Biomedicine @ CRS4

04.05.2011 - 11:00

Sardegna Ricerche - Sala Conferenze (Building 2)

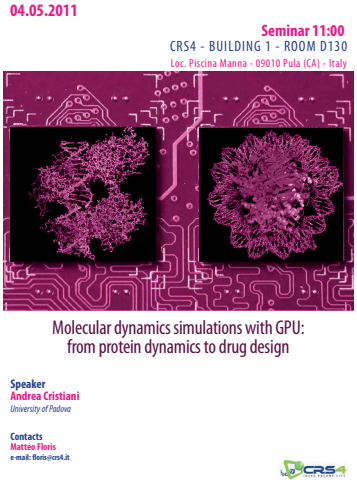
SEMINAR: ***Molecular dynamics simulations with GPU: from protein dynamics to drug design***

SPEAKER: Andrea Cristiani, *Université de Genève - University of Padova.*

ABSTRACT:

The exploration at the molecular level of the conformational changes of a protein can help to elucidate and explain its functionality. This knowledge is tremendously important for a successful drug design. Molecular Dynamics is a high-computing resource demanding technique largely used to explore the conformational space of molecular objects. Nowadays, the introduction of Graphics Processing Unit (GPU) as High Performance Computing tools allows to much larger conformational spaces compared to the traditional CPUs.
We present two multidisciplinary kinase studies [1] where the use of molecular dynamics coupled to the speed of GPU permit the achievement of a fast and accurate convergency in the results. ClickMD [2], an integrated web-oriented platform for processing and analyzing the time dependent behaviour of a bio-molecular system in a molecular dynamic workflow, will also be presented.

1. A. Cristiani, G. Costa, G. Cozza, F. Meggio, L. Scapozza and S. Moro, "The Role of the N-Terminal Domain in the Regulation of the 'Constitutively Active' Conformation of Protein Kinase CK2α: New Insight from a Molecular Dynamics Investigation" ChemMedChem, 2011, 10.1002/cmdc.201100046.
2. A. Cristiani, N. Brisotto, F. Chatwin Cedrati, M. Floris, L.Scapozza, S. Moro, "ClickMD : an Intuitive Web-Oriented Molecular Dynamics Platform", Future Medicinal Chemisty, 2011, accepted.



BIOGRAPHY :

Andrea Cristiani obtained his M.Sc degree in Medicinal Chemistry at the University of Padova. He was teaching assistant in the laboratory of Organic Chemistry Synthesis at the School of Pharmacy at the University of Geneva.

He is approaching the end of his PhD in Computational Medicinal Chemistry both at the University of Geneva and at the Molecular Modeling Session Lab at the University of Padova. He is system manager of the computational section of the Pharmaceutical Biochemistry Group of EPGL and system manager of the MMS Lab at the University of Padova.

He has working experience as external scientific collaborator with: Nestlé Research Center, The Genetics Company, EOS. He is interested in macro molecular dynamic simulation and drug design. He was selected as start-up project manager in the Venture Challenge Class at Venture Lab 2010.

KEYWORDS:

GPU, parallel computing, molecular dynamics, kinase, protein plasticity, interdisciplinarity

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