The TOP500 and Computational Science

A not-so-simple matter of software

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The TOP500 project was started in 1993 to provide a reliable basis for tracking and detecting trends in high-performance computing. Twice a year, a list of the sites operating the 500 most powerful computer systems is assembled and released. As predicted several years ago, only systems exceeding the one teraflop-per-second mark on the Linpack benchmark were able to enter the list.

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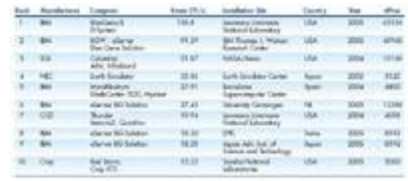
Figure 1: TOP500 Performance Trend, June 2005

The 25th TOP500 List was released during the 20th International Supercomputer Conference (ISC2005), June 21-24, 2005 in Heidelberg, Germany.

General highlights from the TOP500 since the last edition:
• As predicted several years ago, only systems exceeding the 1 TFlop/s mark on the Linpack were able to enter the list.
• The last system on the list - with 1.166 TFlop/s - would have been listed at position 299 in the last TOP500 just six months ago. This exemplifies the continuous rapid turnover of the TOP500.
• The last system (number 500) in June 2005 has about the same compute power as ALL 500 systems combined, when the list was first created 13 years ago in June 1993.
• Total accumulated performance has grown to 1.69 PFlop/s, compared to 1.127 PFlop/s six months ago.
• Entry level is now 1.166 TFlop/s, compared to 850 GFlop/s six months ago.
• The entry point for the top 100 moved from 2.026 TFlop/s to 3.412 TFlop/s.
• A total of 333 systems are now using Intel processors. Six months ago there were 320 Intel-based systems on the list and one year ago only 287.
• The second most common processor family is the IBM Power processor (77 systems), ahead of PA RISC processors (36) and AMD processors (25).
• 304 systems are labeled as clusters, making this the most common architecture in the TOP500.
• At present, IBM and Hewlett-Packard sell the bulk of systems at all performance levels of the TOP500.
• IBM remains the clear leader in the TOP500 list and increased its lead to 51.8 percent of systems and 57.9 percent of installed performance.
• HP is second with 26.2 percent of systems and 13.3 percent of performance.
• SGI is third with five percent of systems and 7.45 percent of performance.
• No other manufacturer is able to capture more than five percent in any category.
• The U.S is clearly the leading consumer of HPC systems with 294 of the 500 systems installed there. A new geographical trend, which started a few years ago, now emerges more clearly. The number of systems in Asian countries other than Japan is rising quite steadily. In this list, Japan is listed with 23 systems and all other Asian countries combined have an additional 58 systems. However, Europe is still ahead of Asia, with 114 systems installed.

• Ninteen of the systems in Asia are installed in China — up from 17 systems six months ago.
• The number of systems installed in the U.S. has increased to 294, up from 267 six months ago.
• In Europe, Germany reclaimed the number one spot from UK again, with 40 systems compared to 32. Six months ago UK was in the lead with 42 compared to Germany's 35 systems.



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The World's Top 10 Most Powerful Commercially Available Computer Systems (June 2005)

The top10 machines in the current list again show a major shake-up. Only half of the top 10 systems from November 2004 are still large enough to hold on to a TOP10 position, five new systems entered it. The new and previous number one is the U.S. Department of Energy's (DOE) IBM BlueGene/L system now installed at DOE's Lawrence Livermore National Laboratory (LLNL). It has doubled in size and has now achieved a Linpack performance of 136.8 TFlop/s. The new number two is a second IBM eServer Blue Gene Solution system, installed at IBM's Thomas Watson Research Center with 91.20 TFlop/s Linpack performance. The Columbia system at NASA/Ames built by SGI slipped to the number three spot from the number two spot, which it had gained just six month ago, with an equally impressive 51.87 TFlop/s. The Earth Simulator, built by NEC and which held the number one spot for five lists, is now number four. The number five spot was barely captured by the upgraded MareNostrum system at the Barcelona Supercomputer Center. It is an IBM BladeCenter JS20-based system with a Myrinet connection network and achieved 27.91 TFlop/s - just ahead of a third Blue Gene system, owned by ASTRON and installed at the University of Groningen with 27.45 TFlop/s. The number ten spot was captured by an early measurement of Cray's Red Storm System at Sandia National Laboratories with 15.25 Tflop/s. This is also the new entry level for the TOP10 up from just under 10 TFlop/s Linpack performance six months ago.

The world's most powerful supercomputer, BlueGene/L, is installed at Lawrence Livermore National Laboratory.

Of course, the general and widespread obsession with hardware is understandable, especially given exponential increases in processor performance, the constant evolution of processor architectures and supercomputer designs and the natural fascination that people have for big, fast machines. I am not exactly immune to it. But when it comes to advancing the cause of computational modeling and simulation as a new part of the scientific method, there is no doubt that the complex software "ecosystem" it requires must take its place on the center stage. Many of us today who want to hasten that growth believe that the most progressive steps in that direction require much more community focus on the vital core of computational science: software and the mathematical models and algorithms it encodes.

At the application level, the science has to be captured in mathematical models, which in turn are expressed algorithmically and ultimately encoded as software. Accordingly, on typical projects, the majority of the funding goes to support this translation process that starts with scientific ideas and ends with executable software, and which over its course requires intimate collaboration among domain scientists, computer scientists and applied mathematicians. This process also relies on a large infrastructure of mathematical libraries, protocols and system software that has taken years to build up and must be maintained, ported and enhanced for many years to come if the value of the application software that depend on it are to be preserved and extended. The software that encapsulates all this time, energy and thought routinely outlasts (usually by years, sometimes by decades) the hardware on which it was originally designed to run, as well as the individuals who designed and developed it.

Thus the life of computational science revolves around a multifaceted software ecosystem. But today there is (and should be) a real concern that this ecosystem,
including all of its complexities, is not ready for the major challenges that will soon confront the field. Domain scientists now want to create much larger, multi-dimensional applications in which a variety of previously independent models are coupled together, or even fully integrated. They hope to be able to run these applications on Petascale systems with tens of thousands of processors, to extract all performance that these platforms can deliver, to recover automatically from the processor failures that regularly occur at this scale, and to do all this without sacrificing good programmability. This vision of what Computational Science wants to become contains numerous unsolved and exciting problems for the software research community. Unfortunately, it also highlights aspects of the current software environment that are either immature, under funded or both.[1]

BlueGene/L during construction on the IBM floor.

Advancing to the next stage of growth for computational simulation and modeling will require us to solve basic research problems in computer science and applied mathematics at the same time as we create and promulgate a new paradigm for the development of scientific software. To make progress on both fronts simultaneously will require a level of sustained, interdisciplinary collaboration among the core research communities that, in the past, has only been achieved by forming and supporting research centers dedicated to such a common purpose. However, a stronger effort is needed by both government and the research community to embrace such a broader vision. I believe that the time has come for the leaders of the computational science movement to focus their energies on creating such software research centers to carry out this indispensable part of the mission. The community has always been in the vanguard of efforts to catalyze and organize precisely the kind of interdisciplinary research partnerships that we now require to transform the future of scientific software. I have every confidence that this community stands ready to step up again to this momentous new effort.

1. D. E. Post and L. G. Votta, "Computational Science Demands a New Paradigm," *Physics Today*, vol. 58, no. 1, pp. 35-41, January, 2005.

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