



Topic: Evolutionary optimization for creation of new molecule structures

Speaker: Prof. Pavel Ošmera
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Date: 22 November 2013, Friday

Time: 2.00pm to 3.00pm

Venue: EA-06-02 (map of NUS can be found at <http://map.nus.edu.sg/>)

Host: Prof T.T.Lim

Abstract

We tried to combine the basic principle of grammatical evolution with vortex-ring-fractal structures of atoms to create new molecule structures. This approach combines knowledge of evolutionary optimization with physical chemistry.

We use a new method of grammatical evolution that is named Transplant Evolution (TE). The transplant evolution is the two-level Grammar-Differential Evolution of Object Sub-trees, which is created by linking the grammatical and differential evolution together, whose individual is represented by the form of an object tree structure without the genotype. The individual in TE only generates phenotype without saving the genotype. This approach allows dynamically change the production rules without losing already generated phenotype of the individual, further use an appropriate method of reducing the tree structure of the object, e.g. using algebraic operations. In consequence of advantages of TE it was possible to create a new method of crossover, called the method of crossover by linking of sub-trees. This method is suitable for creation of new molecule structures.

Allotropy is the property of some chemical elements to exist in two or more different forms, known as allotropes of these elements. Allotropes are different structural modifications of an element; the atoms of the element are bonded together in a different manner. For example, the allotropes of carbon include diamond (where the carbon atoms are bonded together in a tetrahedral lattice arrangement), graphite (where the carbon atoms are bonded together in sheets of a hexagonal lattice), graphene (single sheets of graphite), and fullerenes (where the carbon atoms are bonded together in spherical, tubular, or ellipsoidal formations).

The carbon atom consists of two parts (every part has 3 protons and 3 neutrons). A plane arrangement of electrons in the graphene has all electrons above the structure with parallel axes. These electrons have no gyroscopic problem with movement in the plane that is parallel with the plane of the graphene. It explains high mobility of these electrons and high conductivity of the graphene. For testing this approach will be available demo version of TE on [1].

[1] Ošmera P.: <http://www.pavelosmera.cz>

About the Speaker

Prof. Pavel Ošmera, is currently a professor in the Institute of Automation and Computer science, Brno University of Technology, Czech Republic. His research interests include Vortex-fractal-ring structures, Fractal-ring model of the electron, Vortex structure of light, Automatic generation of programme, Evolutionary Optimization and soft computing.

Admission is free. All are welcome to attend.