Research Center for Scientific Simulations

Introduction

The Research Centre for Scientific Simulations (RCSS) is part of the "Network of Research Supporting Laboratories" at the University of Ioannina. The mission statement of the Centre is to provide computer time for running large scale parallel simulations. The basic infrastructure of the Centre was installed in December 2006, in the framework of the project "*Development of the Research Centre for Scientific Simulations*" and was financed by the Region of Epirus. The system is an important computational asset that contributes in research and educational activities carried out at the University Ioannina.

Facilities & Infrastructure

The hardware infrastructure (Figure 1) consists of 200 worker nodes, each having two (2) independent central processors AMD Opteron™ 248 2.2 GHZ. Consequently, the total number of available processors is four hundred (400). Each worker node includes 4GB ECC memory, 80GB local disk and two 1Gbps network ports. The worker nodes are interconnected by a high capacity (>380Gbps) ethernet switch. Central storage for the applications is provided by a disk array (raid 5) over NFS.

Figure 1: Research Centre of Scientific Simulations

The infrastructure is supported by cooling systems with capability up to 400 KBTU/h and uninterrupted power supply (UPS) with capability up to 120 KVA. Also, the installation includes a set of systems and services that monitor the operation of the infrastructure. Moreover, for handling and distributing user jobs, an appropriate resource management software is installed.

Services

The RCSS provides the opportunity for academic researchers at the University of Ioannina, to perform large scale parallel simulations in various research fields (Chemistry, Materials Science, Medicine, Mathematics, Biology, Economics, Computer Science, etc). Access to the infrastructure has been requested by 50 users, 26 of them consumed more the 1000 hours and are considered by convention as regular users. During the past three years, user applications consumed a total of 5630 Khours.

Indicatively, it is reported that during the past three year (Figure 2), the computational resources of the Centre have been used by researchers in the Departments of Chemistry, Materials Science and Engineering, Mathematics, Economics, Computer Science and the School of Medicine. In addition the Centre contributes in the training of post graduate students.

Finally, in the framework of the European project "Enabling Grids for E-sciencE" (EGEE III), part of the infrastructure was connected with the European Computational Grid (EGEE).

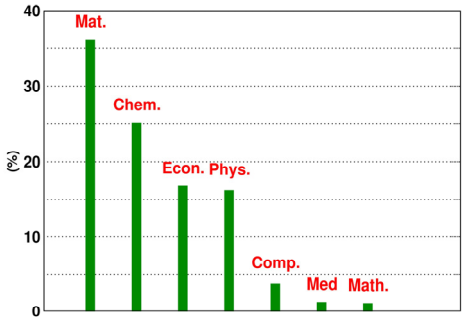

Figure 2: Indicative time distribution of RCSS's resources

Staff & Contact Information

The RCSS is supervised by a Scientific Committee composed of academic staff members from the

University of Ioannina. Information can be obtained by contacting Prof. I. Lagaris.

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Representative Publications

1. Stavrakoudis A.,"Computational modelling and molecular dynamics simulations of a cyclic peptidemimotope of the CD52 antigen complexed with CAMPATH-1H antibody", Molecular Simulation, in press, (2010).
2. Fadouloglou V.E., Stavrakoudis A., Bouriotis, V., Kokkinidis, M., Glykos, N.M., "Molecular dynamics simulations of bczbp, a deacetylase from bacillus cereus: Active site loops determine substrate accessibility and specificity" Journal of Chemical Theory and Computation", 5, 3299 (2009).
3. Stavrakoudis A.,"Conformational studies of the 313-320 and 313-332 peptide fragments derived fromthe αiIb subunit of integrin receptor with molecular dynamics simulations" International Journal of Peptide Research and Therapeutics, 15, 263 (2009).
4. A. C. Tsipis,"Upright or In-Plane Conformational Preference: Dilemma of η^2-Coordinated C=C Double Bond in $PtX_2(CO)(\eta^2$-ene) (X=H, Cl or C_6F_5) Complexes",Organometallics 27, 3701 (2008).
5. A. T. Chaviara, E. E. Kioseoglou, A. A. Pantazaki, A. C. Tsipis, P. A. Karipidis, D. A. Kyriakidis, C. A. Bolos, "DNA interaction studies and evaluation of biological activity of homo- and hetero-trihalide mononuclear Cu(II) Schiff Base complexes", Quantitative structure-activity relationships J. Inorg. Biochem. 102, 1749 (2008).
6. K. Christopoulos, K. Karidi, A. C. Tsipis and A. Garoufis,"Synthesis, characterization, DNA-binding properties and electronic structure (DFT) of Ruthenium oligopyridine complexes", Inorganic Chemistry Communications 11, 1341 (2008)
7. E. Lidorikis and A.C. Ferrari, "Photonics with Multi-Wall Carbon NanotubeArrays", ACS Nano 3, 1238 (2009).
8. M. Guffey, E. Lidorikis, X.-M. Lin, J.D. Joannopoulos and N.F. Scherer, "Plasmon Delocalization in Au Nanoparticle Monolayer Arrays Established by Optical Experiments and Simulation", to be submitted Journal of Physical Chemistry C.
9. S. Egusa, E. Lidorikis, M. Guffey, X-M. Lin, J.D. Joannopoulos, and N.F. Scherer, "Resonant transmission of coherent light through 2D metallic nanocrystal arrays", to be submitted in Phys. Rev. B.
10. D.A. Kilimis, D.G. Papageorgiou, "Density functional study of small bimetallic Ag–Pd clusters", Journal of Molecular Structure: THEOCHEM , in press, (2010).
11. D.A. Kilimis and D.G. Papageorgiou, "Structural and electronic propertiesof small bimetallic Ag–Cu clusters", Eur. Phys. J. D 56, 187 (2010).
12. C. Voglis , P.E. Hadjidoukas , I.E. Lagaris , D.G. Papageorgiou, "A numerical differentiation library exploiting parallel architectures" Computer Physics Communications, in press (2009).
13. I.G. Tsoulos and I.E.Lagaris, "GenMin: An enhanced genetic algorithm for global optimization", Computer Physics Communications 178, 843, (2008).
14. I.G. Tsoulos, I.E. Lagaris,"MinFinder v2.0: An improved version of MinFinder,Computer Physics Communications", 179, 614, (2008).
15. G. V. Papamokos , I. G. Tsoulos , I.N. Demetropoulos , E. Glavas, "Locationof Amide I mode of vibration in computed data utilizing constructed neuralnetworks", Accepted for publication in Expert Systems With Applications.
16. G.A.Almyras, Ch.E. Lekka, N. Mattern and G.A. Evangelakis, "On the microstructure of the Cu65Zr35 and Cu35Zr65 metallic glasses", Scripta Materialia 62, 33 (2010).
17. Ch. E. Lekka, Jun Ren, Sheng Meng, Efthimios Kaxiras, "Structural, electronic and optical properties of representative Cu-flavonoid complexes", Journal of Physical Chemistry B 113 (18), 6478 (2009).
18. Ch. E. Lekka, N. Panagiotopoulos, Ph. Komninou, P.Patsalas, G.A.Evangelakis, "Electronic properties and bonding characteristics of AlN:Ag Thin Film Nanocomposites; a computational and experimental study", to be submitted in Acta Materialia.