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QUANTITATIVE ANALYSIS OF FIBER COMPOSITE MICROSTRUCTURE

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Summary: *This work is concerned with the description of the process of retrieving color images from real composite systems together with their transformation into binary images. The fiber composites were used as a real composite, because of its future perspective use. The main part is dedicated to the comparison of various boundary conditions and processes for obtaining the two-point probability function with various boundary conditions. The dominant purpose of this work is to determine the differences in three boundary conditions. In particular, the plain (no condition), mirror and periodic boundary conditions are considered. The possible computational methods are taken in consideration, too. The speed of evaluation is one of the most important issues and as such is emphasized.*

1.two-point probability functions

Fundamental function and statistical moments. Consider an ensemble of a two-phase random medium. To provide a general statistical description of such a systems it proves useful to characterize each member of the ensemble by a stochastic function – characteristic function $\chi_r(\mathbf{x},\alpha)$, which is equal to one when point **x** lies in the phase r of the sample and equals to zero otherwise,

$$\chi_r(\mathbf{x},\alpha) = \begin{cases} 1, & \text{if } \mathbf{x} \in D_r(\alpha), \\ 0, & \text{otherwise}, \end{cases} \tag{1}$$

where $D_r(\alpha)$ denotes the domain occupied by the r-th phase. Except where noted, composites consisting of clearly distinguishable continuous matrix phase are considered. Therefore, $r = m, f$ is further assumed to take values m for the matrix phase while symbol f is reserved for the second phase. For such a system the characteristic functions $\chi_f(\mathbf{x},\alpha)$ and $\chi_m(\mathbf{x},\alpha)$ are related by

$$\chi_m(\mathbf{x},\alpha) + \chi_f(\mathbf{x},\alpha) = 1 \tag{2}$$

We write the ensemble average of the product of characteristic functions

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$$S_{r_1,\dots,r_n}(\mathbf{x}_1,\dots,\mathbf{x}_n)=\overline{\chi_{r_1}(\mathbf{x}_1,\alpha)\cdots\chi_{r_n}(\mathbf{x}_n,\alpha)}, \tag{3}$$

where function $S_{r_1,\dots,r_n}$ referred to as the general n-point probability gives the probability of finding n points $\mathbf{x}_1, \dots, \mathbf{x}_n$ randomly thrown into a medium located in the phases $r_1, \dots, r_n$.

Functions of the first and second order. Hereafter, we limit our attention to functions of the order of one and two, since higher-order functions are quite difficult to determine in practice. Therefore, description of a random medium will be provided by the one-point probability function $S_r(\mathbf{x})$

$$S_r(\mathbf{x})=\overline{\chi_r(\mathbf{x},\alpha)}, \tag{4}$$

which simply gives the probability of finding the phase r at $\mathbf{x}$ and by the two-point probability function $S_{rs}(\mathbf{x}_1, \mathbf{x}_2)$

$$S_{rs}(\mathbf{x}_1,\mathbf{x}_2)=\overline{\chi_r(\mathbf{x}_1,\alpha)\chi_s(\mathbf{x}_2,\alpha)}, \tag{5}$$

which denotes the probability of finding simultaneously the phase r at $\mathbf{x}_1$ and the phase s at $\mathbf{x}_2$. In general, evaluation of these characteristics may prove to be prohibitively difficult. Fortunately, a simple method of attack can be adopted when accepting an assumption regarding the material as statistically homogeneous, so that

$$S_r(\mathbf{x})=S_r, \tag{6}$$

$$S_{rs}(\mathbf{x}_1,\mathbf{x}_2)=S_{rs}(\mathbf{x}_1-\mathbf{x}_2). \tag{7}$$

Further simplification arises when assuming the medium to be statistically isotropic. Then $S_{rs}(\mathbf{x}_1,\mathbf{x}_2)$ reduces to

$$S_{rs}(\mathbf{x}_1-\mathbf{x}_2)=S_{rs}(\|\mathbf{x}_1-\mathbf{x}_2\|). \tag{8}$$

Finally, making an ergodic assumption allows a substitution of the one-point correlation function by its volume average, i.e., volume concentration or volume fraction of the r-th phase c_r,

$$S_r=c_r. \tag{9}$$

Limiting values. In addition, the two-point probability function S_{rs} incorporates the one-point probability function S_r for certain values of its arguments such that

$$\text{for } \mathbf{x}_1=\mathbf{x}_2 \quad : \quad S_{rs}(\mathbf{x}_1,\mathbf{x}_2)=\delta_{rs}S_r(\mathbf{x}_1), \tag{10}$$

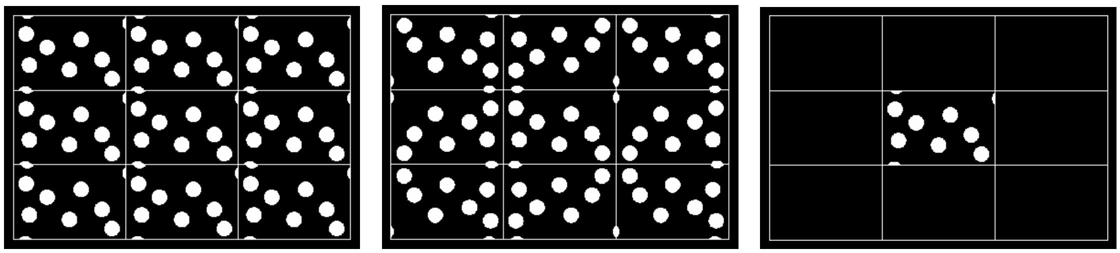
$$\text{for } \|\mathbf{x}_1-\mathbf{x}_2\|\to\infty \quad : \quad \lim_{\|\mathbf{x}_1-\mathbf{x}_2\|\to\infty} S_{rs}(\mathbf{x}_1,\mathbf{x}_2)=S_r(\mathbf{x}_1)S_s(\mathbf{x}_2), \tag{11}$$

where symbol δ_{rs} stands for Kronecker's delta. Relation (10) states that the probability of finding two different phases at a single point is equal to 0 (see also Eq. (2)) or is given by the one-point probability function if phases are identical. Equation (11) manifests that for large distances points $\mathbf{x}_1$ and $\mathbf{x}_2$ are statistically independent. This relation is often denoted as the no-long range orders hypothesis

2.Boundary conditions

There are many possibilities how to statistically describe microstructure. In this work the attention is focused on the two-point probability function. This function is quite simple and easy to compute when compared with other descriptors. The two point probability function can be determined applying various boundary conditions. The literature offers the three main possibilities. Recall that the two point probability function can be obtained by throwing a needle of certain length in the image and counting how many times the ends fall in the selected color. The question is what to do, when one end of the needle falls out of the image.

The first possibility is to expect that the image of microstructure is periodically repeated in each direction. This condition is the simplest one, as it allows using very efficient computational method described below. This first possibility is shown in Figure 1a.



a b c

Figure 1: a) Example of binary image of microstructure with periodical boundary conditions.

b) Example of binary image of microstructure with mirror boundary conditions.

c) Example of binary image with no mirroring or repeating.

The second possibility is to expect that the microstructure is mirrored. This approach is more time consuming, but is presented for the sake of comparison with other results. In case of unidirectional fibers it is probably not very efficient, but research of microstructure consists of many others fields of research, where technique can be very useful(Figure 1b)

The third possibility, here termed as plain boundary conditions, is to disregard the throws, where at least one of the ends of the needle falls out of the image. This approach is probably the most accurate one, but significantly reduces the amount of obtained information. It is evident that long needles can be thrown just a few times to be totally contained in the image. If the needle with length of the diagonal of the rectangle is used, it can be thrown just one time. That is the reason, why the data of two point probability function have to be reduced of data with low reliability. (The needle is too long and therefore can be thrown just few times.) (Figure 1c)

Based on the previous work it was possible to use 25 images, but only 18 images were eventually selected for the analysis. The visual evaluation consists of elimination samples which seem to be unuseful. If about one fifth of the image was fiber free it was clear, that the image experienced some error.

3.Evaluation of the two-point probability function using Fast Fourier Transform method

The fast Fourier transform method can be used only with the periodic boundary conditions. This method is much faster than the classical Monte-Carlo method and was used to as a basis to compare effectiveness of both methods.

After selecting suitable inputs the two point probability function was calculated. In the first step the edge of the input image was cut to obtain a square bitmap. The reason was that the edge could be influenced by inaccuracy when taking images. That means that the largest image had size of 1 148 x 1 148 pixels. In the next step the size was reduced by 70 pixels in both directions to 1 078 x 1 078 pixels. The smaller image was selected 10 times from random positions of the largest image. The step 70 pixels was chosen, because the average size of fibers in images is c. 70 pixels. In each subsequent step the size was reduced by 70 pixels in both directions and the random selection was increased 10 times compared to the previous case

After preparation and sorting of bitmaps the two point probability function was calculated for each bitmap. The results of this calculation were stored in the matrix of the same dimensions as the bitmap. Next step was to create the average result for each size. The average was calculated not only on the whole set, but also on partial sets constructed from *2, 3, 4, … , Number of bitmaps of the specified size* bitmaps. The value of average two-point probability function at the position *ij* was obtained as average value of independently computed two-point probability functions at the position *ij*.

The last step was to determine a suitable measure of a difference among the two-point probability functions. As “an exact” two point probability function the function calculated on the largest image was chosen. To calculate the measure *M*, the following formula was used

$$M = \frac{1}{W.H} . \sum_{i=0}^{W-1} \sum_{j=0}^{H-1} \frac{\left| S_{ij} - P_{ij} \right|}{\left| S_{ij} \right|} . \tag{13}$$

In equation (13) *W* means the number of used points in the direction of width of the bitmap, *H* the number of used points in the direction of height of the bitmap. If every point of bitmap is used for evaluation of the measure *W* means the width of bitmap and *H* is the height of bitmap. S_{ij} is the value of the two point probability function of an image taken in the point with coordinates *i* and *j*. P_{ij} is the value of the two point probability function of the largest bitmap. This enables comparison of measures taken from bitmaps with variable sizes.

Another measure M_M was also considered and compared to measure *M*. The used formula follows

$$M = \frac{1}{W.H} . \sum_{i=0}^{W-1} \sum_{j=0}^{H-1} \frac{\left| S_{ij} - P_{ij} \right|}{\left| S_{ij} \right| . dist(i, j)} \tag{14}$$

in which

$$dist(i, j) = \begin{cases} 1 & , i = 0 \wedge j = 0 \\ \sqrt{i^2 + j^2} & , \text{otherwise} \end{cases} \tag{15}$$

The variable *dist* should guarantee that the values of the two point probability function, which are more distant from the origin, have smaller significance than those which are closer. Quite surprisingly, this correction results in rather negligible difference.

Because the measure M and measure M_M were the same, just multiplied by almost a constant value, in the subsequent research, only the measure M was used as it is more simple to compute.

4.Graphs of measures

This part presents an overview of the measures M evaluated from the computed two point probability functions. It is evident that bigger bitmaps allow getting results with better reliability. Quite surprisingly, even for lower resolutions there is no common value, where all measures stabilize. The measure of the two point probability function oscillates around different value.

The resolution displayed above each graph represents the area over which the measure M was evaluated. The values at horizontal axis are the numbers of used bitmaps for evaluation of the average two point probability function. The accuracy does not gain zero value at numbers of repeats 11, 21, 31, … . The line connecting the value of measure with zero is displayed just for the lucidity of graphs. The described example follows.

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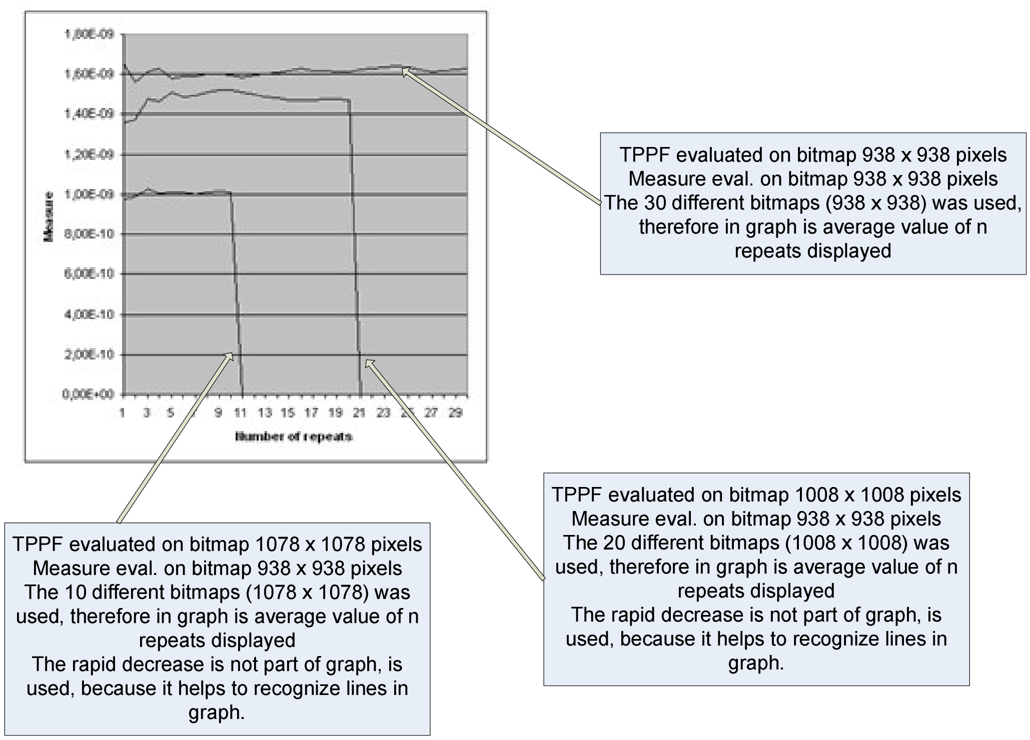

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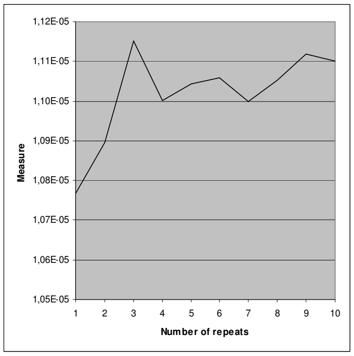

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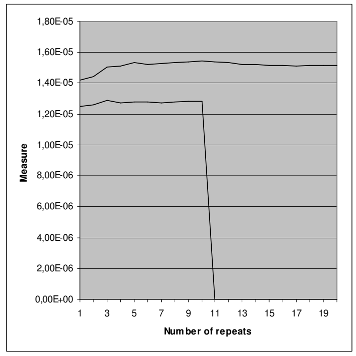

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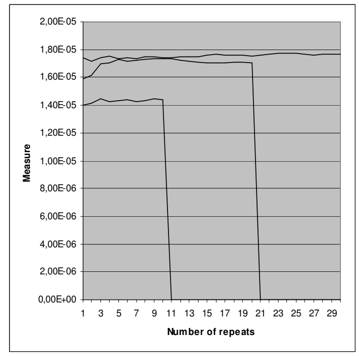

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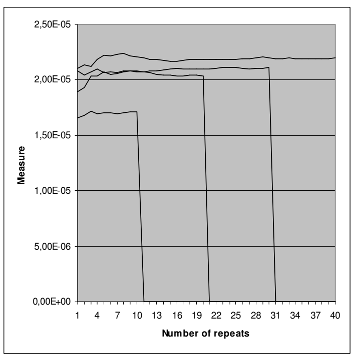

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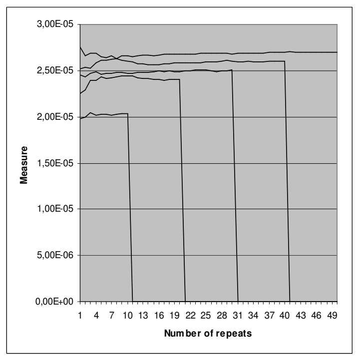

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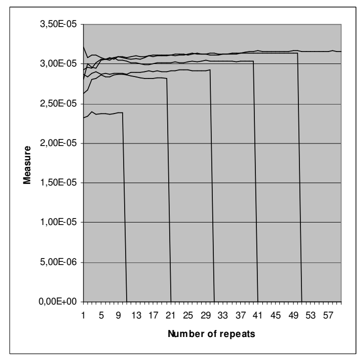

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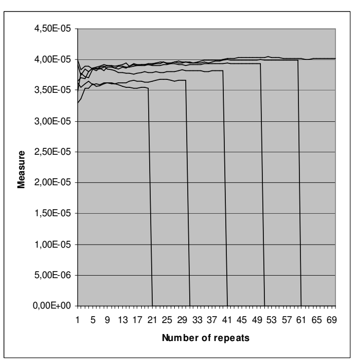

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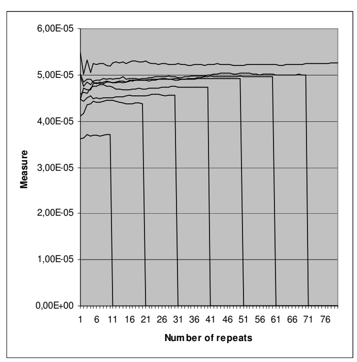

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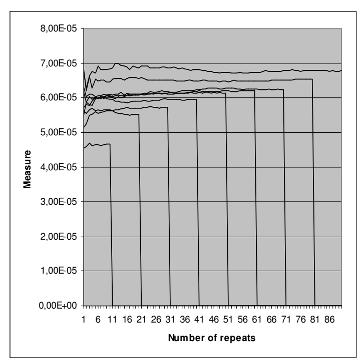

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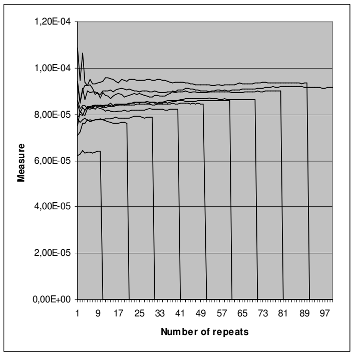

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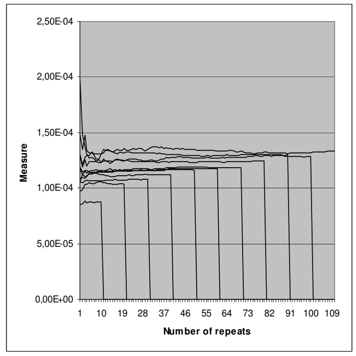

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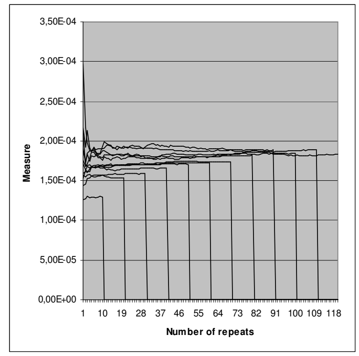

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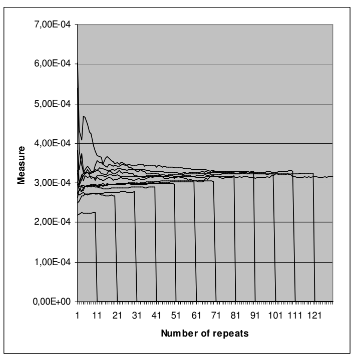

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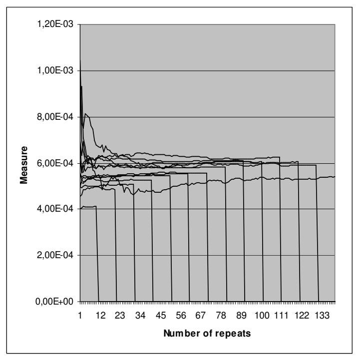

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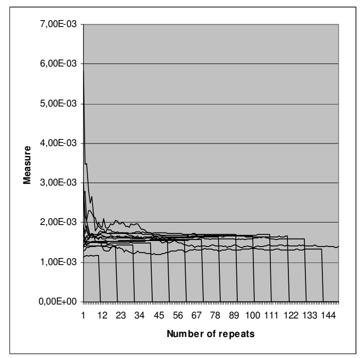

5.Evaluation of the two-point probability function using the Monte Carlo Method

Due to computational demands of the Monte-Carlo method the simplifying conditions had to be applied to the evaluation. The detail description of the used algorithm is presented in this section. Two possibilities of simplification were considered. First, the value of the two point probability function could be computed for all available vectors of function, but not all data contained by the graph are used for the function evaluation. In other words the needles of every available length are used but just limited numbers of throws are done. Other possibility is to evaluate the function just for a few specific vectors, but all data stored in the bitmap are used for evaluation. In other words to throw the needles of just few chosen lengths but the needles are thrown into every point of bitmap.

In the present work the second possibility was employed. The reason was that this approach allows comparison with results obtained by Fast Fourier transform method, which evaluates the function with use of all data stored in the image. This property is important as the goal of this research is to compare different boundary conditions.

The step used through the bitmap was based upon the average size of one fiber. The average diameter of fiber was c. 70 pixels and one quarter of the diameter is approximately 17 pixels. The used step was 15 pixels. For obtaining the step in horizontal direction the same relation was used and since the fibers are circles, both steps were the same.

Another difference compare to the Fast-Fourier transform method is that the step reducing the bitmaps sizes was bigger. Recall that in Fast Fourier transformation method the step 70 pixels was used which in the Monte Carlo method was set to 140 pixels and just one half of bitmap size reductions was done.

6.Periodic boundary conditions

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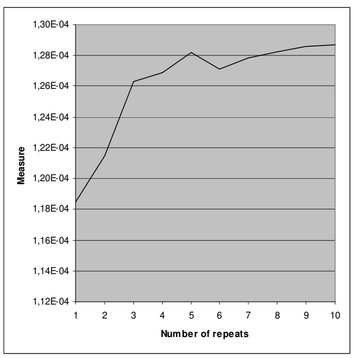

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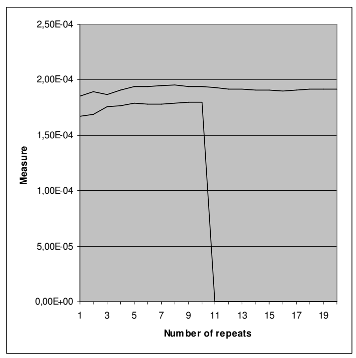

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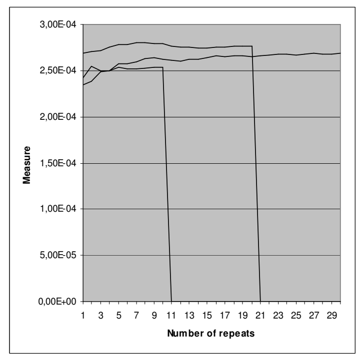

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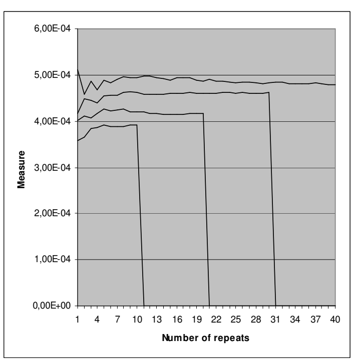

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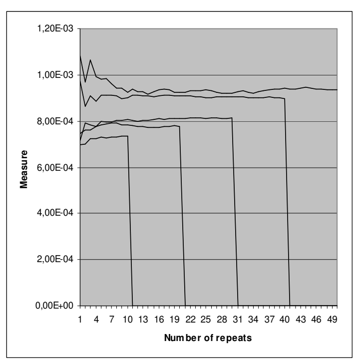

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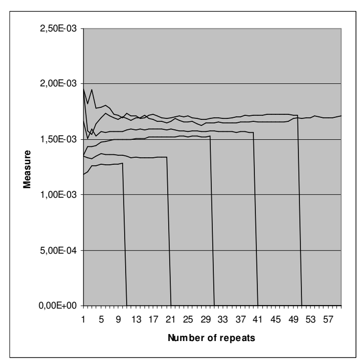

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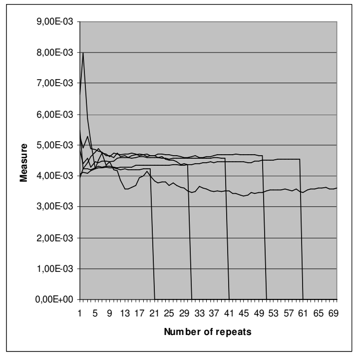

7.Plain boundary conditions

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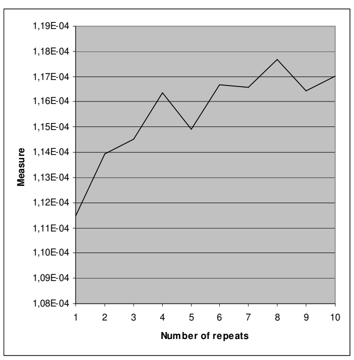

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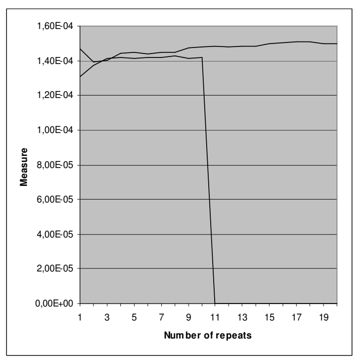

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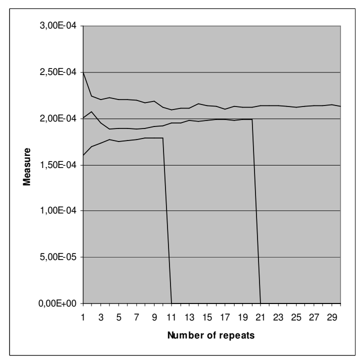

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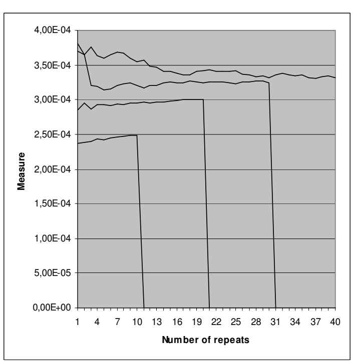

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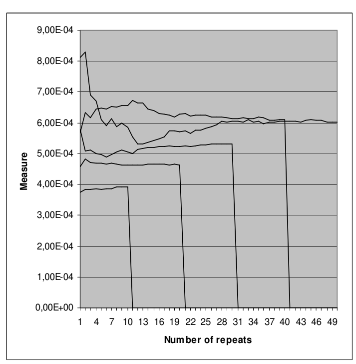

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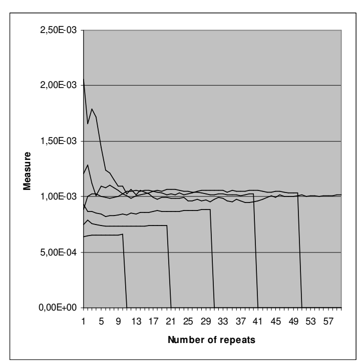

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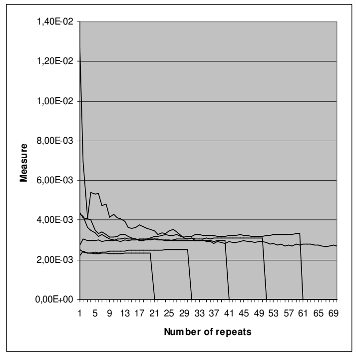

8.Mirror boundary conditions

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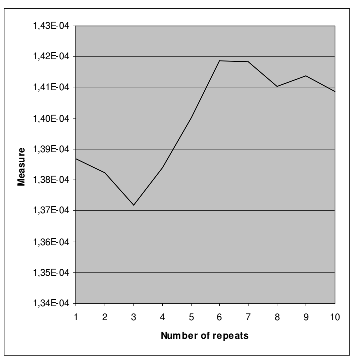

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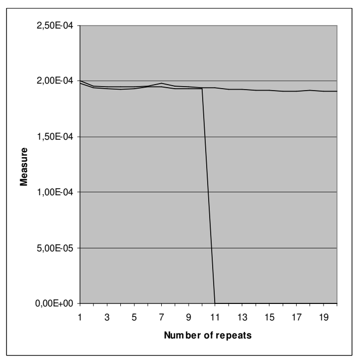

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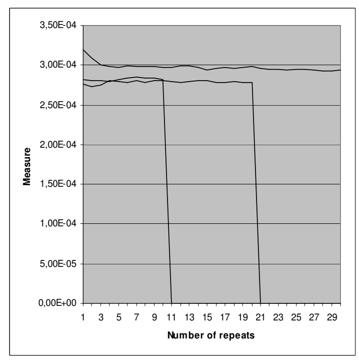

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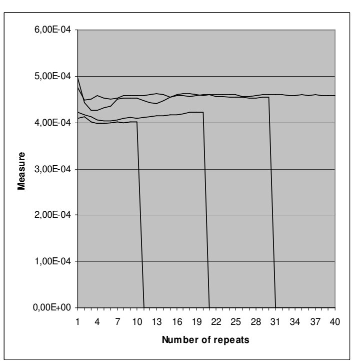

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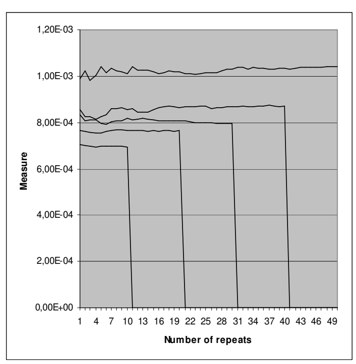

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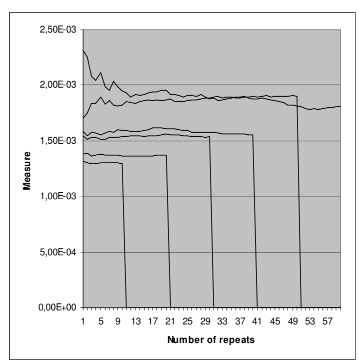

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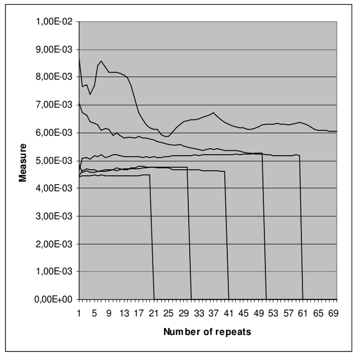

9.Comparison of periodic boundary conditions with others

In previous section statistical characteristics for different boundary conditions were compared. In this section the two-point probability functions with periodic, mirror and plain boundary conditions derived from one bitmap are shown. The difference between different boundary conditions presented, too. The difference is provided in a absolute value, since it is confusing to show negative and positive values with just one color. The two point probability functions are shown in first quadrant. The enormous computational demand associated with an exact evaluation of the function in every point is the main reason for this simplification.

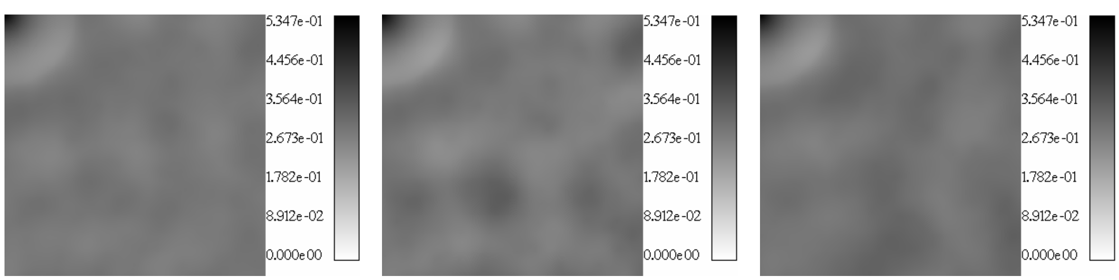

Figure 2: a) Two point probability function with periodic boundary conditions.

b) Two point probability function with plain boundary conditions.

c) Two point probability function with mirror boundary conditions

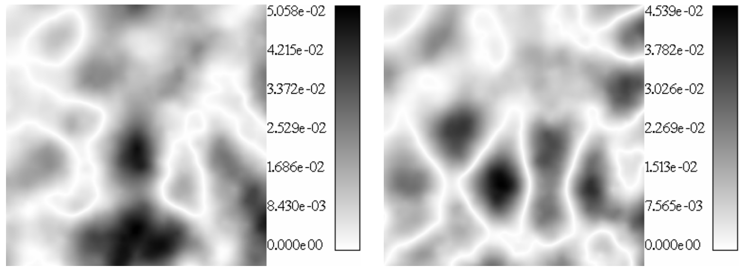

Figure 3: a) Comparison of periodic and mirror boundary conditions.

b) Comparison of periodic and plain boundary conditions.

10.Conclusions

It is obvious from graphs that all boundary conditions can be considered as equal. The measure used for comparison is almost the same and behaves in a similar manner. The suggested measure cannot fully contain the difference between functions set at different resolutions of bitmaps. The reason is explained in the next paragraph at parable.

The two point probability function behaves little bit like surface of water in pond after being hit by stone in the middle of the pond. If stones of different shapes, but quite similar size are thrown in pond, the waves close to place of hit are quite different but in a farther distance from the place of hits the waves are small. If the wave is small, the difference is small too. If the observer is monitoring just small area of the surface close to the place of hit, he will see that the differences between shapes of waves made by stones of different shapes are bigger than if he monitors larger area. The results from this research are same. The average values of measure are always smaller if determined from functions computed for large bitmaps.

It is shown that the difference between periodic and plain or mirror boundary conditions are random and do not follow any regular pattern. Recall that the more important values of the two-point probability functions are close to the origin. The origin of graphs displayed in this work is in the left upper corner. All graphs look to be very similar in this area and even the differences are close to zero (are bright) in this part.

Providing no boundary condition is superior to the other the only objective then remains the speed of evaluation. The periodic boundary conditions can be determined with the use of Fast Fourier transform, which is significantly faster than the classic Monte-Carlo method. The largest bitmaps in this work have resolution about 1000 x 1000pixels. FFTM is approximately 125 000 times faster than MCM for these dimensions. In particular, when using FFTM the evaluation lasted two minutes, while with MCM it would have taken almost half a year.

The speed of evaluation with use of Monte-Carlo method is heavily influenced by the dimensions of input bitmap. Out of the measures M it follows that it is faster to use a set of smaller sections of the largest bitmap. The results of one big bitmap and set of sections are comparable but the result for one big bitmap is nevertheless more accurate. Due to the Fast Fourier method small time consumption I generally recommend to use this method on the largest bitmap, because it is still very simple.