Dr. Daniel Rotimi, Registrar, Prof. James Katende, Dean, College of Science and Technology, and in-fact the entire Board of Regents are to be thanked for their support in making this event possible. The Workshop Steering Committee (Dr. Ezekiel Adebiyi, Ms. Ijeoma Dike, Mr. Conrad Omonimiyin, Dr. Wande Daramola, Mr. Oluwagbemi, Mrs. Ogunlana and Dr. Segun Fatumo) are to be thanked for the efforts invested in making this a successful and smoothly run event, the Workshop Resource Persons (Drs. Valverde, Rebai, Bewaji, Adebiyi, Osamor and Fatumo) are thanked for their labor in steering the workshop, and all participants are to be acknowledged and congratulated for the big efforts and great undertakings achieved during it.

References:

- Larkin MA, et al. (2007). Clustal W and Clustal X version 2.0. Bioinformatics, 23, 2947-2948.
- Galtier et al. (1996) SEAVIEW and PHYLO _ WIN: two graphic tools for sequence alignment and molecular phylogeny, Bioinformatics, 12-6, 543-548
- 3. Valverde, J. R. (2007) IBS-ES-07 course: The making of. embnet.news, vol 13, no. 4. 11-17
- 4. Rice et al. (2000) EMBOSS: The European Molecular Biology Open Software Suite, Trends in Genetics, 16(6), 276-277.
- Felsenstein, J. 2005. PHYLIP (Phylogeny Inference Package) version 3.6. Distributed by the author. Department of Genome Sciences, University of Washington, Seattle
- Prokop et al. (2008) TRITON: a graphical tool for ligand-binding protein engineering. Bioinformatics. 24(17): 1955–1956.
- Sali, A. and Blundell, T.L. (1993) Comparative protein modelling by satisfaction of spatial restraints. J. Mol. Biol. 234(3):779-815.
- 8. Wahab et al. (2009) On Elucidating Isoniazid Resistance Using Molecular Modeling, J. Chem. Inf. Model. 49, 97-107
- Johnson et al. (2006) Drug Resistance in Mycobacterium tuberculosis. Curr. Issues Mol. Biol. 7: 91-112
- Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S. and Olson, A. J. (2009) J. Comput. Chem. in press. "Autodock4 and AutoDockTools4: automated docking with selective receptor flexibility."
- MOPAC2009, James J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA, http://openMOPAC.net (2008)

Personal Account: Training in Grid Computing for Bioinformatics



Kanchana Senanayake

Institute of Biochemistry, Molecular Biology and Biotechnology (IBMBB), University of Colombo, Cumaratunga Munidasa Mawatha, Colombo, Sri Lanka

Since the Institute of Biochemistry, Molecular Biology and Biotechnology (IBMBB) was elected as the Sri Lankan EMBNet node at the EMBNet AGM in 2006 we have been in close contact with the Swedish EMBNet node. As a result of this association I was fortunate enough to get an invitation for a short visit to the Swedish University of Agricultural Sciences (SLU), Uppsala, Sweden. This visit was funded by SIDA/SAREC and IBMBB. In this article I will be giving a brief insight in to my visit from an academic and a personal point of view.

Academic

The main objective of my visit was to get hands on training in grid computing and its applications in Bioinformatics. A 14 node cluster was given to the IBMBB under the NorduGrid project in 2006. NorduGrid is a Grid Research and Development collaboration aiming at development, maintenance and support of the free Grid middleware, known as the Advance Resource Connector (ARC)¹. The aim of this collaboration was to use grid computing for bioinformatics applications as well as porting existing bioinformatics tools on to the grid. These tools then can be used for high volume data processing application in various fields of Biology. Unfortunately the know-how was not there to make the best use of this resource at the IBMBB. The best way of describing this situation the Sri Lankan way is:

"Like giving an elephant, without the goad to control it"

So for the last three years this was not utilized at all for any type of research. In order to utilize this resource IBMBB needed someone with hands on

¹ http://www.nordugrid.org/middleware/

knowledge on Grid computing. As a result of this requirement I was requested to go to Sweden by Prof. Kamani Tennekoon, Director of IBMBB and Node Manager of the EMBNet Sri Lanka to gain the necessary knowledge and experience to better utilize this resource at IBMBB.

With help and support of the UPPMAX personnel I managed to assemble a 5 node cluster and install the OS and the middleware. The UPPMAX was kind enough to provide me 5 spare nodes to construct a fully functional cluster. These nodes had the same hardware configuration as the cluster that is at the IBMBB. The purpose of this exercise is to create a 5 node replica of the cluster in Sri Lanka but with the updated versions of the OS and the middleware, so I could do the same to our node and upgrade the cluster in Sri Lanka. After installing the cluster I managed to install and configure few bioinformatics tools and databases with the support of Prof. Erik Bongcam-Ruddloff. This bioinformatics cluster can be accessed with the URL http://biocluster.hgen.slu.se/.

Although the main objective of this visit was Grid computing I was fortunate enough to get exposed to several other aspects of Bioinformatics as a result of the collective research culture at the Bioinformatics lab headed by Prof. Erik Bongcam-Rudloff. I was initially involved in a sequence assembly project with an MSc student at the lab which was his research project of the MSc. Through this exercise I learned different techniques and tools used for sequence assembly and their problems in execution for Illumina data. This made me realize the importance of a bioinformatics cluster to do these big data analysis work. I also got a chance to learn about Microarray data analysis using R and Bioconductor. This knowledge was gained through the participation in the one week course "DNA expression microarray data analysis using R and Bioconductor" conducted by the CSC - IT Center for Science in Finland, I also had a brief introduction to Weblab as the creators of this bioinformatics workflow had a visit to the SLU to do a local installation of the Weblab at the SLU.

Personal

From a personal point of view I thoroughly enjoyed the visit to this wonderful country and made some good and interesting friends both from Sweden and from other countries like Pakistan, China, Iran and Kenya.

The Swedish are very friendly people and a great host. I found that they are very serious about two things other than work, which are holidays and Coffee. The support that I got from these people for my work is maximum, specially from the people from SLU and UPPMAX. Without their support I could not have completed this training successfully.

Probably the highlight of this trip from a personal point of view is my visit to the Linnaeus Gardens. He is known as the father of modern taxonomy, and one of the fathers of modern ecology and happens to be my Favorite scientist. I think he was one of the greatest logical minds of the 18th century. This was one of those rare opportunities that you get to see your idol. I will also never forget the trip to Finland on a ship. This was the first time I was on a cruise ship which was a great experience for me. During this trip I saw so many wonderful sceneries and had expensive but excellent food.

I like to take this opportunity to thank the Department of Animal Breeding and Genetics of the Swedish University of Agricultural Sciences who was my host for providing me with all the facilities and the staff who provided me with all the support. I also like to thank the Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX), University of Uppsala and the staff for providing me with the resources and the know how to make this training a sucsess. I also like to thank SIDA/SAREC for funding this visit and the staff at International Science Program office who looked after me while I was in Sweden.

I look forward to continued and enhanced collaboration with Swedish EMBNet node and the other nodes in the EMBNet.