Name: Kalyan Basu
Chief Scientist, CarlBio
Cellular Automata Research Lab
URL: www.CarlBio.org
E-mail: kalyanbasu12@msn.com

Research Interest:

1. Research on development of computational tools for Structured Drug Discovery [1]. We are working on Cellular Automata (CA) [2] based Transform Domain algorithms to determine the 2D and 3D protein structures and discovery of protein-Ligand binding sites for pre-screening of drug molecules. The current state of the art on this research is homologue based algorithms [3] to map the structure from existing database of the known proteins in combination with force field simulation and rigid body geometrical modeling technique for protein-protein docking. Currently researchers submit their algorithms for CASP evaluation to test the accuracy for an unknown primary sequence. The present algorithms are highly computation intensive and require super computers to compute the 3D structure. Also proteins, those are not suitable for crystallography (e.g. membrane proteins) is difficult to handle in the current modeling technique because few matching sequences are found in PDB. Most of the protein that bind to drug molecules are membrane proteins, as a result the effectiveness of these algorithms are limited in Structured Drug Discovery. Moreover as these algorithms work on physical domain, as a result the complexity is overwhelming. We transform the primary Amino Acid Chain of a protein molecule into a CA machine and try to derive the physical characteristics of the protein molecule from the dynamic properties of the CA machine. Our objective is to develop a set of algorithms those are independent of availability of PDB sequence and computationally order of magnitude faster.

References:

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[3] "Computational Methods of Protein Structure Prediction and Modeling: Volume-1: Edited by Y. Xu, D. Xu and J. Liang, Springer 2007, ISBN 0-387-33319-3.

2. Research on the development of new generation of education and training software and processes by using wireless, sensors, Internet, audio, video, animation, game and virtual Lab technologies. The integrated product will be compatible to the current cognition models. The systematic use of human cognition in learning process in designing the learning product to make it compatible to the human brain is lacking today. At present models like ACT-R [1] are available for evaluating the effectiveness of the simple learning objects. In addition many concepts of cognitive loops important for learning like (i) Phonological loop for language, (ii) Visuomotor loop for learning a task like driving a car [2], (iii) Numerosity for learning numbers are available. These models are suitable to become part of modeling framework for computer evaluation. Moreover wireless devices penetration has reached to a point, when it is possible to use it as an extension of human brain for knowledge capacity. The rural education in the poor and developing countries is a challenge due to shortage of good teachers and the lack of good schools. Only way to change this situation is using technology. Because of deep penetration of wireless technology; internet based remote education and training products are now appearing in the market. The present generation of remote education products are not taking full advantage of the existing technology like search engine, collaborative learning through social network. At the same time these education products are neither designed for effectiveness and quality nor suitable for customization based on the learners' current knowledge. The customization will make the teaching effective for the learning retarded students. The research incudes effective use of sensors, wireless connections, search engine and social networks [3], [4] for developing the effective learning process suitable for multiple mode learning (on-campus, remote, trial and error, collaborative, etc.)

References

[1] "How Can the Human Mind Occur in the Physical Universe?", John R. Anderson, Oxford University Press, 2007, ISBN: 978-0-19-539895-3.

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[3] "Computer skills development by children using 'hole in the wall' facilities in rural India". P. Inamdar, (2004), Australasian Journal of Educational Technology, 20(3), pp 337-350.

[4] "Can kids teach themselves?", Sugata Mitra, www.youtube.com/watch?v=xRb7_ffl2D0