## NANOSCIENCE AND NANOTECHNOLOGY

## Theory and modelling of real-time physical and bio- nanosensor systems

Yu Shunin, D Fink, A Kiv, L Alfonta, A Mansharipova, R Muhamediyev, Yu Zhukovskii, T Lobanova-Shunina, N Burlutskaya, V Gopeyenko, S Bellucci

## Computer Modelling & New Technologies 2016 20(4) 7-17

Our research pursues two important directions of real-time control nanosystems addressed to ecological monitoring and medical applications. We develop physical nanosensors (pressure and temperature) based on functionalized CNTs and GNRs nanostructures. The model of nanocomposite materials based on carbon nanocluster suspension in dielectric polymer environments (epoxy resins) is regarded as a disordered system of fragments of nanocarbon inclusions with different morphologies. Using the effective media cluster approach, disordered systems theory and conductivity mechanisms analysis we have formulated the approach of conductivity calculations for carbon-based polymer nanocomposites and obtained the calibration dependences. We also develop bio-nanosensors based on polymer nanotracks with various enzymes, which provide the corresponding biocatalytic reactions and give reliably controlled ion currents. Particularly, we describe a glucose biosensor based on the enzyme glucose oxidase (GOx) covalently linked to nanopores of etched nuclear track membranes. Using simulation of chemical kinetics glucose oxidation with GOx, we have obtained theoretical calibration dependences. Our objective is to demonstrate the implementation of advanced simulation models providing a proper description of electric responses in nanosensoring systems suitable for real time control nanosystems. Comparisons with experimental calibration dependences are discussed. Prospective ways of developing the proposed physical and bio- nanosensor models and prototypes are considered.

Keywords: real-time nanosensors, functionalized nanocomposites, physical nanosensors bionanosensors

#### INFORMATION AND COMPUTER TECHNOLOGIES

## Development of the augmented reality applications based on ontologies

Yersain Chinibayev, Tolganay Temirbolatova

Computer Modelling & New Technologies 2016 20(4) 18-22

This article presents an analysis of the existing popular libraries for the development of augmented reality applications. Based on the analysis we propose a universal technology of construction of augmented reality applications using ontology. The technology is based on the geolocation using GPS and communicates with the resource through Linked Open Data.

Keywords: Augmented reality, ontological modelling, ontological engineering, Linked Open Data

## Comparison of Cuckoo Search, Tabu Search and TS-Simplex algorithms for unconstrained global optimization

Ghania Khensous, Belhadri Messabih, Abdellah Chouarfia, Bernard Maigret

Computer Modelling & New Technologies 2016 20(4) 23-29

Metaheuristics Algorithms are widely recognized as one of the most practical approaches for Global Optimization Problems. This paper presents a comparison between two metaheuristics to optimize a set of eight standard benchmark functions. Among the most representative single solution metaheuristics, we selected Tabu Search Algorithm (TSA), to compare with a novel population-based metaheuristic: Cuckoo Search Algorithm (CSA). Empirical results reveal that the problem solving success of the TSA was better than the CSA. However, the run-time complexity for acquiring global minimizer by the Cuckoo Search was generally smaller than the Tabu Search. Besides, the hybrid TSA-Simplex Algorithm gave superior results in term of efficiency and run-time complexity compared to CSA or TSA tested alone.

Keywords: Metaheuristic Algorithms, CSA, TSA, Global Optimization, Nature Inspired Algorithms

## Handwritten offline Hindi character recognition using advanced feature extraction techniques

Dayashankar Singh, J P Saini, D S Chauhan

Computer Modelling & New Technologies 2016 20(4) 30-36

Feature extraction technique plays an important role in character recognition since last so many years. In this paper, two advanced feature extraction techniques namely 16-Directional Gradient Feature Extraction Technique (16-DGFET) and 24-Directional Gradient Feature Extraction Technique (24- DGFET) have been proposed and implemented. This paper demonstrates the concept of Handwritten Hindi Character Recognition (HCR), feature extraction mechanisms adopted for character recognition starting from Conventional Feature Extraction Technique (CFET), Gradient Feature Extraction Technique (GFET), and Directional Gradient Feature Extraction Technique (DGFET). In DGFET, few techniques have been initiated which involve dividing the gradient values to 8/16 directional values, these techniques attained recognition accuracy of around 94%. We have aimed at further splitting of the gradient values in 24 parts in order to find if it achieves the objective of increasing the performance of character recognition with more accurate analysis and acceptable training time. An experimental evaluation and comparative analysis have been made at the end of the paper to prove the result whether further splitting is providing a better result in comparison to 8 or 16 parts division taking in account the training time, the accuracy of recognition and performance appraisal. The network used here is Multilayer Perceptron (MLP) with Error Back Propagation (EBP) algorithm to train the network.

A sample of count 1000 has been taken for experimentation including the personnel of different age groups involving both male and female handwriting. A comparative synthesis is made for 8/16-Directional and 24-Directional input values comparing the recognition

performance and training time.

*Keywords:* Pattern Recognition, Hindi Character Recognition, Gradient Feature Extraction Technique (GFET), Directional Gradient Feature Extraction (DGFET), Multilayer Perceptron (MLP), Error Back Propagation (EBP)

### MATHEMATICAL AND COMPUTER MODELLING

## Modelling of non-point source pollution transport for the Charyn River Basin

Jalal K Jamalov, Daniyar B Nurseitov, Kairat A Bostanbekov Computer Modelling & New Technologies 2016 20(4) 37-43

The results of pollution transport simulation for the Charyn river (the Republic of Kazakhstan, Central Asia) obtained using software package BASINS 4.1 are shown in this article [1]. Modules created in the process of the study as well as the method of adaptation of the model of pollution transport are described. The calculations include the modeling of the hydrology of the river basin and the calculation of the concentration of non-point sources of pollution. The comparison with the data of natural hydrological observation post.

Keywords: Simulation, BASINS, Watershed Delineation, HSPF, pollution transport in water, BOD, nitrate, dissolved oxygen

# Performance evaluation of computer-aided knit design using software package based on ontological knowledge model

#### O Kochetkova, A Kaznacheeva, A Kochetkov

Computer Modelling & New Technologies 2016 20(4) 44-47

The article represents the original approach to computer-aided warp knit fabrics on the base of universal algorithms and modern methodology which allows to apply the methods of projecting with the given technologies. The ontological approach is represented for development and improvement of knowledge model which provides the description of object domain of computer-aided warp knit fabrics and its formalized presentation. The elaborated software allows to perform fully the proceedings of art and technological and parametric projecting of warp knit fabrics. The performance evaluation of computer-aided warp knit fabrics on the basis of algorithmical and ontological approach is elaborated. To solve this problem we used the method of hierarchy analysis of Thomas Saati. The results of the evaluation represent that software grounded on ontological approach in totality of functional means is more effective than CAD on the base of algorithmical approach.

Keywords: warp knit fabrics, ontological approach, knowledge model, program-methodical package

#### Effect of texture on mechanical and magnetic properties of steel from the petroleum distillation column

E Dragomeretskaya

Computer Modelling & New Technologies 2016 20(4) 48-51

Texture, mechanical properties and coercive force of steel 09G2S from the column fragment of petroleum distillation after prolonged use studied. Anisotropy of mechanical properties and coercive force take place. Significant pair wise linear correlations and appropriate regression equations with coefficients reliability of approximation not less than 0.90 were found between magnitudes of the coercive force, tensile strength, yield strength, elongation and texture characteristics. Found correlations may be used for non-destructive mechanical properties control of investigated steel by means of monitoring of coercive force.

Keywords: Texture, anisotropy, mechanical properties, coercive force, correlation