11th Machine Evaluation Workshop (2000)

Summary

The 11th annual Daresbury Machine Evaluation Workshop was held on the 22nd, 23rd and 24th of November 2000 at the Daresbury Laboratory, near Warrington, Cheshire. This event is an important part of the Distributed Computing Support Programme (DisCo) of the Engineering and Physical Sciences Research Council (EPSRC) operated by Daresbury Laboratory.

The first Daresbury Machine Evaluation Workshop took place in 1990 as part of the SERC Computational Science Initiative and the Workshop is now well established as a leading national event dedicated to distributed high-performance scientific computing. The principal objective is to encourage close contact between the research communities supported by the EPSRC grant lines (Mathematics, Physics, Chemistry, Materials and Engineering), and the major vendors of PCs, workstations, mid-range and high-end systems, software and peripherals.

The Workshop comprises three main activities, (i) a two day programme of short talks, (ii) a two day technical exhibition, and (iii) an opportunity for delegates to access loaned systems and benchmark their own codes via the internet and on site.

The lecture programme provides a forum for delegates to receive an update from all the major vendors. The technical exhibition runs in parallel and includes demonstrations of a wide range of technology of importance to scientists using distributed computing. We consider the Workshop benchmarking exercise to be of particular importance. There are many standard performance measures available, such as SPEC, MFLOPS, Whetstones and timings on standard codes. Whilst providing very useful information, these can never be as indicative as results from the code to be used in production.

The DisCo support team (Drs. Steven Andrews and Barry Searle) worked with the machine suppliers prior to the workshop to make a number of systems available for benchmarking. These included:

- SGI 8 x1200 dual PIII Linux cluster
- HP Visualize J6000 dual PA-8600 552 MHz and Visualize X1000 NT workstation (1GHz PIII)
- IBM Netfinity 4000R/4500R rack-mount cluster
- Workstations UK 4 x dual PIII 800 MHz SCI based MIM cluster

The DisCo team also created and managed a set of new accounts for delegates to log in remotely over SuperJANET, transfer their own codes and run benchmarks. Help on doing this was provided via the Web with pages accessible from the main DisCo site at URL http://www.cse.clrc.ac.uk/Activity/DisCo. Further information on DisCo activities, archives and benchmarks and the Beowulf cluster is also available from this source.

The lecture programme started on the first day after lunch. A closed delegates' session provided an opportunity for speakers and workshop delegates to discuss experiences and the results of the benchmarking trials. Dr. Martyn Guest (Daresbury) presented his benchmark results which are included, in full, in the Workshop proceedings. In summary, these benchmarks, which are taken mostly from computational chemistry, include the most important intensive operations found in this kind of scientific code, i.e. vector and scalar matrix operations both with and without optimised BLAS where available. Raw matrix operation benchmarks are complimented by a set of codes taken from the numerically demanding kernels of larger applications including self-consistent field calculations using Gaussian basis functions, molecular dynamics, quantum Monte-Carlo, and an iterative Jacobi linear equation solver. The paper also includes results on full production runs of both the GAMESS-UK *ab initio* electronic structure code and DL_POLY molecular dynamics simulation code.

To a lesser extent than last year the Alpha offerings led the field, this time with the 833MHz version but the 667MHz EV67-based machines now have competition from the 552MHz PA8600 from Hewlett Packard (in

the Vizualize J6000). These processors continue to out perform the leading CPUs from the other workstation vendors. The latter included the 375MHz Power3 from IBM (in the RS/6000 44P Model 270), the 400MHz R12k from SGI (in the Octane2) and the 750MHz UltraSPARC-III from Sun (in the Blade 1000). Very cheap high performance PC-based hardware is now a reality, with a 1GHz Athlon K7 typically delivering 60% of the performance of the 667MHz Alpha processor.

In the second presentation the theme of commodity cluster computing was picked up by Themis Bowcock of Liverpool University, who gave a talk on the construction and running of the MAP System at Liverpool.

A total of 25 companies were represented at the Workshop including major workstation, PC and HPC manufacturers: SGI, HP, IBM, Cray, NEC, Fujitsu, Compaq and Sun. Cluster integrators included Workstations UK, Streamline Computing and Compusys. A cross section of resellers and distributors of these systems were present: Keltec, Compusys/API, TBC, OCF, Prolinx, ABC Workstations and E-Net Technology. Software specialists were represented by Pallas and Platform Computing, and network specialists by Quadrics, Scali, Dolphin Interconnect and Extreme Networks.

The first day's open presentations included contributions from:

- Chris Brown of IBM (*RS/6000 Technology Roadmap);*
- Martyn Guest *(Application Performance on High-End and Commodity-class Computers);*
- Andy Grant of SGI (*SGI: Technology Curves and Product Roadmaps);*
- Toine Beckers of NEC *(NEC's HPC Technology and Product Roadmap);*
- Bill McMillan of Platform (*Distributed Resource Management).*

Through the generosity of our sponsors, the lectures were followed by a wine reception in CLRC's "Science Centre" where delegates could find out more about work done at the Daresbury and Rutherford-Appleton Laboratories and continue their in-depth discussions with vendors.

Lectures resumed in the morning of the second day with two sessions including:

- Bill Blake of Compaq (*Compaq's HPTC Direction*);
- Ian Gilbert of Hewlett Packard (*HP Technology Roadmap*);
- Peter Thomas of Fujitsu (*Fujitsu Linux Beowulf Cluster Plans*);
- John Taylor of Quadrics (*Quadrics in Linux Clusters*);
- Chris Franz of Extreme Networks (*Extreme Architecture*);
- Peter Thomas of Fujitsu (*Fujitsu HPC Strategy*).

After a lunch sponsored by Compaq, delegates returned to the vendor demonstrations at the Exhibition. The latter again proved to be a very successful component of the Workshop and several newly announced systems were on show (see above). A list of hardware and software demonstrated may be found here.

Later in the day there were further talks from:

- Paul Calleja of Compusys (*Commodity HPC clusters: current status*):
- Werner Krotz-Vogel of Pallas (*Cluster Performance Modelling*);
- Nic Harrison of Imperial College London and Daresbury Laboratory (*A Cluster for UKCP Materials Modelling*).

The last year has seen an explosion of curiosity in cluster computing as a cost effective alternative to large departmental SMP machines. As a consequence we felt it would be useful to extend the Workshop by an extra day to cater for those considering such a solution. The huge amount of interest generated meant that not only was the third day dedicated to this topic but the presentations spilled over into the previous day as may be seen form the programme above. Presentations on Day 3 were from:

- David Beagle of SUN (*SUN Cluster Technology*);
- Mike Rudgyard of Streamline Computing (*Cluster Procurement, Integration and Support - a Streamlined Approach*)
- Nick Davis of IBM (*Linux and the Next Generation of e-Business*)
- Kåre Løchsen of Dolphin Interconnect Solutions (*SCI Network Hardware*)
- Einer Rustad of Scali (*ScaMPI, Shmem and Management*)

- David Spillane of API Networks (*API's High Performance Computing Solutions*)
- Martyn Foster of SGI (*SGI Linux Cluster Technology*)

A total of 168 delegates registered for this 11th Workshop, a record number for the event. 63 delegates were from Universities around the country, 26 from CLRC and the other Research Councils and their representatives, 5 "non-academic" and 74 from participating vendors and resellers.

During the two weeks preceding the Workshop, a number of delegates registered to use systems for benchmarking by accessing the systems via SuperJANET. Local disk space and fileservers were used to provide room for compilations and for benchmark runs. Most of the systems were available at the Workshop for closer evaluation and comparison.

We would like to thank all those who attended as delegates and those who represented resellers or manufacturers. According to informal feedback, this event was again a success and we hope that the attendees found the Workshop useful and profitable. Many staff at Daresbury put in extra effort to make the event run smoothly including the Staff of Security, Stores the Restaurant, Network Team, the Riggers and our Department Secretary and assistant, Mrs. Shirley Miller and Damian Jones. Our thanks go to them all.

We especially thank the EPSRC for their continued funding and support and also the event sponsors: API Networks, Compaq, Quadrics, IBM and SGI.

With a growing number of participants we are confident that the Machine Evaluation Workshop remains a leading national event in distributed high performance computing, bringing together as it does both suppliers and users in technical and productive fashion. We look forward to continuing Distributed Computing Support for the community and to future Workshops at Daresbury.

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