Blue Gene supercomputer installed at IBM Zurich Research Laboratory

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One of the world's fastest supercomputers was officially inaugurated at IBM's Zurich Research Laboratory (ZRL). The so-called BlueGene/L system has the same performance as the computer ranked 21st on the current list of the world's top 500 supercomputers. It will be used to address some of the most demanding problems faced by scientists regarding the future of information technology, such as how computer chips can be made even smaller and more powerful. Thanks to this new supercomputer, ZRL researchers can now run large-scale simulations of systems having a complexity similar to that of real semiconductor structures in microchips.

Supercomputers of the Blue Gene family comprise modules of multiple racks. ZRL's two-rack BlueGene/L system has a peak performance of 11.2 Teraflops (i.e. 11.2 trillion calculations per second). In Switzerland, this performance is topped only by the four-rack BlueGene/L system at the Ecole Polytechnique Fédérale de Lausanne, which has a maximum performance of 22.9 Teraflops.

The ZRL supercomputer will be used for emerging Deep Computing and research applications, primarily for simulations in computational materials science. This field is of special importance in view of the continuing miniaturization of microchips. Microchip structures and elements have become smaller and smaller, resulting in better and faster performance. This development so far has largely followed "Moore's Law", which predicts that the number of transistors on an integrated circuit will double every two years.

Progressive miniaturization, however, raises new issues. Integrated circuits of microchips are composed of transistors, which serve as switches. They typically have a sandwich-type structure of insulating and conducting layers, some of which are only a few atomic layers thick. This means that leakage currents through the insulation layers will pose an ever more serious problem as chips become increasingly smaller. Efforts are underway to design novel materials with better insulation properties than the currently used silicon dioxide

The suitability of such materials for silicon-based microchips critically depends on their characteristics when implemented in a transistor. To investigate these features, ZRL researchers will use the new supercomputer to produce simulations based on first-principles molecular dynamics. In other words, they will model the behavior of a material solely using quantum mechanics. These simulations are very complex and thus require a significant amount of processing capability. For example, to calculate all interactions in a system of about 100 to 500 atoms using a time step of 0.1 femtoseconds (one femtosecond equals one millionth of a millionth of a millisecond), it took the previous ZRL supercomputer — the most powerful system in Switzerland three years ago — two minutes of calculation time. Today, with BlueGene/L, the same calculation can be done in about 10 seconds.

To achieve such performance, software is also a crucial factor. The CPMD code used for such simulations has been tuned to exploit the unique features of the modular BlueGene/L hardware. This means that not only the speed but also the complexity of simulations can be increased with BlueGene/L. Simulations can be conducted on systems that involve anywhere from 1000 up to 5000 atoms, a number that is necessary to obtain a realistic model of the chemistry and physics of the relevant materials in a microchip.

The ability to design novel materials with tailored properties is crucial to the further improvement of computer chips. Research efforts in this field are therefore aimed at achieving further miniaturization in semiconductor technology and may eventually contribute to the development of next-generation supercomputers. Thanks to BlueGene/L technology, a possible breakthrough has come closer.

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