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Discrete mean square approximation applied to error calculation in biomolecules and brownian motion

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Advanced research frontiers are extended from biophysics relations on the Earth upto the discovering any type of alive matter within the whole space. Microorganisms' motion within the molecular biology processes integrates variety of microorgnisms functions. In continuation of our Brownian motion phenomena research, we consistently build molecular-microorganisms structures hierarchy. We recognize everywhere biomimetic similarities between the particles in alive and nonalive matter. The research data are based on real experiments, without external energy impulses. So, we develop the analysis, inspired by fractal nature Brownian motion, as recognized joint parameter between particles in alive and nonalive biophysical systems. This is also in line with advance trends in hybrid submicroelectronic integrations. The important innovation in this paper is that we introduced approximation of trajectory and error calculations, using discrete mean square approximation, what cumulatively provide much more precise biophysical systems parameters. By this paper, we continue to generate new knowledge in direction to get complex relations between the particles clusters in biophysical systems condensed matter.

Keywords: Microorganisms; biomolecules; Brownian motion; fractals; approximation; error.

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1. Introduction

The subject of molecular biology is morphological structures and functional processes in living organisms at the molecular and submolecular level; thus, phenomena like electron and molecular motion belong within its scope. On the other hand, these phenomena are the subject of microelectronic and bioelectronic science; therefore, they can be observed and examined from various aspects, in order to compile the results and provide biophysical systems further integration. It is very important to predict and control physical systems' particles motion from the aspect of further miniaturization and integration, and we can obtain significant data by this multidisciplinary approach.

Nowadays, alive and nonalive matter structures' integration is one of the major issues in advanced complex materials and technologies' scientific research because it provides the possibility for higher level integrations. If we take into consideration the fact that the electrons, atoms and molecules are constituents of both alive and nonalive matter systems, we can approach this subject from the biomimetic aspect. It implies joint examination of biosystems' and condensed matter systems' micro and submicroparticles, based on the fractal nature of their Brownian motion.[1,2]

The insight into the electron motion could be obtained indirectly by examining the molecular and bacterial motion, because molecules "carry" electrons, and bacteria "carry" molecules with them. These electron transport processes are the same, regardless of molecules as constituents of physical systems, or biomolecules, which underlines the molecule as the central factor. Also, due to bacterial size and motion behavior regarding Brownian motion, they can be observed in relation with condensed matter systems particles in order to connect these two systems, which is our goal.

The final aim of our research is the mathematical characterization of molecular and microorganisms' motion, with Brownian motion fractal nature similarities as their joint motion characteristic. Our intention is to define the relation between the particles, which leads to defining the relation between biophysical systems as well.[3–7]

2. Experimental Methods and Procedures

Bacterial trajectories are random and unpredictable, and they can be influenced by different factors, such as temperature, light, pH, etc. In our experimental research, we examined the influence of various energetic impulses on bacterial motion,[8] in order to obtain significant data regarding bacterial Brownian motion, which we used for further mathematical processing. We introduced two bacterial species (*Staphylococcus aureus* and *Pseudomonas aeruginosa*) into a liquid phase (see Fig. 1), and observed their motion patterns. In our theoretical experiment, we studied the molecular motion, according to available, previously published data.[2,8]

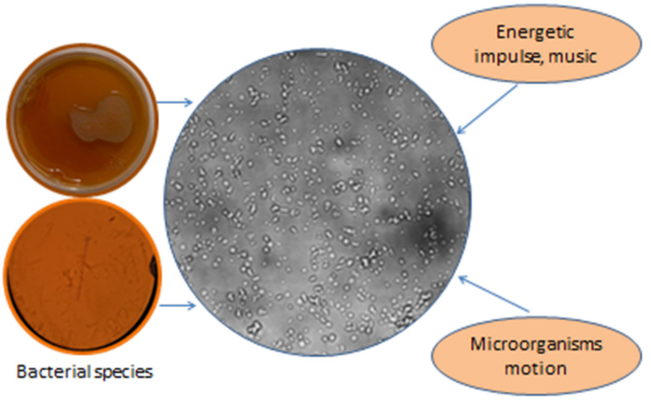

Fig. 1. (Color online) Schematic presentation of the microorganisms' motion experiment.

We obtained some interesting results regarding both the bacterial and molecular motion, and we used them for creating mathematical analytical forms, with the idea to connect electrons and microorganisms' motion via molecular level.[9]

2.1. *Mathematical background*

The relationship between several quantities is a very good mathematical model for describing some dependencies. If we consider one of them as dependent variable (we will denote it with y) and one or more of them, as the independent variables (we can denote them with $x_1, x_2 \dots x_n$), we obtain a linear relationship between the dependent variable and independent variables, as a model in the form

$$y = a_1x_1 + a_2x_2 + \cdots + a_nx_n + b,$$

where $a_1, a_2 \dots a_n, b$ are real (or complex) numbers. If the value of the variable y depends only on one independent variable x, then previous formula has a form

$$y = ax + b.$$

We can use various numerical approximation methods in order to obtain such a formula. One of very useful approximation models is the mean square approximation. The mean squares method (also called discrete mean square approximation[10]) belongs to the class of, so-called, best approximations. In this approximation method, the criterion is the minimization of the error according to some of the norms. Specifically, in this research, we will use the norm L^2, i.e., minimization of the total sum of the squares of the errors in the approximation nodes.[10,11] There are various applications of this method. Some of the them are given in Refs. 12–14.

If we decide to use more precise formula, more precise minimization of the error, and better results in application of obtained formula, we can use approximation

formulas with higher degrees and with more independent variables

$$y = a_{00} + \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij} x_i^j \right).$$

Those formulas could be even more complex

$$y = a_{00} + \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij} x_i^j \right) + \sum_{i=1}^{m-1} \left(\sum_{k=1}^{n} \left(\sum_{j=i+1}^{m} \left(\sum_{l=1}^{n} a_{ikjl} x_i^k x_j^l \right) \right) \right).$$

Using approximation formula of higher order, we can get better precision and accuracy.

2.2. *Main results*

For analysis of the data in Table 1, which describes the coordinates of bacteria locations, during movement through coordinate system,[8] we applied our technique.

Table 1. Bacteria location coordinates.

i	x_i	y_i	z_i
1	0	0	0
2	0.1043	−0.3698	−0.2869
3	0.0521	−0.4622	−0.3641
4	0.0521	−0.2773	−0.4809
5	0.0521	−0.2773	−0.7842
6	0.0521	−0.1849	−0.7605
7	0.1564	−0.5547	−0.7709
8	0.2607	−0.7396	−0.7757
9	0.5213	−0.7396	−1.0163
10	0.4170	−0.8320	−0.9330
11	0.3649	−0.8320	−0.9349

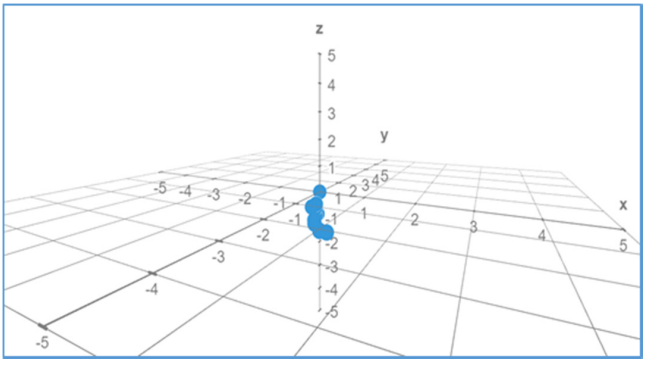

Fig. 2. (Color online) The points of the bacteria locations in 3D.

Table 2. Molecule location coordinates.

i	x_i	y_i	z_i
1	2	5.8	4
2	2.2	2	4.2
3	2.5	4.4	4.5
4	2.8	3.2	5.2

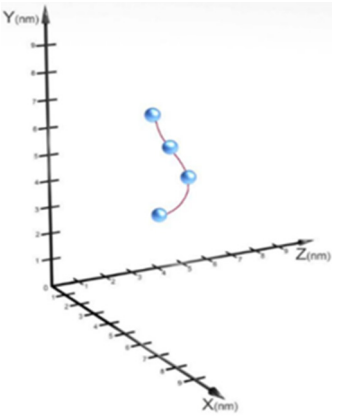

Fig. 3. (Color online) 3D diagram of molecule motion in different time intervals.

Based on the data from Table 1, we obtained the 3D diagram presented in Fig. 2. Next, we considered four molecule location points in 3D given in Table 2 and presented in Fig. 3.

2.3. *Results and discussion — linear fit*

In this section, we applied multiple linear regression to determine the mutual dependence of the coordinates and to obtain explicit formula for predicting and calculating positions. Based on the data from Table 1, we will apply the procedure of forming an approximation function

$$\varphi(x, y) = ax + by + c,$$

by using the least squares method. Thus, by applying the least square approximation on the given data sets, we obtained next results considering the best linear fit for the presented model: the coefficients of the resulting linear function are respectfully $a = -0.746871$, $b = -0.421536$ and $c = -0.3306160$ and the estimated regression function is of the form

$$\varphi(x, y) = -0.746871x - 0.421536y - 0.306160.$$

We can compare values and precision of dependent variables $\mathbf{z_i}$ in given points and results obtained by formula through the absolute and relative error (Table 3).

Table 3. Comparison between real and approximate coordinates, absolute and relative error.

x_i	y_i	z_i	φ_i	Δ	%
0	0	0	−0.3061600	0.3061600	
0.1043	−0.3698	−0.2869	−0.5399426	0.2530427	−88.20%
0.0521	−0.4622	−0.3641	−0.5399059	0.1758059	−48.29%
0.0521	−0.2773	−0.4809	−0.4619639	0.0189361	−3.94%
0.0521	−0.2773	−0.7842	−0.4619639	0.3222361	−41.09%
0.0521	−0.1849	−0.7605	−0.4230139	0.3374860	−44.38%
0.1564	−0.5547	−0.7709	−0.6567966	0.1141034	−14.80%
0.2607	−0.7396	−0.7757	−0.8126373	0.0369373	−4.76%
0.5213	−0.7396	−1.0163	−1.0072718	0.0090281	−0.89%
0.4170	−0.8320	−0.9330	−0.9683232	0.0353232	−3.79%
0.3649	−0.8320	−0.9349	−0.9294112	0.0054888	−0.59%

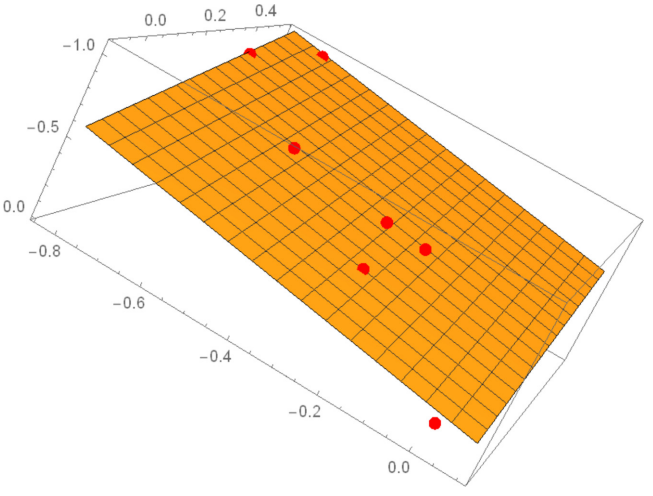

Fig. 4. (Color online) The approximation plot with marked red points from Table 3.

The plot obtained with the least squares method is presented in Fig. 4.

Similarly, as in previous procedure applied on bacterial motion experimental data, we obtained next results for molecule motion in different time intervals, considering the best linear fit for the presented model: the coefficients of the resulting linear function are respectfully $a = 1.4685067$, $b = 0.0035386$ and $c = 0.973673$ and the estimated regression function is of the form

$$\varphi = 1.4685067x + 0.0035386y + 0.973673.$$

Next, by using the estimated regression function (5) and by implementing the 2D coordinates, we obtained the estimated dependent values of the z-coordinates, presented in Table 4, together with the evaluated absolute and relative error of this approximation.

The plot obtained with the least squares method is presented in Fig. 5.

Table 4. z-coordinates with the absolute and relative error.

x_i	y_i	z_i	φ_i	Δ	%
0	0	0			
2	5.8	4	3.9312102	0.0687898	1.72%
2.2	2	4.2	4.2114649	0.0114649	0.27%
2.5	4.4	4.5	4.6605095	0.1605096	3.57%
2.8	3.2	5.2	5.0968150	0.1031850	1.98%

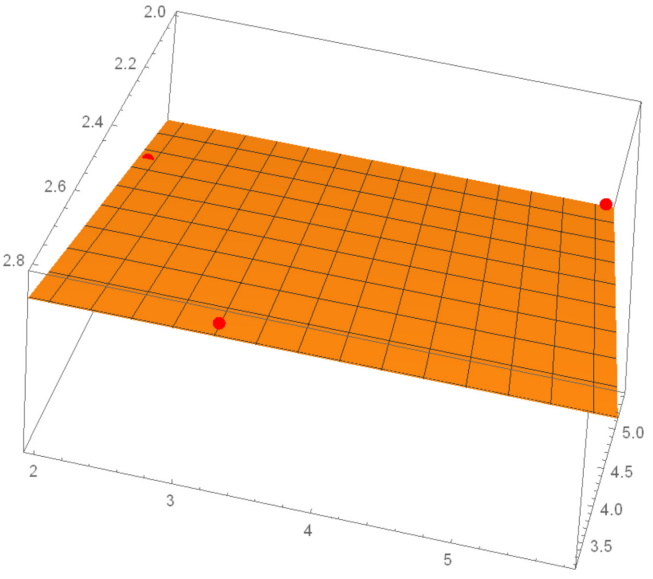

Fig. 5. (Color online) The approximation plot with marked red points from Table 4.

If we observe alive and nonalive matter particles as a hierarchical phenomenon, we can consider an atom as a cluster of electrons and other particles. Next, we can consider a molecule as a cluster of atoms with already mentioned particles, which are penetrating each other from their orbitals in interatomic relations within the molecule.[15] Finally, in this hierarchy, a microorganism could be considered as a cluster of molecules. Nowadays, fundamental research and science do not have high-tech and also resolution possibilities to recognize separately the electron motion. We can consider only the indirect effects. Here, we must stress the complexity in the matter based on quantum mechanical principles and Heisenberg uncertainty principle, as well, in all of these considerations.

Each bacterial cell comprises 2–4 millions of protein molecules,[16] which implies that the total number of molecules per bacterial cell is much higher. This is just one comparison. We can observe the effect of electron motion at the molecular and microorganisms' level. So definitely, the particles' motion based on Brownian motion fractals effects is the base for deeply understanding all of these processes

within the submicroscale sizes with the joint characteristic which we can nominate as "action in distance" in motion.

In this paper, we introduced two mathematical analytical forms: one for bacterial and second for molecular motion, which are characterized by Brownian motion. In that sense, we would like to establish a relation between these two mathematical analytical forms considering molecule number ratio. In this way, we could determine asymptotic approaching[17] of two mathematical functions towards fractals' biomimetical self-similarity. This is the idea for our further research.

2.4. *Results and discussion — nonlinear fit*

We applied multiple linear regression to determine the mutual dependence of the coordinates and to obtain explicit formula for predicting and calculating positions.[18,19] Based on the data from Table 1, we will apply the procedure of forming an approximation function

$$\varphi(x, y) = a + bx + cx^2 + dxy + ey + fy^2,$$

by using the least squares method. Thus, by applying the least square approximation on the given data sets, we obtained next results considering the best linear fit for the presented model: the coefficients of the resulting linear function are respectfully $a = -0.113743$, $b = 0.610584$, $c = 10.672648$, $d = 13.512006$, $e = 2.686915$, $f = 5.657841$, and the estimated regression function is of the form

$$\varphi(x, y) = -0.113743 + 0.610584x + 10.672648x^2 + 13.512006xy + 2.686915y + 5.657841y^2.$$

We can compare the values and precision of dependent variables $\mathbf{z_i}$ in given points and results obtained by formula trough the absolute and relative error (Table 5).

The plot obtained with the least squares method is presented in Fig. 6. Similarly, as in previous procedure applied on bacterial motion experimental data, we obtained

Table 5. Comparison between real and approximate coordinates, absolute and relative error.

x_i	y_i	z_i	φ_i	Δ	%
0	0	0	−0.113743	0.113743	
0.1043	−0.3698	−0.2869	−0.675016626	0.388116626	−135.28%
0.0521	−0.4622	−0.3641	−0.411553216	0.047453216	−13.03%
0.0521	−0.2773	−0.4809	−0.558194246	0.077294246	−16.07%
0.0521	−0.2773	−0.7842	−0.558194246	0.226005754	−28.82%
0.0521	−0.1849	−0.7605	−0.486506962	0.273993038	−36.03%
0.1564	−0.5547	−0.7709	−0.678978436	0.091921564	−11.92%
0.2607	−0.7396	−0.7757	−0.726859953	0.048840047	−6.30%
0.5213	−0.7396	−1.0163	−0.997072159	0.019227841	−1.89%
0.4170	−0.8320	−0.9330	−1.01020275	0.07720275	−8.27%
0.3649	−0.8320	−0.9349	−0.8910781	0.0438219	−4.69%

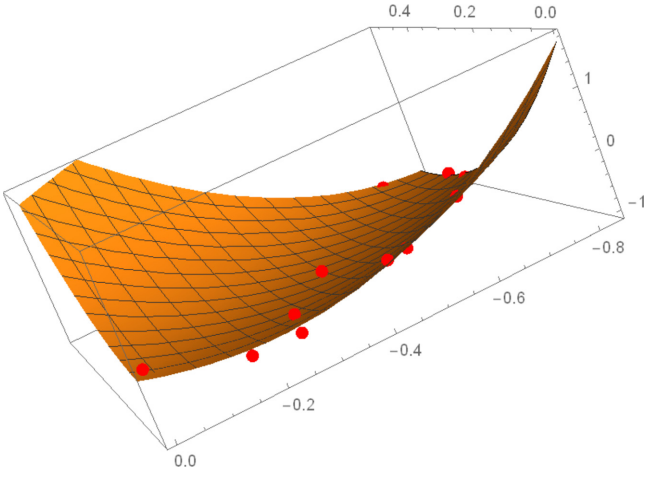

Fig. 6. (Color online) The approximation plot with marked red points from Table 5.

Table 6. z-coordinates with the absolute and relative error.

x_i	y_i	z_i	φ_i	Δ	%
0	0	0			
2	5.8	4	3.999999120	0.000000880	0.000022000%
2.2	2	4.2	4.199996920	0.000003080	0.000073333%
2.5	4.4	4.5	4.499998180	0.000001820	0.000040444%
2.8	3.2	5.2	5.199996160	0.000003840	0.000073846%

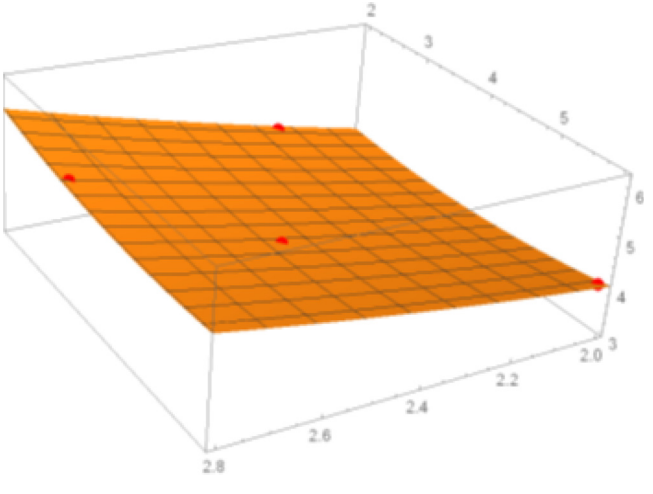

Fig. 7. (Color online) The approximation plot with marked red points from Table 6.

the next results for molecular motion in different time intervals, considering the best linear fit for the presented model: the coefficients of the resulting linear function are respectfully $a = 1.561174$, $b = 0.640807$, $c = 0.390808$, $d = 0.199523$, $e = -0.008767$ and $f = 0.058243$, and the estimated regression function is of the form

$$\varphi(x, y) = 1.561174 + 0.640807x + 0.390808x^2 - 0.199523xy - 0.008767y + 0.058243y^2.$$

Next, by using the estimated regression function (5) and by implementing the 2D coordinates, we obtained the estimated dependent values of the z-coordinates, presented in Table 6, together with the evaluated absolute and relative error of this approximation.

The plot obtained with the least squares method is presented in Fig. 7.

3. Outlook

Furthermore, we will implement similar mathematical methods of discrete mean square approximation, for linear and quadratic case, on experimental results with bacteria,[1,2] treated with energetic impulses in the frame of different musical rhythms.

4. Conclusion

In this paper, we presented experimental results for Brownian motion of n particles, for cases $n = 4$ and $n = 11$, without external influence of music. We performed discrete mean square approximation method with linear and quadratic formula, and we provided mathematical analytical expressions, that substantially characterize this motion. The main point of this paper is calculation of absolute and relative error of approximation formula in both cases. This is quite a new application and further innovative advancement in this field.

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References

1. V. V. Mitic *et al.*, *Mod. Phys. Lett. B* **35**, 2150076 (2021).
2. V. V. Mitic *et al.*, *Mod. Phys. Lett. B* **34**, 1 (2020).
3. Z. B. Vosika *et al.*, *Ferroelectrics* **531**, 38 (2018).
4. J. Mei *et al.*, *Adv. Funct. Mater.* **31**, 2100299 (2021).
5. V. V. Mitic *et al.*, *Mod. Phys. Lett. B* **34**, 2150172 (2020).
6. V. V. Mitic *et al.*, *Integr. Ferroelectr.* **212**, 135 (2020).
7. V. V. Mitić *et al.*, Biomolecules and brownian motion, *Int. Conf. IcETRAN 2021*, September 08–10, 2021 (accepted).

8. V. V. Mitic, G. Lazovic, D. Milosevic, J. Manojlovic, E. Ristanovic, D. Simeunovic, S.-C. Tsay, M. Milosevic, M. Sokovic and B. Vlahovic, Brownian motion fractal nature frontiers within the matter, in *Biocompatible and Biomimetic Features of Materials for Biomedical Applications–New Insights*, Chapter 10 (Springer, Switzerland, 2021).
9. S. Bhunia *et al.*, *J. Am. Chem. Soc.* **140**, 9444 (2018).
10. G. V. Milovanović, *Numerical Analysis II*, 3rd edn. (Naucna Knjiga, Belgrade, Serbia, 1991), VIII+210 pp.
11. G. V. Milovanović and M. A. Kovačević, *A Collection of Solutions for Problems in Numerical Analysis*, 3rd edn. (Naucna Knjiga, Belgrade, Serbia, 1991), IV+278 pp.
12. B. Ranđelović, I. Radojković and B.Gajić, *Appl. Math. Comp. Sci.* **5**, 7 (2020).
13. I. D. Radojkovic, B. Gajic and B. M. Randjelovic, *J. Econ. Social Dev.–Resilient Soc.* **8**, 2 (2021).
14. I. D. Radojkovic, B. M. Randjelovic and I. D. Ilic, *Ekonomske teme* **59**, 243 (2021).
15. S. Kruchinin and T. Pruschke, *Phys. Lett. A* **378**, 157 (2014).
16. R. Milo, *BioEssays* **35**, 1050 (2013).
17. P. Kruchinin, V. Novikov and N. N. Bogolyubov, *Int. J. Mod. Phys.* **22**, 2025 (2008).
18. S. Kruchinin, V. Klepikov and V. Novikov, *Mater. Sci.* **23**, 1009 (2005).
19. S. Kruchinin, V. Novikov and V. Klepikov, *Metrol. Meas. Syst.* **15**, 281 (2008).