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3-D modelling of fractal nanoclusters using the iterated affine transformations systems method

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Abstract— In the current work an approach for fractal nanocluster 3-D modelling is proposed using the iterated affine transformations system method. The symmetry of regular polyhedra concept is applied. It is shown that the models can be used to interpret experimental results.

Keywords— fractal, nanocluter, symmetry, polyhera, modelling, iterated affine transformations

I. Introduction

THE concept of reflection, turn and translation symmetries is widely used in crystallography to describe the formation principles of crystals [1,2]. However, nanosystems do not conform with Euclidean geometry's principles and often form a variety non-Euclidean structures, including fractal structures with adaptive and biogenic properties [3-5]. These structures may seem chaotic, however it was found that the addition of components such as CNTs into a dispersed system can modify the morphology and properties of the resulting hybrid system without affecting the chemical composition [6,7]. Nowadays there is no universal method to describe such complex systems, which could characterize their symmetrical transformations combined with chaotic quality.

II. METHOD

A new 3-D modeling method based on the iterated affine systems algorithm [8,9] is proposed to describe the morphology of fractal nanosystems. The choice of the symmetry is of primary importance for the fractal formation, thus by defining the relative spacial arrangement of the contracting affine reflections of a primary space it is possible to create a kernel cluster that will define the symmetry of the resulting dot fractal structure.

For instance, to describe the morphology of a GaSb [10,11] cluster with an icosahedral fractal symmetry [3,12] 12 reflections of a singular cube in Cartesian space are placed in the vertices of an icosahedron and one additional reflection is placed in the middle denoting a central cluster (Fig. 1). Each of the reflections have a primarily defined contraction ratio. The used system of affine transformation matrixes is the following:

$$T_1\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.333 \\ 0.333 \\ 0.333 \end{bmatrix}$$

$$T_2\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.333 \\ 0.475 \\ 0.421 \end{bmatrix}$$

$$T_3\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.333 \\ 0.475 \\ 0.246 \end{bmatrix}$$

$$T_4\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.333 \\ 0.192 \\ 0.421 \end{bmatrix}$$

$$T_5\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.333 \\ 0.192 \\ 0.246 \end{bmatrix}$$

$$T_6\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.421 \\ 0.333 \\ 0.475 \end{bmatrix}$$

$$T_7\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.421 \\ 0.333 \\ 0.192 \end{bmatrix}$$

$$T_8\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.246 \\ 0.333 \\ 0.475 \end{bmatrix}$$

$$T_9\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.246 \\ 0.333 \\ 0.192 \end{bmatrix}$$

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$$T_{10}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.475 \\ 0.421 \\ 0.333 \end{bmatrix}$$

$$T_{11}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.475 \\ 0.246 \\ 0.333 \end{bmatrix}$$

$$T_{12}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.192 \\ 0.421 \\ 0.333 \end{bmatrix}$$

$$T_{13}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.333 & 0. & 0. \\ 0. & 0.333 & 0. \\ 0. & 0. & 0.333 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.192 \\ 0.246 \\ 0.333 \end{bmatrix}$$

After the kernel cluster is defined, a random point is generated inside the primary cube. The affine transformation matrix functions that were used to build the icosahedral reflections are in series randomly applied to the point's coordinates and the generated coordinates are stored in an array, which is then displayed (Fig. 2).

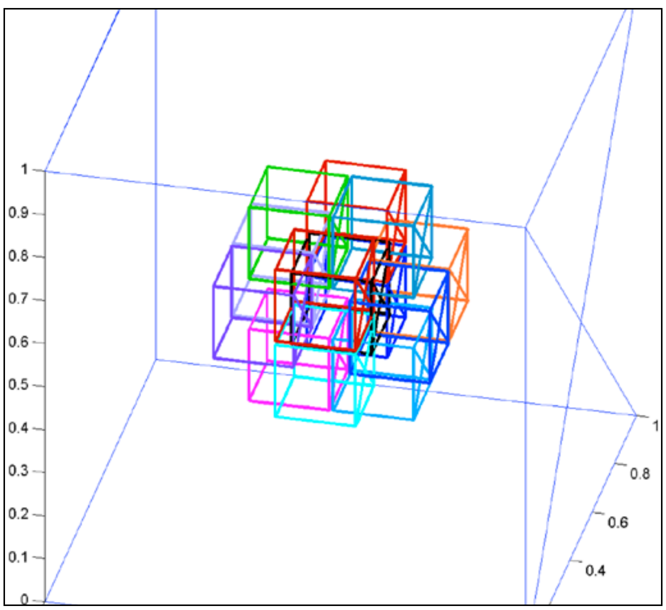

Fig. 1. The 13 affine reflections of a singular cube.

The achieved model being randomly generated has the chaotic properties of real systems. However every next generated model can not be clearly singled out due to the invariance, achieved by the large number of points.

The model conforms with the used RVE-based modelling method [13] where after generating a law for particle space occupation the space is extrapolated to larger scale levels. However, the presented model clearly describes the intrinsic symmetry of nanoclusters, conforms to their finiteness and fractal scale independency.

In [6] a CNT doped dispersed hydrated system $CaSO_4 - H_2O$ – CNT was studied where a chaotic fractal system of short CNTs turned into a symmetrical fractal system with the

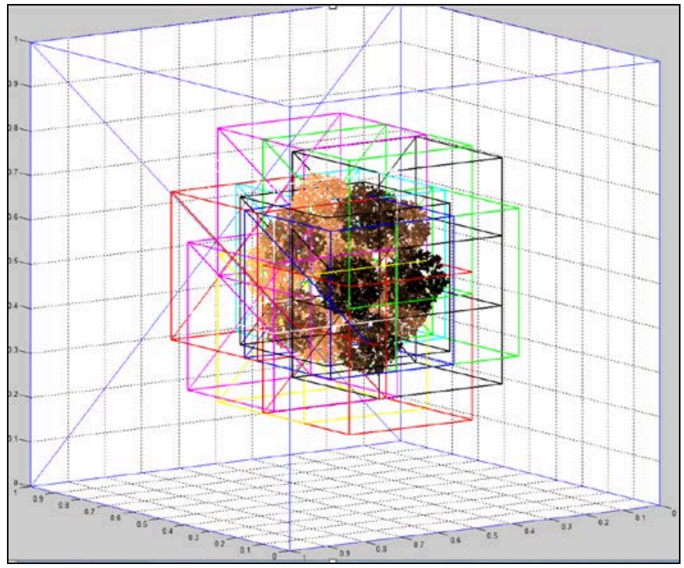
Fig. 2. The fractal dot model with an icosahedral symmetry, 30 000 dots with the corresponding affine reflections of a singular cube.

introduction of gyps. The symmetry of the resulting hybrid clusters can be described by the octahedral symmetry using the following affine transformations system

$$T_{1}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.500 & 0. & 0. \\ 0. & 0.500 & 0. \\ 0. & 0. & 0.500 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.250 \\ 0.250 \\ 0.250 \end{bmatrix}$$

$$T_{2}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.125 \\ 0.375 \\ 0.375 \end{bmatrix}$$

$$T_{3}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.375 \\ 0.625 \\ 0.375 \end{bmatrix}$$

$$T_{4}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.625 \\ 0.375 \\ 0.375 \end{bmatrix}$$

$$T_{5}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.375 \\ 0.125 \\ 0.375 \end{bmatrix}$$

$$T_{6}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.375 \\ 0.375 \\ 0.125 \end{bmatrix}$$

$$T_{7}\left(\begin{bmatrix} x \\ y \\ z \end{bmatrix}\right) = \begin{bmatrix} 0.250 & 0. & 0. \\ 0. & 0.250 & 0. \\ 0. & 0. & 0.250 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0.375 \\ 0.375 \\ 0.625 \end{bmatrix}$$

which generates the following affine reflections and resulting model (Fig. 3).

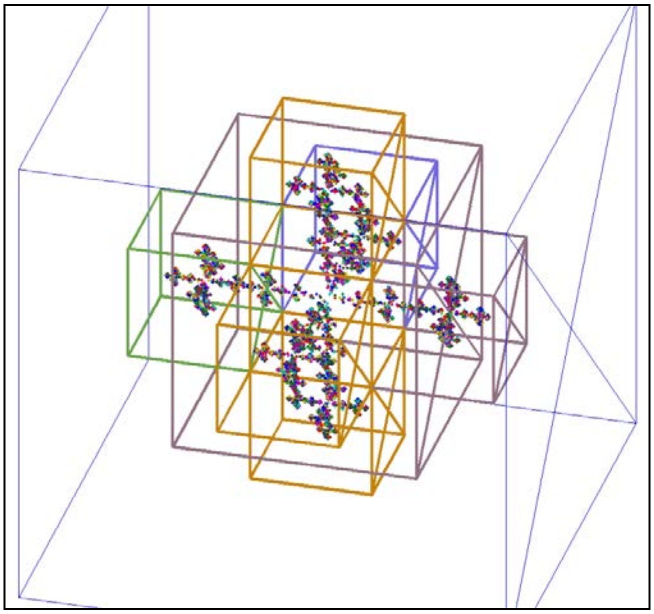

Fig. 3. The affine reflections for an octahedral symmetric system and the generated fractal dot model, 20 000 dots.

By introducing random deformations to the primary reflections the morphology of the resulting cluster is also affected (Fig. 4, 5).

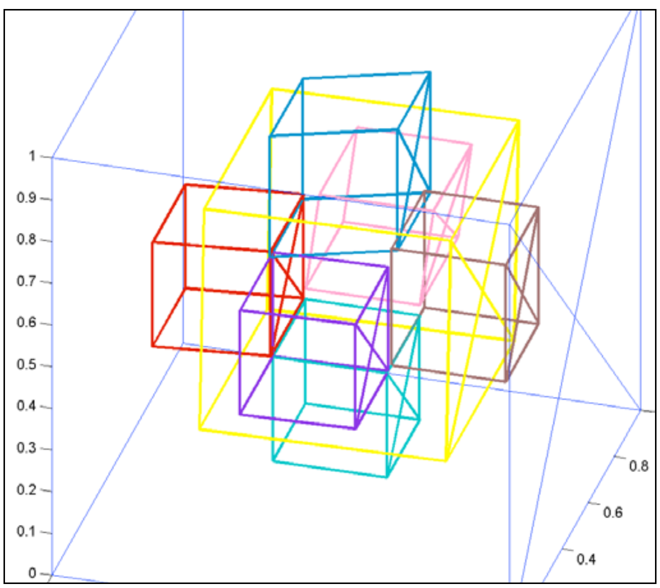

Fig. 4. An octahedral symmetrical model. The randomly modified affine reflections of a singular cube.

III. Conclusion

The obtained symmetrical objects qualitatively better represent real structures, keeping the chaotic properties of natural objects, that are not represented in purely deterministic fractal models. The further development of the method can show the importance of the regular polyhedra symmetries for the formation of nanoclusters. The method is capable of describing fractal systems of different kinds and could be used for fractal nanosystems' symmetry characterization.

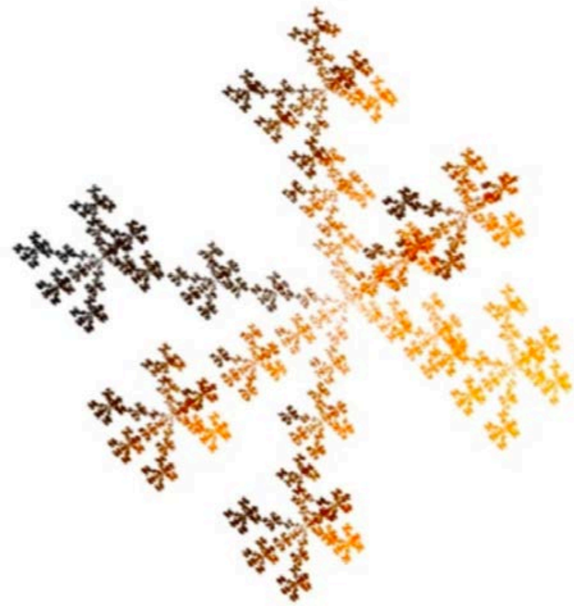

Fig. 5. The 3-D dot symmetrical octahedral model generated with minor random modifications to the affine transformations system.

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