Press Release

I-SCALARE LABORATORY IN MIPT ACHIEVED FURTHER SUCCESS IN RESEARCH WITH RSC SUPERCOMPUTER

Moscow, May 29, 2012. *— I-SCALARE (Intel super computer applications laboratory for advanced research), a supercomputing technology laboratory for biomedicine, pharmacology and small-scale structures created in 2010 as a part of the Russian Government grant in Moscow Institute of Physics and Technology (MIPT), introduced new successful results of its scientific research achieved using an upgraded energy efficient computer with a peak performance of 41.57 TFLOPS (trillion floating point operations per second) created on the basis of RSC Tornado advanced architecture and new Intel® Xeon® E5-2600 server processors. The project is implemented with participation of MIPT and Intel Corporation employees; RSC developed and installed the innovative computing cluster to perform a full range of research as a part of the laboratory activities.*

Bioinformatics and pharmaceutical modeling are one of the fast-growing areas with an acute need for high-performance supercomputing calculations. The research carried out on the basis of I-SCALARE laboratory is very important, as breakthroughs in new methods of diagnosis and medical treatment, creation of new pharmaceuticals etc. are possible only through the development of new calculation methods and platforms that take into account specific nature of biological, medical and pharmaceutical tasks. Joint implementation of this project by MIPT, Intel and RSC Group's specialists will bring the research in this area to the next level.

"The main goal of I-SCALARE laboratory led by Vladimir Pentkovsky is solving most important problems in modern bioinformatics. Professionalism, commitment and enthusiasm shown by the team facilitates successful achievement of the goal", said Nikolay Kudryavtsev, Rector, Moscow Institute of Physics and Technology.

New scientific results achieved by the laboratory with the help of the upgraded supercomputer and further development prospects were presented as a part of a press conference held in MIPT with participation of Intel Corporation and RSC Group. Sergey Garichev, dean of radio technology and cybernetics department (RTCD), a MIPT unit where I-SCALARE has been created, welcomed the press conference participants and told about the goals and development prospects of the department.

Kamil Isayev, managing director for research and development, Intel Russia, introduced the major activities of I-SCALARE held in MIPT with Intel's participation. The laboratory's main interest area is the development of task-oriented architectures for

computing systems used in biomedicine, pharmacology and small-scale structures. Several computing applied tasks related to the modeling of viruses and cell membranes, as well as interaction between proteins and external fields with cell membranes were selected as the primary goal. On the one hand, all these tasks have a great practical value, and on the other hand they cannot be solved with the existing computing resources, as such tasks require a new approach to the cluster architecture.

For example, a research team led by Prof. **Roman Yefremov**, Biochemistry Institute, RAS, uses I-SCALARE's upgraded computing cluster in MIPT to carry out research in the area of constructing a new class of antimicrobial compounds based on natural lantibiotics. As a part of calculations and modeling during the project, microsecond-long trajectories of molecular dynamics (MD) for antibiotic targets (lipid II molecules) in the bacteria membrane were calculated. The upgraded supercomputer in I-SCALARE laboratory allows calculating such trajectories for systems that contain more than 50,000 atoms within just a week. For comparison, the same calculations using a computing cluster on the basis of the previous-generation Intel® Xeon® E5450 processors actively used by RAN Biochemistry Institute would take about 100 days. This means that thanks to the high performance of the new computing cluster the scientific results can be achieved more than 14 times as faster. The analysis of MD trajectories allowed to determine special features of the bacterial membrane structure. This year a more detailed modeling of interaction between lantibiotics and lipid II in the membrane will be held using I-SCALARE's upgraded supercomputer. In future such research could lead to the creation of a new class of antibiotics not susceptible to bacteria resistance.

A. Palyutin, a senior researcher in a research group led by Academician N. Zefirov at the chemical department of Lomonosov's Moscow State University, presented details of modeling the protein coat and molecular dynamics of dangerous Flaviviruses (e.g. bouquet fever virus) and the processes of their interaction with human body cells. During the research, molecular models of virion's membrane and a fragment of the protein coat consisting of millions of atoms were built. This gave the scientists information about three-dimensional structure of the protein virus that they could not obtain using experimental methods. Then the specialists analyzed its dynamic behavior and molecules that could bind with it and prevent Flaviviruses from conjugation with human body cells. Based on such models, a computerized search of potential conjugation inhibitors for tick-borne encephalitis virus was held and prospective compounds showing the necessary activity in *in vitro* tests were indentified. As a part of works to design new neuroprotection substances, full-fledged NMDA receptor models were created. The modeling of its molecular dynamics in a phospholipid membrane with aquatic environment, as well as interaction with the known neuroprotectors was performed (the system includes hundreds of thousands atoms). The principles of interrelation between their structure and activity, as well as a prospective mechanism for receptor's modulators action were studied. Based on this data, the scientists continue to search for new prospective structures having neuroprotector activity. Such structures can form a basis for medicines to cure serious neurodegenerative diseases, such as Alzheimer's disease.

Grigory Rechistov, post-graduate student, MIPT, told about the principles of architecture modeling and the outcomes of this process. The main result achieved by the modeling group is the development of a method that allows to study the operation of a supercomputer application in next-generation systems before they become physically available. The experimental results received as of today allow for fully describe the ability of an application to work on computing complexes that include 16 times as many

processing cores as are physically available in the cluster. This method can be used to study computer systems with the performance of up to 665 TFLOPS. Computing system modeling technologies developed on the basis of Wind River Simics product give supercomputer system architects and users the tools to measure the full performance of such system, determine bottlenecks and evaluate optimization effects. As a result of such analysis the specialists can decide on the suitability of the selected configuration for practical scientific tasks.

Creating an innovative computing cluster at MIPT

In 2011, as a part of a contract with MIPT, RSC Group, Russia's and CIS leading full-cycle developer and integrator of next-generation supercomputing solutions based on Intel architecture and advanced liquid cooling has developed and installed a pilot system on the basis of RSC Tornado advanced architecture and previous-generation Intel® Xeon® 5600 processors in I-SCALARE, a supercomputing technology laboratory that performs research in biomedicine, pharmacology and small-scale structures. This year the system was upgraded to the level of a powerful computing cluster that represents a complete RCS Mini Datacenter-class solution with a peak performance of 41.57 TFLOPS. The system holds the 20th position in the current edition of Top50 rating of most powerful supercomputers in Russia and CIS countries (as of March 2012).

I-SCALARE's upgraded cluster consists of 112 computing clusters with two new generation Intel® Xeon® E5-2690 processors per node (in total 224 processors with 1792 cores). The use of Intel® Xeon® E5-2600 family of best-performing processors became possible due to advanced liquid cooling, which is the basis of RSC Tornado architecture. Additionally, larger RAM capacity per node was achieved - 64 GB (the pilot system had 36 GB of RAM per node), which totals to 7.1 TB of RAM.

Alexander Moscovsky, general manager of RSC Technologies, a part of RSC Group, told that MIPT's supercomputer is based on RSC Tornado innovative architecture. This is the world's first energy efficient supercomputing solution with advanced liquid cooling for generally available standard server boards based on Intel® Xeon® processors initially designed for traditional systems with air cooling of electronic components. RSC Tornado ensures flexible configuration of computing nodes with standard interfaces, ensures simple creation of a solution, high serviceability (simple replacement of RAM modules and RAM extension, as well as processor upgrades), and integration with any external products having standard PCI Express interfaces.

Currently the upgraded cluster system at MIPT has a data storage system of 10 TB and a communication network implemented on the basis of a high-speed Infiniband QDR interface. RSC Tornado architecture provides for the following unique characteristics of the cluster:

- Simplicity and high reliability;
- Cost effectiveness;
- High energy efficiency - a record Power Usage Effectiveness (PUE) of less than 1.2. This means that maximum 20% of energy consumption will be used for cooling;
- Compact size and high density;
- High computing effectiveness ratio - more than 90 % in LINPACK benchmark;
- High scalability;
- Accelerator support (Intel® MIC architecture).

The history of I-SCALARE laboratory creation in MIPT

In 2010, during a competition announced by the Ministry of Education and Science of the Russian Federation as a part of Russian Government's Decree #220**, Vladimir Pentkovsky, an employee of Intel Corporation, together with MIPT scientists introduced a program to study hardware and software architectures that would show maximum effectiveness when solving complex task in bioinformatics and pharmacology that require a lot of processing resources. Vladimir Pentkovsky, a famous software and hardware architecture developer, Intel research fellow, has extensive experience in creating scientific teams in Russia, USA and India. He has 40 international patents, which confirms its high authority. The project by Dr. Pentkovsky, who acted as the project team leader, ranked among 40 winners and received a grant in the amount of 150 million rubles to create a laboratory in MIPT and carry out research under the proposed project. In total, over 500 applications were submitted for the contest.

Intel actively collaborates with Russian universities in the area of scientific research, implementation of new learning programs and creating an innovation ecosystem through cooperation with higher education institutions and the industry. Intel is a base organization for MIPT's radio technology and cybernetics department, so the state-funded joint project became a logic development of such cooperation.

It is worth noting that I-SCALARE laboratory carries out both scientific and educational activities. Its employees developed a learning course to use simulators in modeling of various computing systems. Additionally, the laboratory regularly holds scientific seminars, and Vladimir Pentkovsky became a research advisor for several MIPT's post-graduate students and undergraduates.

Press Contacts:

Oleg Gorbachov
Corporate Communications Director,
RSC Group
Mobile: +7 (967) 052-50-85
Mobile: +38 (067) 501-25-94
Email:
oleg.gorbachov@rsc-skif.ru

Mikhail Rybakov
Mikhail Rybakov, Intel PR director Russia/CIS.
Tel.: 8 (495) 641-45-00
Email:
mikhail.a.rybakov@intel.com

Maria Kibkalo
Intel PR manager Russia/ CIS
Tel.: 8 (495) 641-45-65
Email:
Maria.Kibkalo@Intel.com

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About RSC Group

RSC Group is Russia's and CIS leading full-cycle developer and integrator of next-generation supercomputing solutions based on Intel architecture and technology, advanced liquid cooling

and its own extensive know-how. The company's potential allows for practical creation of the most energy efficient solutions with record PUE, realization of industry-highest computing density based on x86 standard processors, completely green design, the highest reliability of solutions, complete noiselessness of computing modules, 100 percent compatibility and guaranteed scalability, while ensuring lowest total cost of ownership and small energy consumption. Additionally RSC specialists are experienced in development and implementation of a complete software solution stack for increased effectiveness and usability of supercomputer systems ranging from system software to vertically oriented platforms on the basis of cloud computing technology.
RSC is the Platinum Partner of the Intel® Technology Provider Program. For additional information please visit www.rscgroup.ru.

About MIPT

Moscow Institute of Physics and Technology was founded in 1951 on the basis of MSU department of physics and technology (1946-1951). The institute prepares highly qualified specialists in various areas of modern science and technology. The Nobel prizewinners P. Kapitsa, N. Semenov and L. Landay were co-founders and employees of the Institute. Many leading Russian scientists are professors at MIPT. Over 80 academicians and corresponding fellows of the Russian Academy of Science are among them.
Since its inception, Moscow Institute of Physics and Technology uses a unique specialist training system widely known as the Fiztekh System. For additional information about MIPT please visit http://mipt.ru/.