that  $r$  displays direct connection. If correlation  $r = 0$ , it does not mean that there is no connection at all. Non-linear connection may appear in this case. We may conclude that because  $r$  is close to zero, there is no suitable line by the data.

To check  $H_0$  hypothesis, values of  $t$  were checked (see Table 4).

When  $\alpha = 0.4$ , all values of  $t$  exceeding 0.855 are considered significant correlations and they are worth attention. Values lower than 0.855 are considered insignificant. That means that it is useful to analyse connections between following indicators:

- i)  $M$  and  $R_3$  (1.080),  $R_3 = f(M)$ ; see Fig. 4;
- ii)  $M$  and  $R_4$  (0.913),  $R_4 = f(M)$ ; see Fig. 5;
- iii)  $M$  and  $R_5$  (1.308),  $R_5 = f(M)$ ; see Fig. 6;
- iv)  $M$  and  $R_6$  (1.308),  $R_6 = f(M)$ ; see Fig. 7.

Choice of variables was done according the following schema:  $X$  - indicator of metrical organization  $M$ ,  $Y$  - indicator of informational organization  $R$ .

Fig. 4 and Fig. 5 represent the dependences  $R_3 = f(M)$  and  $R_4 = f(M)$  respectively. Following linear equations were established from mentioned Fig. 4 and Fig. 5 respectively (red line):

$$Y = 0.27678 \cdot X + 0.11983 \quad (39)$$

$$Y = 0.19999 \cdot X + 0.10764 \quad (40)$$

We set Student's coefficient to 5% and see that the reliability of correlation is 95%, but 67% of data is unreliable for  $R_3$  and 27% of data is reliable for  $R_4$ . Such data allow us to conclude that connection between metrical and informational organization is insignificant or there are no indicators when

Table 2. Dependencies between indicators of metrical ( $M$ ) and informational organization ( $R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8$ ).

$Nr$	$M$	$R_1$	$R_2$	$R_3$	$R_4$	$R_5$	$R_6$	$R_7$	$R_8$
1.	0.53	0.05	0.45	0.10	0.005	0.08	0.15	1.30	1.18
2.	0.58	0.21	0.06	0.21	0.32	1.43	1.20	1.08	1.25
3.	0.60	0.16	0.01	0.12	0.30	1.79	1.52	1.52	1.90
4.	0.38	0.21	0.35	0.35	0.40	1.27	1.53	1.02	1.10
5.	0.42	0.10	0.003	0.25	0.53	1.71	1.55	1.38	2.19
6.	0.47	0.01	0.30	0.77	0.38	1.11	1.55	3.15	1.16
7.	0.50	0.09	0.14	0.30	0.28	1.38	1.46	1.46	1.43
8.	0.68	0.06	0.02	0.06	0.23	0.98	0.94	1.14	1.40
9.	0.64	0.01	0.12	0.16	0.11	0.94	1.05	1.32	1.23
10.	0.56	0.04	0.01	0.14	0.43	1.07	1.02	1.03	1.55
11.	0.64	0.05	0.13	0.04	0.10	1.35	1.46	1.42	1.50
12.	0.59	0.13	0.42	0.74	0.24	1.28	1.93	3.58	1.22
13.	0.63	0.004	0.07	0.11	0.11	0.85	0.92	1.08	1.08
14.	0.32	0.01	0.34	0.31	0.11	0.46	0.69	0.78	0.61
15.	0.51	0.11	0.36	0.10	0.06	1.18	1.64	1.42	1.36
16.	0.60	0.08	0.35	0.14	0.06	1.23	1.72	1.67	1.52
17.	0.54	0.01	0.34	0.20	0.10	0.82	1.22	1.31	1.16
18.	0.48	0.03	0.17	0.15	0.09	1.29	1.51	1.60	1.49
19.	0.60	0.07	0.27	0.22	0.22	1.15	1.48	1.67	1.66
20.	0.63	0.06	0.30	0.18	0.13	1.16	1.55	1.23	1.17
21.	0.66	0.05	0.28	0.32	0.25	0.98	1.30	1.31	1.19
22.	0.51	0.04	0.47	0.17	0.01	0.83	1.52	1.34	1.12
23.	-0.09	0.02	0.36	0.07	0.09	0.43	0.66	1.23	1.27
24.	0.63	0.01	0.53	0.41	0.14	0.45	0.95	1.38	0.95
25.	0.65	0.05	0.47	0.29	0.08	0.05	0.29	1.33	1.03
26.	0.63	0.004	0.17	0.57	0.69	0.21	0.25	0.76	1.06
27.	0.71	0.02	0.12	0.58	0.36	1.70	1.88	1.66	1.09
28.	0.61	0.40	0.64	0.06	0.02	1.51	2.48	1.92	1.85
29.	0.54	0.12	0.53	0.33	0.08	1.24	2.32	2.00	1.44
30.	0.78	0.10	0.42	0.72	0.61	1.55	2.41	2.21	1.59

probabilities are calculated by using areas of forest groups that are classified by fractal dimension of forests ( $R_3$ ) or by perimeter of forests ( $R_4$ ).

Fig. 6 and Fig. 7 represent dependences  $R_5 = f(M)$  and  $R_6 = f(M)$  respectively. Following linear equations were established from Fig. 6 and Fig. 7 (red line):

$$Y = 0.66599 \cdot X + 0.66504 \quad (41)$$

$$Y = 0.89736 \cdot X + 0.84422 \quad (42)$$

We set Student's coefficient to 5% and see that the reliability of correlation is 95%, but 37% of data is reliable for  $R_5$  and 36% - for  $R_6$ . Such data allow us to conclude that connection between metrical and informational organization is insignificant but direct when values of informational organization are calculated by using expression of negentropy, where probabilities are calculated by using amount of elements and divided by entropy, which is calculated:

- i) by using element number in class, classified by fractal dimension of forests ( $R_5$ ) or
- ii) by numbers of elements in a class, classified by fractal dimension of forests ( $R_6$ ).

Although all indicators suggest that observed structures

are more or less organized, no connection between indicators was noticed after reviewing all charts, because neither way of examination showed strong direct dependence. Analytically, both methods are similar - they both depend on connection between the variables. Unfortunately analysis of correlation did not confirm this assumption. Why there is no connection between them? Organization of spatial structures is a term that has multiple meanings. There is a possibility that this property may not be represented by any single indicator and needs multivariable characteristics. If, for example, one indicator shows homogeneity, another may show anisotropy. In

Table 3. Correlations for indicators.

Indexes	Correlation coefficients	Pearson $T$ -criteria
$M$ and $R_1$	0.07	0.371
$M$ and $R_2$	-0.10	0.532
$M$ and $R_3$	0.20	1.080
$M$ and $R_4$	0.17	0.913
$M$ and $R_5$	0.24	1.308
$M$ and $R_6$	0.24	1.308
$M$ and $R_7$	0.13	0.694
$M$ and $R_8$	0.09	0.478

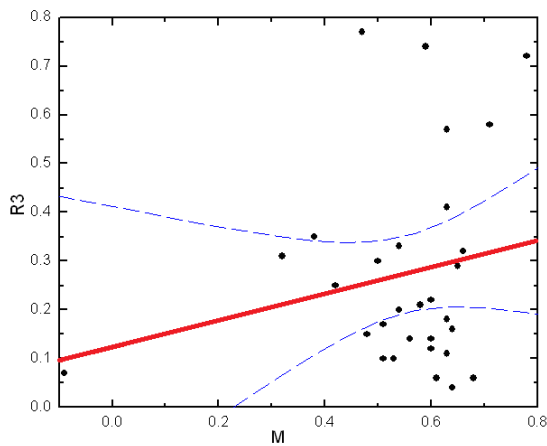


Fig. 4.  $R_3 = f(M)$ . Dependency of metric organization indicator from information organization indicator when probabilities are calculated based on the areas of forest groups that are classified by fractal dimension of forests.

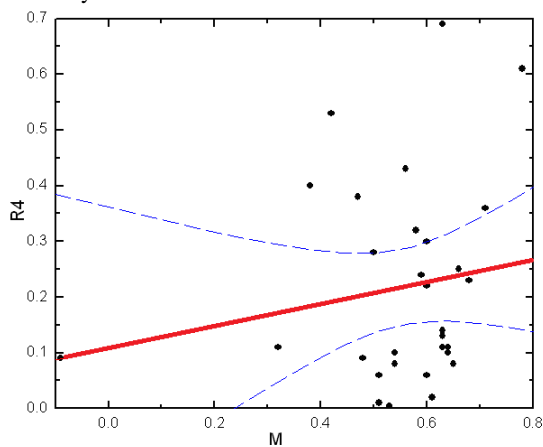


Fig. 5.  $R_4 = f(M)$ . Dependency of metric organization indicator from information organization indicator when probabilities are calculated based on the areas of forest groups that are classified by perimeters of forests.

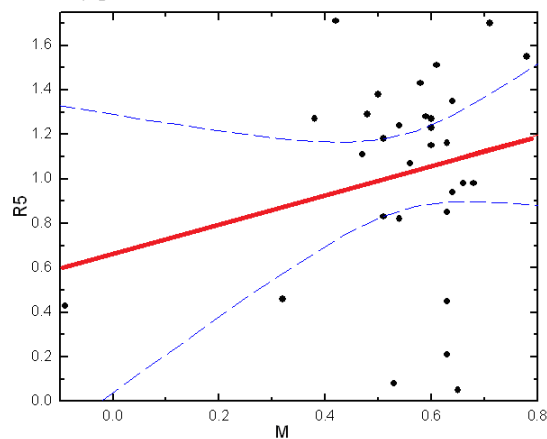


Fig. 6.  $R_5 = f(M)$ . Dependency of metric organization indicator from information organization indicator when values of information organization are calculated by using negentropy where probabilities are calculated by the amount of elements and divided by entropy which is calculated by the amount of elements in a class, classified by the fractal dimension of forests.

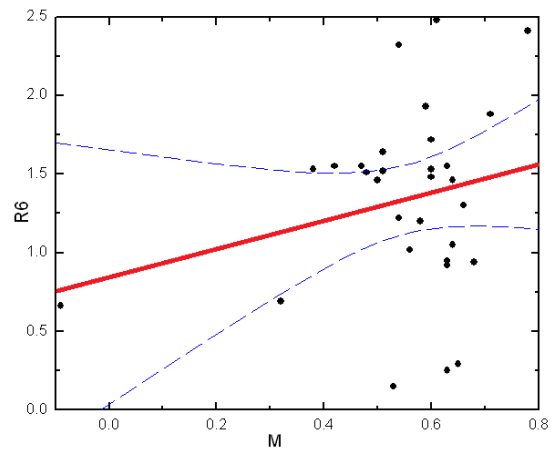


Fig. 7.  $R_6 = f(M)$ . Dependency of metric organization indicator from information organization indicator when values of information organization are calculated by using negentropy where probabilities are calculated by the amount of elements and divided by entropy which is calculated by the amount of elements in a class, classified by the perimeter of forests.

this case, there may be no correlation between them and only future research will perhaps will solve this problem.

### Conclusions

1. Research of cartographic layers in two different ways (19 000 km<sup>2</sup> territory was observed in total) shows that there are no statistically significant correlations between informational and metrical organization indicators. Two conclusions come of this:
  - i) these indicators show different aspects of spatial organization;
  - ii) research done (variety of layers and numbers) is insufficient to measure the correlation.
2. Variation of informational indicator values is bigger than the characteristics of metrical indicator ( $C_u > C_v$ ). This difference is the significance of a structure.
3. Observation of real layers is not sufficient to determine the sensitivity of indicators. Research should be done by changing properties of layers by applying Moran and Getis indicators in order to compare results. That would help to determine the susceptibility of objects for spatial heterogeneity, anisotropy and of metrical and topological properties of layers.
4. In order to improve the research it is preferable to apply both: GIS and statistical computation routines for estimation of spatial organization in cartography.

### Acknowledgments

This work was prepared as a part of the Master Thesis. Author would like to thank Assoc. Prof. Algimantas Tiknius (Klaipėda university) for suggestions and comments.

## References

1. Jelena Nesterova. Spatial self-arrangement of expanding structures. 1. Overview of assessment concepts – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 17-22.
2. Jelena Nesterova. Spatial self-arrangement of expanding structures. 2. Structure model construction – *Innovative Infotechnologies for Science, Business and Education*, ISSN 2029-1035 – **2(9)** 2010 – Pp. 23-29.
3. Algimantas Tiknius, Kęstutis Dučinskas, Benediktas Jankauskas. Deriving the spatial traits of organized land structures. – In: I. Petrosillo et al. Use of landscape sciences for the assessment of environment security. – Springer, 2008. – 121-130. – <<http://www.springerlink.com/content/q6u8m2m545582162/>>, accessed 2010 08 05.
4. G. Boffetta, M. Cencini, M. Falcioni, A. Vulpiani. Predictability: a way to characterize complexity. – <<http://arxiv.org/abs/nlin.CD/0101029>>, accessed 2010 04 09.
5. J. Bogaert, A. Farina, R. Ceulemans. Entropy increase of fragmented habitats: A sign of human impact? – <<http://www.springerlink.com/content/hw2784516085402x/fulltext.pdf>>, accessed 2010 04 09.
6. Ambedkar Dukkipati. On Generalized Measures of Information with Maximum and Minimum Entropy Prescriptions. – <<http://etd.ncsi.iisc.ernet.in/bitstream/2005/353/1/G20346.pdf>>, accessed 2010 04 09.
7. Bronislovas Martinėnas. Eksperimento duomenų statistinė analizė (in lith.) – Vilnius: Technika, 2004.