

Report on LinkSCEEM Users Meeting, Amman, Jordan, 6th November, 2008. Hosted by JUNET courtesy of the University of Jordan.

This meeting was the 3rd users meeting for the LinkSCEEM project. It took place in the Wadi Rum Auditorium at the University of Jordan and was hosted by JUNet on behalf of LinkSCEEM. The meeting was attended by over 55 participants from universities and research organizations in Jordan, Cyprus, Syria, Palestine and the Lebanon.

Network connectivity (both of itself and indirectly through discussions on large data transfers) was a recurring topic throughout the day. Also discussed was the necessity for sufficient stimulation of the user base to ensure full utilization of large scale facilities. It was also argued that systems, both locally and at the Cyprus Institute, should be put in place to deal with capacity as well as capability computing needs since there were institutions in the region where these needs were not being met.

Of the 9 presentations, 2 were user presentations, one from Balqa Allied University in Jordan and one from the University of Jordan. These presentations are outlined below along with relevant comments made by the participants.

The panel discussion, which consisted of Prof. Victor Jongeneel of the Cyprus Institute, Dr. Norbert Attig of the Julich Supercomputing Center, Dr. Assad Sakhel of Balqa Applied University and Dr. Mohamad Gharaibeh of SESAME, took place after the user presentations. During this discussion Prof. Nabil Nassif reiterated his belief that, based on their experience at the American University of Beirut, significant resources should be placed in the adequate preparation and training of a suitable user base for any proposed facility. Also discussed was the date the SESAME facility would begin operations and what its data requirements would be at that time. There was also discussion on GRID facilities in the area and the possibility of using cycle-scavenging systems to deal with some of the capability computing requirements at the university level. Prof. Jongeneel commented that multiple solutions for such a system existed but suited only a small subset of applications. Dr. Attig made the point that a smaller scale facility should exist to deal with capacity computing and also as a proving ground for users prior to applying for resources to use the larger facilities.

Prof. Victor Jongeneel, Cyprus Institute “The Cyprus Institute, CSTRC and LinkSCEEM”

Prof. Jongeneel contextualized the meeting by introducing the Cyprus Institute (CyI), the Computational Science and Technology Research Center (CSTRC) and the LinkSCEEM project. He discussed how the LinkSCEEM EU funded Support Action aims to ensure that, in planning and developing the CSTRC, strong links are created both to the European ICT infrastructure and the Eastern Mediterranean scientific community. The projects thereby acts as a facilitator to build scientific and technological bridges between Europe and the Middle East and to narrow the digital gap between the Eastern Mediterranean and the Western World.

He also outlined the estimated time-line for the acquisition of facilities. In the Tier system utilized in the PRACE initiative, a Tier 2 facility (with 10s of Tflop capability) is expected to be in place by the end of 2009, with a Tier 1 facility (100s of Tflops) available in 2012. Since Cyprus is now a general partner in the PRACE initiative it can provide indirect access to Tier 0 (PetaFlop) facilities in Europe, and also in America, through its collaborative agreement with the NCSA.

He also made the point that the Cypriot government has made a commitment to SESAME to analyze data created there which will require the upgrading of network connectivity in the region to deal with

the necessary data traffic.

Dr. Mohamad Gharaibeh, SESAME
“SESAME Light Source as an International Research Center”

Dr. Gharaibeh outlined the technical operation of a synchrotron facility and how it leads to a high intensity coherent light in the ultraviolet to x-ray region. Since there is a large wavelength bandwidth in the resulting light, it is possible to service multiple users simultaneously using multiple beam lines. He provided a list of the coordinators of various beam lines and their areas of expertise.

With respect to computing facilities, he detailed how crystallographers and those involved in medical imaging would have huge data storage requirements that cannot be addressed at the SESAME facility (in the medium to long term). It is intended that this data will be sent to Cyprus to be analyzed, visualized and archived there. Such a scenario would require dramatic improvements in network connectivity between the two countries.

Prof. Nabil Nassif, American University of Beirut
“Computational Sciences at the American University of Beirut”

Prof. Nassif discussed the development of computational sciences at the AUB. An undergraduate program in Computational Science was introduced in 2001 and a Masters program began in 2007. The programs focus on the mathematical basis and methods for simulation and are aimed at preparing a new generation of students to address emerging demands.

He listed the computer facilities available at the AUB, the most powerful of these being at the Center for Advance Mathematical Sciences. In this particular case, he noted that the facility (when purchased) was expensive but suffered from severe underutilization because few users with the necessary skills existed. It was for this reason that a more practical approach was adopted, where students are instructed in the use of tools such as MatLab rather than high-level programming languages and root project development. He warned that unless significant educational support was provided, the investment in a facility in Cyprus could turn into a white elephant. Prof. Jongeneel assured him that the development of an educational program and sophisticated user support was a core function of the CSTRC.

Dr. Radha Nandkumar, National Center for Supercomputing Applications
“International Cooperation in Computational Sciences and infrastructures”

Dr. Nandkumar explained the current infrastructure in place at the NCSA to assist in the growth and development of supercomputing facilities and usage at national and international levels. She outlined some of the programs that NCSA have implemented to promote collaboration and project advancement. Particular programs included the Summer Fellowship program where researchers are invited to NCSA for a 3 month period, enabling them to become familiar with the environment and the facilities as well as develop their particular applications. This has operated on a national level for many years and has recently been expanded to the international level.

She also spoke of the partnerships that NCSA has fostered with emerging supercomputer facilities throughout the world, and stated that the cooperation with Cyprus is in a similar vein.

Dr. Alan O'Cais, Cyprus Institute
“Scientific Applications on High Performance Platforms”

Dr. O'Cais described the likely make-up of large scale computer facilities in the near future. In particular he focused on the new types of accelerators that are emerging in these platforms at present.

He discussed the basic makeup and functionality of GPUs, the Cell processor and FPGAs. Explicit examples of their successful utilization in Lattice QCD were given.

He also spoke of the necessary steps in developing an application for these platforms. Such steps include choosing a programming language, library utilization, compilers, profilers, repository use, documentation and other topics.

Dr. Norbert Attig, Jülich Supercomputing Center (JSC)
“The users and applications portfolio of a tier-1 HPC center”

Dr. Attig spoke of the development of the supercomputing center in Jülich. The current installation, including a purpose-built building, was completed in 2004. The center itself has been operational for almost 20 years. The Jülich Supercomputing Center is in charge of operation of the facility. The allocation of facilities to users is implemented by the John von Neumann-Institut für Computing (NIC) which operates independently of the center. The NIC allocation is based on scientific merit of the project and the judgment process is conducted independently of the JSC. The JSC still has veto rights once the NIC has approved a project, but these are only based on technical considerations such as the actual suitability of the project for implementation on the system architecture.

Dr. Attig also outlined how the support structure for users has developed in recent times. Previously, it operated as a three tier system with a help desk providing immediate technical support, a specialist tier for help with computational methods and optimization and an advisor to guide scientific partnerships. The newly implemented system is that of a Simulation Laboratory (SL). An SL is a targeted research and support organization for a scientific community. It cooperates with its community and supports it in performing simulations on supercomputers. The SL are adjusted according to the needs of the scientific communities and each SL is itself part of its community and strengthens it. An SL consists of a core group located at a supercomputer and a number of associated scientists at universities and research institutes.

Dr. Attig reinforced earlier comments on the need for a large educational effort when running a supercomputing center. He also stressed that a Tier 1 facility must be fully embedded in the educational network and that active and strong collaborations are essential to the active utilization of such a system.

Dr. Yousef Torman, Jordan Universities Network (JUNET)
“Providing computational power and connectivity in the Eastern Mediterranean”

Dr. Torman's main focus was on the network connectivity in the Eastern Mediterranean region. He listed some of the national connectivity bodies in countries in the area (such as MARWAN in Morocco and AARN in Algeria). He also discussed regional connectivity efforts and in particular Consortium of Arab and Mediterranean Research and Education Networks (CAMREN).

He showed the extremely limited bandwidth available in the area. He stressed however that, apart from Libya, there exists dark fiber connections throughout the region, but unfortunately political and economic considerations are stunting the growth of the research connectivity.

Users Presentations:

Dr. Assad Sakhel, Balqa Applied University
“Tunneling of bosons in optical lattices: A Monte Carlo Investigation”

Dr. Sakhel described some of his recent research in the area of tunneling in optical lattices. Optical lattices are formed by the interference of counterpropagating laser beams, which creates a periodic (in space) intensity pattern. Atoms are cooled and congregated in the potential minima. The resulting

system of trapped atoms resembles a crystal in the sense that the atoms are in a periodical potential. Because of quantum tunneling, atoms can move in the optical lattice even if the well depth of the lattice is higher than the energy of the atoms. Atoms in an optical lattice provide an ideal quantum system where all parameters can be controlled. Thus they can be used to study effects that are difficult to observe in real crystals.

With respect to his own particular research, Dr. Sakhel stressed that he had nowhere near enough computational power to simulate interesting systems (with 100000s of bosons). He has limited use of a GRID facility in Italy and his needs cannot be met locally.

Dr. Iyad Al-Qasir, University of Jordan

“Thermal and Neutronic Properties of Crystalline Materials”

Dr. Al-Qasir described his work which is based on first principle calculations in nuclear engineering. He uses the density functional theory formalism to address these problems and utilizes the VASP software package to perform simulations. This package performs ab initio quantum mechanical molecular dynamics (MD) using Vanderbilt pseudopotentials.

He commented that the University had contacted IBM to assist in setting up a center for computational physics but that a solution for funding it had not been found.