# A monitoring system for supercomputers of SUSU

*Alexander Safonov, Pavel Kostenetskiy, Kirill Borodulin and Fedor Melekhin*

**Keywords:** supercomputer, management, slurm, mysql

A new system capable of monitoring and processing data for the Supercomputer Simulation Laboratory of South Ural State University is described. This system allows administrators and managers to create many different reports and provides tools to robust reaction to problems of an urgent character. This article is devoted to issues concerning with collecting and visualizing statistical data obtained from supercomputers.

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# A multilevel approach to algorithm and software design for exaflops supercomputers

*Boris Glinskiy, Igor Kulikov, Aleksey Snytnikov, Igor Chernykh and Dmitry Weins*

**Keywords:** high performance computing, scalability simulation, exaflops supercomputers

A strategy is proposed for the development of algorithms and software for Exaflops supercomputers. The strategy contain three stages. The first stage is the co-design, which is defined as considering the architecture of the supercomputer at all stages of the development of the code. The second is the forward-looking development of algorithms and software for the most promising Exaflops supercomputers. The forward-looking development is based on the simulation of the algorithm behavior within the given supercomputer architecture. The thrird stage is the estimation of the energy efficiency of the algorithm with different implementation for one single architecture or with different supercomputer architectures. The strategy is shown by the example of two problems from astrophysics and plasma physics.

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# A parallel multiple-precision arithmetic library for high performance systems

*Konstantin Isupov and Knyazkov Vladimir*

**Keywords:** computer arithmetic, precision, rounding errors, residue number system, modular-positional format, program library

The IEEE 64-bit floating-point arithmetic is often not sufficient to correctly solve large problems on high performance systems. In this case, high-precision computations should be used. In this paper an actual high-precision applications are presented. A review of the existing software is given. The requirements to prospective high-precision software are discussed. A new multiple-precision arithmetic library MF-Library is considered. A residue number system is used to represent arbitrary-length floating-point numbers in this library. This provides effective implementation of main high-precision arithmetic operations with parallel processing of significand digits. MF-Library implements the thread-safety concept that allows you to use it in shared memory systems. Results of an experimental study on the efficiency of MF-Library are presented.

# A technology for the design of hybrid supercomputer simulation codes for relativistic particle electrodynamics

*Alexey Snytnikov, Ekaterina Mesyats, Marina Boronina and Alexey Romanenko*

**Keywords:** relativistic plasma physics, templates, GPU

For the development of simulation codes for a group of similar physical problems one needs a tool of fast and flexible modification of the critical parts of the code. In the present work the modification is performed with C++ templates and inheritance. With inheritance one can transform a code for plasma simulation into a code for relativistic beam simulation. Moreover, the GPU plasma simulation code itself was built by means of C++ templates. Finally, the virtual methods is used to improve accuracy of the simulation. In such a way, C++ templates facilitate the quick and easy computation method replacement and also the transition from one supercomputer architecture to another.

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# A technology of 3D elastic wave propagation simulation using hybrid supercomputers

*Dmitry Karavaev, Boris Glinsky and V. Kovalevsky*

**Keywords:** parallel algorithm, seismic waves, simulation, hybrid cluster, Xeon Phi, supercomputers

We present a technology of 3D seismic field simulation for high-performance computing systems with great number computing cores that are placed on graphical processors or Intel Xeon Phi coprocessors. This technology covers the adaptation and development of mathematical modeling method and development of a parallel algorithm. We describe the parallel realization designed for simulation based on using staggered-grids and 3D domain decomposition method. We present the new simulation code for supercomputers equipped with Intel Xeon Phi coprocessors. In the paper, we study the parallel algorithm behavior on computing devices such as CPUs or GPUs and either Intel Xeon Phi coprocessors. We consider the results of experiments of program codes for 3D seismic simulation that were carried out on clusters for different tests for parallel algorithm. The first results of applying the technology to the Intel Xeon Phi coprocessors architecture are presented. Experiments are conducted on the NKS-30T cluster of the Siberian Supercomputer Center of SB RAS and the cluster MVS-10P of the Joint Supercomputer Center of RAS. The acceleration archived gives a good opportunity of using of such computing devices in scientific computations based on scalable parallel implementation of a difference method. The developed scientific HPC software can be used to study the structure of seismic field, to interpret geophysical data, to compare modeling data with geophysical data to develop most appropriate model of a geophysical object under research. This work was partially supported by RFBR grants No. 13-07-00589, 14-07-832, 14-05-867, 15-07-06821, 15-31-20150.

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# Accelerator numerical calculations based on modular-systolic microprocessor

*Ilya Osinin*

**Keywords:** accelerator, residue number system, homogeneous computing environment, microprocessor

The article describes the main technical solutions accelerator numerical calculations of the developed based on quad-systolic modular microprocessor MIMD-architecture, with the distributed cache, oriented to the mass-balanced, arithmetic and logical processing of fixed-point numbers. He has a number of unique features, such as dynamic group-rangement processor cores to build the capacity of processed numbers. At the same time, the same operations and the processing itself is extremely parallelized, which is achieved through the implementation of operations in parallel-pipelined over nonpositional numbers.

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## Application of modern high-performance techniques for solving local and global seismic problems

*Nikolay Khokhlov and Igor Petrov*

**Keywords:** MPI, OpenMP, CUDA, OpenCL, grid-characteristic method, finite-volume method, seismic

This paper discusses the parallelization of software, designed for dynamic modeling of the spread of wave disturbances in solids, using various advanced high-performance techniques. The software package supports two-dimensional and three-dimensional structural block meshes, explicit reference irregularities and the apparent isolation of contact boundaries. For numerical integration used grid-characteristic and finite volume methods of high order. The algorithm is parallelized using technology MPI, CUDA, OpenMP and OpenCL. Described some aspects of optimization of code using SIMD instructions of CPUs such as SSE and AVX. Comparative tests for the acceleration are given. As an example of the software system provides results of a series of test calculations.

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## Arrowhead decomposition for a block-tridiagonal system of linear equations

*Pavel Belov, Eduard Nugumanov and Sergey Yakovlev*

**Keywords:** arrowhead decomposition method, block-tridiagonal matrix, system of linear equations, parallel solution, computational speedup, matrix sweeping algorithm

The arrowhead decomposition method which allows efficient parallel solution of a block-tridiagonal system of linear equations is presented. The computational speedup with respect to the matrix sweeping algorithm is analytically estimated by taking into account the number of elementary operations of multiplication for the parallel and serial parts of the decomposition method. It is shown that the maximal speedup is achieved for the finite number of parallel processors. For a given size of the initial system of linear equations, the parameters of the computational system which give the maximal speedup are obtained. Computational experiments confirm the analytical estimations of the computational speedup.

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## Automated parallelization of sequential C-programs on the example of two applications from the field of laser material processing

*Maxim Baranov, Dmitry Ivanov, Nikita Kataev and Alexander Smirnov*

**Keywords:** parallelization, automation, transformation of sequential programs, analysis of programs

It is important to understand the information structure of programs for their parallelization. This helps to realize which kind of transformations may be necessary, and which parts of source code can be executed in parallel. Systems for automated analysis and transformation of programs may be useful to explore the structure of programs and to improve the performance of parallelization within a reasonable period of time. The paper proposes an approach to developing of such kind of systems. The process of program transformation is split into a set of basic operations. These operations are performed automatically in the order which is determined by the user. The offered approach has been successfully applied to parallelize two applications from the field of laser material processing.

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## Case study of using Intel Xeon Phi for solving particle-in-cell plasma simulation problems

*Iosif Meyerov, Sergey Bastrakov, Igor Surmin, Arkady Gonoskov, Evgeny Efimenko, Aleksei Bashinov, Artem Korzhimanov, Anton Larin, Alexander Muraviev, Anatoly Rozanov and Mikhail Savichev*

**Keywords:** Plasma simulation, Particle-In-Cell, Intel Xeon Phi, Case study, Performance optimization, High Performance Computing, Parallel programming, Optimization techniques

This paper considers efficient utilization of computational systems equipped with Intel Xeon Phi coprocessors for laser-plasma simulation. We analyze features of Xeon Phi architecture that influence performance of Particle-in-Cell plasma simulation. Description of the parallel plasma simulation code PICADOR previously optimized for Xeon Phi is provided. We study performance on Xeon Phi compared to CPU on three computationally intensive plasma simulation problems. A ratio of computational time on Xeon Phi to CPU is given for the main stages of the Particle-in-Cell method. Our study shows that depending on features of the physical problem using Xeon Phi can be both advantageous and disadvantageous compared to CPU.

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## Charge qubit inversion in combined laser and cavity field

*Alexander Tsukanov and Vadim Chekmachev*

**Keywords:** quantum dots, double quantum dot, qubit, inversion

We address the design and control of the single-electron double-dot charge qubits coherently driven by both laser and cavity mode. The dynamics is modeled via rigorous matrix density Lindblad approach and the inversion (or NOT) gate is shown to be realized with good accuracy.

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## CMF - framework for high-resolution Earth system modeling

*Vladimir Kalmykov and Rashit Ibrayev*

**Keywords:** Earth system modeling, massively-parallel applications, parallel I/O, coupler, coupling, scaling, performance

We present an original framework CMF (Compact Modeling Framework) developed for high-resolution coupled ocean-atmosphere model. Two version of CMF are presented, reflecting progress of our researches. In CMF 2.0 we concentrate on single executable central hub approach with high-level abstract driver, optimized parallel coupler interpolation scheme and

parallel I/O algorithm. CMF 3.0 replaces pure MPI approach with PGAS based communications scheme, while central hub architecture evolves to set of simultaneously working services. Performance tests are presented for "MVS" and "Lomonosov" supercomputers.

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## Combined use of HPC resources and grid infrastructures with Everest cloud platform

*Oleg Sukhoroslov*

**Keywords:** distributed computing, heterogeneous computing environments, grid middleware, job scheduling, cloud platform

Everest is a cloud platform supporting publication, execution and composition of computing applications in a distributed environment. One of distinguishing features of the platform is the ability to run applications across arbitrary combinations of external computing resources attached by a user. This work presents integration of Everest with HPC clusters and EGI grid infrastructure, and also considers problems related to combined use of these resources for running Everest applications.

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## Computer modeling of structure formation in aqueous solutions of lecithin and bile salts

*Anastasia Markina, Viktor Ivanov, Pavel Komarov, Alexei Khokhlov and Shih-Huang Tung*

**Keywords:** computer simulation, nanostructured materials, self-assembly

Recently, much attention is paid to the development of nanostructured materials by self-assembly. The report discusses the results of the first simulation of the effect of adding an inorganic salt on the morphology of supramolecular structures in aqueous solution of a mixture of lecithin and bile salts. All calculations were carried out in the framework of the dissipative particle dynamics. Using a parallelized computation performed on the cluster "Lomonosov" of the Supercomputer Center of Moscow State University, allowed to realize the modeling of large enough cells for extended time intervals over a wide range of parameters. We observed the effect of salt on the change in the morphology of aggregates of lecithin and bile salts. Depending on the concentration of salt, we observed transformation of ellipsoidal or cylindrical structures in long worm-like micelles. These long, flexible worm-like micelles can cause the experimentally observed increase in the viscosity of the solution of lecithin.

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## Computer simulation of excitation conductivity by qubit model

*Yuri Ozhigov and Nikita Skovoroda*

**Keywords:** dephasing assisted transport, quantum bottleneck, JCH model

We describe the computational model of quantum energy transfer in JCH like chains based on qubit representation of quantum states. The chain consists of optical cavities, each of which contains one two level atom interacting with field inside the cavity. Photons can jump between cavities that creates the effect of conductivity in the chain. Mathematical model of the conductivity is based on the qubit representation of quantum states in which any qubit has

the fixed physical sense. This allows to include the dephasing noise, input and output intensity and analyze the contra intuitive quantum effects like dephasing assisted transport (DAT) and quantum bottleneck. The program realization of the model is based on the package Mathematica and utilizes such adventages of object oriented programming as module structure of the programm. We represent the results of numerical simulation: the optimal output and input intensities, DAT and bottleneck.

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## Control and managing the HPC cluster in Siberian Supercomputer Center

*Nikolay Kuchin, Boris Glinsky, Igor Chernykh, Sergey Lomakin and Igor Makarov*

**Keywords:** HPC, Bach system, queue, PBS

The paper presents the experience of exploitation high-performance computing cluster installed in the Siberian Supercomputer Center (SSCC ICMMG SB RAS). SSCC has more than 150 users from more than 20 academic institutions. One important example of virtual computing environment is the integration KVM with batch system PBS Pro.

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## Delay structure mining in computing cluster

*Alexey Gorelov, Archil Maysuradze and Alexey Salnikov*

**Keywords:** communication environment of computing cluster, MPI programming model, message passing delays, information model of delays, communication environment diagnostics, delay data aggregation

We propose a new scheme for the collection and analysis of message passing delays from one MPI process to another. The proposed approach is abstracted from a specific implementation of network interaction between computing cluster nodes. It is argued that it is possible to collect data with special software systems and build adequate information model of delays. It is shown how to use this model in the communication environment diagnostics and the dynamic scheduling problems. All stages of the proposed scheme are illustrated with real data collected at Lomonosov Moscow State University supercomputer systems.

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## Design and development of distributed systems for iterative conjugation of sector hydrodynamic models

*Stanislav Samboretskiy*

**Keywords:** sector modeling, software system, oil and gas fields, distributed computing, parallel programming, fault tolerance, load balancing

This article presents the architecture of software, which is a distributed computing system to hydrodynamic modeling of oil and gas field. The simulation is based on an iterative algorithm of parallel conjugation of sector models by Schwartz's method. The original algorithm was parallelized only the basic steps. To achieve a greater degree of concurrency algorithm it was modified so that its implementation must be a distributed system. Describes of solving the problem of fault tolerance in the distributed system, approach to load balancing and tools for interaction between objects of the system.

# Development of high-performance GPU-based technique for morphological research of biological objects

*Nikolay Gavrilov and Vadim Turlapov*

**Keywords:** GPGPU, astrocytes, cells morphology, Monte-Carlo, surface integral

Surface-to-Volume Ratio, or SVR is one of the most important characteristics of biological objects' morphology. This measure characterizes the metabolism of a bio object and has inverse relation to its radius R as 1/R. We propose a method for local research of spatial morphology of bio objects in SVR terms. A new computational method was proposed to calculate the volume inside arbitrary mesh and a sphere intersection that is four times faster than a conventional Monte-Carlo method giving the same precision. GPU-implementation increased algorithm performance in 60 times.

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# Development of parallel linear solver for reservoir simulation on hybrid computing systems with GPUs

*Arthur Yuldashev, Ratmir Gubaidullin and Nikita Repin*

**Keywords:** graphics processors, sparse linear systems, multi-and many-core systems, parallel computing, reservoir simulation

Problem of hydrodynamic modeling of oil and gas fields is characterized by high consumption of computing resources. The present work aims to accelerate reservoir simulations through the use of hybrid computing systems with graphics processors, mainly to accelerate linear solver for numerical simulations of multiphase filtration.

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# Development of SIGMA software for the supercomputer simulation of coupled aerodynamic and thermomechanical processes in composite structures of high-speed aircraft

*Yury Dimitrienko, Mikhail Koryakov and Andrey Zakharov*

**Keywords:** coupled simulation, aerogasdynamics, thermomechanics, hypersonic flows, heat-and-mass transfer, thermodecomposition, polymer composites, heat displacement, thermotension, layering, parallel processing

An algorithm for the numerical simulation of coupled aerodynamic and thermomechanical processes in composite structures of high-speed aircraft is proposed, which allows to calculate all parameters of the three-dimensional aerogasdynamic flow near the surface of the aircraft, the heat exchange on the surface, the internal heat-and-mass transfer processes in the construction of thermodecomposition polymer composite material, and dynamic processes of heat displacement in the composite construction, including the effects of changes in the elastic characteristics of the composite, variable thermal deformation, shrinkage caused by thermodecomposition, the formation of the internal pore pressure in the composite. The computer-aided software package SIGMA that implements obtained algorithms and is capable to perform calculations on high-performance computers is developed. An example of the numerical solution of the coupled problem of a model composite construction of high-speed aircraft, showing the possibility of the proposed algorithm is given.

# Development of technological solutions in creating and using specialized hardware-software complex based on grid infrastructure supercomputer resources

*Oleg Tchij, Nikolay Paramonov, Marina Kuleshova and Nadzeya Paramonova*

**Keywords:** supercomputer, grid, data processing center

The results of the practical use of hardware-software complexes on the basis of a distributed supercomputing grid infrastructure resources for a variety of demanding applications. As a tool environment for research used an experimental model of the data center (DC) in the National Grid Segment-based cluster SKIF-GPU.

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# Distributed adaptive VoIP load balancing in hybrid clouds

*Andrei Tchernykh, Jorge M. Cortés-Mendoza, Alexander Drozdov, Pascal Bouvry, Ana-Maria Simionovici and Arutyun Avetisyan*

**Keywords:** Cloud computing, Load balancing, Voice over IP

Cloud computing as a powerful economic stimulus widely being adopted by many companies. However, the management of cloud infrastructure is a challenging task. Re-liability, security, quality of service, and cost-efficiency are important issues in these systems. They require resource optimization at multiple layers of the infrastructure and applications. The complexity of cloud computing systems makes infeasible the optimal resource allocation, especially in presence of uncertainty of very dynamic and unpre-dictable environment. Hence, load balancing algorithms are a fundamental part of the research in cloud computing. We formulate the problem of load balancing in distribut-ed computer environments and review several algorithms. The goal is to understand the main characteristics of dynamic load balancing algorithms and how they can be adapted for the domain of VoIP computations on hybrid clouds. We conclude by show-ing how none of these works directly addresses the problem space of the considered problem, but do provide a valuable basis for our work.

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# Domain decomposition method for supercomputer simulation of gravitating systems

*Nikolay Snytnikov and Vitaly Vshivkov*

**Keywords:** particle in cell, Poisson solver, Vlasov equation, gravitational potential

We present a new parallel algorithm for supercomputer simulation of collisionless gravitating systems. The algorithm combines particle-in-cell (PIC) method for solving Vlasov equation with parallel convolution FFT-based method for calculating gravitational potential of an isolated system. It uses a special domain decomposition technique for dynamical assignment of processors to subdomains. It is designed to address the specifics of simulating non-stationary rotating 2D/3D disks, in which PIC particles, representing collisionless matter, may cross computational domain for many times during the numerical experiment. Therefore there is a need to have an efficient load-balancing method. The parallel algorithm is suitable for running on supercomputers with different types of architectures: traditional (CPU-based), and hybrid (CPU with NVIDIA GPU and Intel Xeon Phi).

# Dynamic tuning methods of DVMH-programs for clusters with accelerators

*Vladimir Bakhtin, Alexander Kolganov, Victor Krukov, Natalya Podderugina and Mikhail Pritula*

**Keywords:** DVMH, high-level programming language, accelerator, coprocessor, GPU, MIC, NAS Parallel Benchmarks

DVM system is being developed at KIAM RAS with active participation of students and postgraduate students of CMC department of Lomonosov MSU. DVM system is designed for computational parallel program development in C-DVMH and Fortran-DVMH languages. These languages are directive-based extensions of standard C and Fortran languages and use a common parallel programming model (DVMH model). DVMH model enables creation of effective parallel programs (DVMH programs) for heterogeneous computational clusters exploiting multicore CPUs as well as various accelerators (GPUs and/or Intel Xeon Phi coprocessors). When using DVMH model, the programmer does not use explicit copy operation of data located in CPU or accelerators memory. For fragments of programs that can be executed on accelerators (regions), the programmer specifies the input and output data, and the data that is modified or used outside the region. This allows to dynamically select the devices that can be used for region execution, distribute the work between the devices in accordance with their performance, repeatedly perform the regions for the selection of the optimal configuration. The article demonstrates the effect of these methods on the effectiveness of some tests (NAS NPB Benchmarks), and real applications.

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# Educational and research systems for studying of parallel methods

*Evgeniy Kozinov, Victor Gergel, Alexey Linev and Anton Shtanyuk*

**Keywords:** parallel programming, high-performance computing, education, computer technology

Teaching supercomputing technologies is very important and complex task. A wide variety of computer systems and technologies complicate training process. Educational and research systems can help. We are presenting two such systems: ParaLab and ParaLib. User can select task from a predefined list. For a given method, and different initial conditions can be performed computational experiments. For tasks can be explored methods of implementation of parallel algorithms. ParaLab allows you visualize the solution of the problem on a simulated computer system, as well as to obtain estimates of the performance and efficiency of algorithms. ParaLib demonstrates the possibility of using various modern technologies of parallel programming and parallel languages for the task (for example OpenMP,MPI,Co-Array Fortran and Chapel). Both systems allow store results for later analysis. The open architecture allows students to add their own implementation of algorithms. ParaLab and ParaLib are used in teaching students in the Nizhny Novgorod State University.

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# Efficiency of ARM processors for classical molecular dynamics calculations

*Vsevolod Nikolskiy and Vladimir Stegailov*

**Keywords:** ARM architecture, floating point operations, efficiency, molecular dynamics

Supercomputing of the exascale era is inevitably limited by power efficiency. Nowadays different CPU architectures are considered as possible choices for these purposes. Recently the development of ARM processors has come to the point when their floating point performance can be seriously considered for a range of scientific applications. In this talk we present the analysis of the floating point performance of the latest ARM cores and their efficiency for the algorithms of classical molecular dynamics.

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## Experience of teaching of supercomputer technologies on the engineering directions in FSSFEI HPE “SUSU” (NRU)

*Natalia Dolganina*

**Keywords:** teaching, supercomputing technology, engineering education

Article is devoted to experience of teaching of supercomputer technologies on the engineering directions in Federal State State-Financed Educational Institution of High Professional Education "South Ural State University" (National Research University). The contents and the program of the course "Supercomputer Modelling of Technical Devices and Processes" which is taught in a magistracy on technical specialties, and also an order of teaching this subject are submitted.

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## Heterogeneous job consolidation for power aware scheduling with quality of service

*Fermin Armenta-Cano, Andrei Tchernykh, Jorge-Mario Cortés-Mendoza, Ramin Yahyapour, Alexander Drozdov, Pascal Bouvry, Dzmitry Kliazovich and Arutyun Avetisyan*

**Keywords:** Cloud computing, Service Level Agreement, Energy Efficiency, Multi-objective Scheduling, IaaS

In this paper, we present an energy optimization model of Cloud computing, and formulate novel energy-aware resource allocation problem that provides energy-efficiency by heterogeneous job consolidation taking into account types of applications. Data centers process heterogeneous workloads that include CPU intensive, disk I/O intensive, memory intensive, network I/O intensive and other types of applications. When one type of applications creates a bottleneck and resource contention either in CPU, disk or network, it may result in degradation of the system performance and increasing energy consumption. We discuss energy characteristics of applications, and how an awareness of their types can help in intelligent allocation strategy to improve energy consumption.

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## High-performance computing in bioinformatic analysis of protein superfamilies to design enzymes with new properties

*Dmitry Suplatov, Nina Popova, Kirill Kopylov, Maksim Shegay, Vladimir Voevodin and Vytas Švedas*

**Keywords:** high-performance computing, bioinformatic analysis, protein superfamilies, enzyme engineering, structure-function relationship

Growing capacity of bioinformatic databases provides new opportunities to study structure-function relationship in large protein superfamilies and greatly increases the demand for high

performance computing. However, the general-purpose parallel computing clusters do not provide optimal accommodation to bioinformatic applications which are usually written using openMP rather than MPI, Java or even Perl and Python. Distributed computing platforms are available as an inexpensive alternative but they lack the power of a dedicated computing cluster. Based on the Lomonosov Moscow State University supercomputer complex we are developing a platform which implements computational methods of bioinformatic analysis, molecular modeling and computational chemistry to study the structure-function relationship in large enzyme superfamilies and produce novel biocatalysts with improved properties. Co-design of cluster's hardware and software according to demands of computational biology will provide a solution for large-scale tasks of biocatalysis. Homologous enzymes have evolved from a common ancestor to retain a general function but diverged in more specific features and can be divided into subfamilies with different functional properties such as catalytic activity, substrate specificity, enantioselectivity, stability, etc. Analysis of sequence and structural information in protein superfamilies is a promising trend in order to rationalize enzyme engineering and move away from unguided evolutionary stochastic approaches and empirical design. We have recently developed a new method of bioinformatic analysis to identify function-related variable residues in protein structures that are responsible for functional divergence within superfamilies of homologous enzymes. The developed methodology has been applied to study structure-functional relationship in various enzyme superfamilies: α/β-hydrolases, Ntn-hydrolases, penicillin-binding proteins, etc. Systematic bioinformatic analysis of genomic and structural information corresponding to each selected superfamily of enzymes has been carried out to identify functionally important amino acid residues as hotspots for enzyme engineering. It has been shown that bioinformatic analysis can be effectively used to design enzyme mutants with improved catalytic properties and to predict functional properties of enzymes. There is a need to implement these computationally demanding algorithms into the common laboratory practice to study the structure-function relationship in proteins and develop novel protein engineering strategies.

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# High-performance simulations of continuously variable transmission dynamics

*Stepan Orlov, Natalia Melnikova, Yury Ispolov and Nikolay Shabrov*

**Keywords:** continuously variable transmission, multi-body dynamics, contact interaction, supercomputing

The paper describes a parallel computational model simulating continuously variable transmission (CVT) dynamics. A specific feature of the CVT model is the combination of relatively small problem sizes (about 1000 unknowns) and high computational costs (up to several weeks of sequential code computations for a thirty seconds simulation period). The main source of computational complexity here is the calculation of non-linear contact forces acting between pulleys and chain parts at each step of the explicit time integration procedure. Below we analyze simulation workflow and runtime load distribution among the application modules. Based on the profiling data, we present a task parallel multithreaded implementation of the model over shared memory and discuss steps towards further parallelization.

# How to reach GreenGraph500 top with FPGA-based supercomputer? Theory and practice

*Anatoliy Sizov and Sergey Elizarov*

**Keywords:** Field-Programmable Gate Array, Hybrid computing systems, application-specific supercomputer, breath first search algorithm, low latency communications processor, low latency memory controller, green graph 500, graph

World achievements in energy-efficient Field-Programmable Gate Array (FPGA), wide experience in reconfigurable application-specific supercomputers field and new FPGA-based low latency communications processors and memory controllers allows us to assume excellent efficiency for custom FPGA-based supercomputers on GreenGraph500 benchmark. In this paper breath first search (BFS) algorithm implementation on FPGA systems are discussed. One node consisting of FPGA Kintex Ultra Scale with 4 RLDRAMIII memory controllers, and BFS algorithm are examined. 32 nodes system performance are estimated, energy-efficient calculated using GreenGraph500 criteria.

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# Hydrogeological modeling in radioactive waste disposal safety assessment using the GeRa code

*Ivan Kapyrin, Igor Konshin, Kopytov German, Kirill Nikitin and Yuri Vassilevski*

**Keywords:** groundwater flow, transport in porous media, reactive transport, density-driven flow, disposal safety assessment

The challenges of hydrogeological modeling in the framework of radioactive waste disposal safety assessment are discussed. Analysis of the ongoing projects shows three major trends in code development: increasing models complexity; codes "born parallel"; adaptive polyhedral grids and suitable high-order numerical schemes. These concepts are demonstrated using the GeRa (Geomigration of Radionuclides) numerical code in terms of a couple of advanced models: reactive transport, unsaturated flow and transport in vadose zone, density-driven flow.

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# Implementation of e-learning management system at the faculty of Computational mathemetics and informatics of South Ural State University for supercomputer technologies learning

*Peter Mekaev and Pavel Kostenetskiy*

**Keywords:** E-learning management system, Personal virtual desktop, Cloud technologies, Moodle

This article describes the experience of implementing e-learning management system supercomputer technologies at the faculty of Computational Mathematics and Informatics of the South Ural State University previously sold under the cloud platform «Personal virtual desktop». The comparison of modern e-learning systems. Described the causes and the transition from a closed source «Competentum» to open source software «Moodle». Describes how to use the software Apache Jmeter as a load-testing tool for of e-learning; examples of parameters for assessing load testing progress results. Discusses the use of Microsoft Windows Server OS and Ubuntu OS as platforms for e-learning management

system installation «Moodle», the results of stress testing the system on OS data. Examples of additional modules that extend the functionality of an e-learning management system «Moodle», established in the course of implementation of the system in the learning process of teachers.

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## Influence of spontaneously formed crystalline inclusions on the mechanical properties of amorphous polymer matrix

*Dmitry Gusarov, Viktor Ivanov, Pavel Komarov, Alexei Khokhlov, Yuung-Ching Sheen, Yang-Shan Lin and Cheng-Hung San*

**Keywords:** multiscale computer modeling, polymer nanocomposites, mechanical properties of polymeric materials

One of the possible ways to increase the strength of the polymeric materials is the formation of reinforcement domains treated in situ during the microphase separation of the polymer matrix after adding various fillers. To narrow the field of experimental research, hybrid calculation schemes can be involved based on the concept of multi-scale modeling. In this approach, you can study almost any material on the basis of their chemical structure, the quantitative ratios of the components and physical conditions. The report discusses the development of the scheme of multiscale modeling of polymer composites with nanoparticles and two-phase heterogeneous polymer systems. Simulation of material samples at different external loads and temperatures allows us to study the response of the internal structure of the material and study thermal and mechanical properties of the material. This requires a fairly large amount of computations that can be implemented on modern supercomputers that allow to study samples of polymer nanocomposites in a wide range of parameters. To illustrate the implementation of the scheme, the report discusses the first results of the calculations on the effect of the chemical structure of polyurethanes formed microdomains in the matrix and the mechanical properties of the sample material.

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## Information and mathematical software for the aerospace systems of remote sensing and the radiation forcing on the Earth's climate to predict the consequences of development of the Arctic region and computing

*Tamara Sushkevich, Sergey Strelkov and Svetlana Maksakova*

**Keywords:** information, mathematical, software, aerospace, systems, remote, sensing, Arctic

In 2015 the world scientific community celebrates the day of memory of the greatest scientists who stood at the origins creation of the great scientific inheritage of the theory of radiation transfer in a natural and artificial environments and its application in space projects, as well as in astrophysics, climatology, meteorology, remote sensing, global monitoring of dangerous objects and consequences of natural and anthropogenic disasters, etc. The report will talk about national achievements at the world level in the theory of radiation transfer in a natural environments and on developing in modern Russia's the modern scientific potential, which adequately provides the methodological basis for the theoretical and computational researches of the radiation processes and the radiation fields in the Arctic region with the use of supercomputers and distributed computing infrastructure with a network computing.

# Integration of Russian Tier 1 center with HPC at NRC "Kurchatov Institute"

*Ivan Tertychnyy, Ruslan Mashinistov, Alexander Novikov, Alexey Poyda, Alexei Klimentov and Eygene Ryabinkin*

**Keywords:** HPC, Grid, Distributed computing

LHC experiments preparing for the precision measurements and further discoveries that will be made possible by much higher LHC collision rates from 2015 (Run2). The need for simulation, data processing and analysis and would overwhelm the expected capacity of WLCG computing facilities unless the range and precision of physics studies were to be curtailed. To meet this challenge the integration of the opportunistic resources into LHC computing model is highly important. Tier-1 facility at Kurchatov Institute (NRC-KI) in Moscow is a part of WLCG and it will process and store up to 10% of total data obtained from ALICE, ATLAS and LHCb experiments. In addition Kurchatov Institute has supercomputers with peak performance 0.12 PFLOPS. Delegation of even a fraction of supercomputing resources to the LHC Computing will notably increase total capacity. In 2014, we have started a pioneer work to develop a portal combining a Tier-1 and a supercomputer in Kurchatov Institute. This portal is aimed to provide interfaces to run Monte-Carlo simulation at the Tier-1 Grid and supercomputer, using common storage. PanDA (Production and Distributed Analysis) workload management system having great results at the ATLAS was chosen as underlying technology.

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# Integrative possibilities of the course "Parallel Programming"

*Irina Zakharova and Alexander Zakharov*

**Keywords:** IT-education, parallel programming, course content

This paper describes the features of the parallel programming course content for the programs "Software and Administration of Information Systems" and "Information Security". We present the experience of teaching algorithms and parallel programming techniques in the general courses and as an independent discipline. We draw the possibilities of integrative separate course for generalization, understanding and applying knowledge of programming, computer graphics and applied mathematics in practice projects.

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# Investigation of graphics processors efficiency on the example of quantum-chemical modeling of the complex of chitosan

*Arthur Yuldashev, Vladimir Lazarev and Vladimir Spele*

**Keywords:** graphics processors, quantum chemical modeling, molecular complex of chitosan

The report presents the experience of using graphics processors for quantum chemical calculation of the optimum geometry of the molecular complex of chitosan.

# Iterative modeling using supercomputer for reengineering semiconductor devices and analyzing their radiation resistance

*Alexander Potehin, Serge Obolenskiy, Alexey Liniov and Alexander Puzanov*

**Keywords:** physic-topological modeling, semiconductors, evaluation of thermal fields

The features of physic-topological modeling of radiation resistance of semiconductor devices are discussed. The composition of software for calculating the parameters of semiconductor devices are defined. The program for calculating thermal fields in semiconductor devices are created and discusses the features of its application in conjunction with the physic-topological model.

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# Massively parallel hybrid algorithm for simulation of seismic wave propagation in complex media

*Victor Kostin, Vadim Lisitsa, Galina Reshetova, Vladimir Tcheverda and Dmitry Vishnevsky*

**Keywords:** Domain decomposition, finite differences, wave propagation, MPI, hybrid algorithm

This paper presents a problem-oriented approach, designed for numerical simulation of seismic wave propagation in models containing geological formations with complex properties such as anisotropy, attenuation, and small-scale heterogeneities. Each of the named property requires special treatment which increases computational complexity of the algorithm in comparison with ideally elastic isotropic media. At the same time these formations are typically relatively small taking up to 25% of the model, thus the computationally expensive approaches can be used only locally to speed-up the simulations. In this paper we discuss both mathematical and numerical aspects of hybrid algorithm paying the main attention to its parallel implementation.

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# Mathematical and numerical modeling of multidimensional quasi-stationary electromagnetic fields in the channel of electrodynamical launchers

*Mikhail Galanin*

**Keywords:** mathematical, modeling, electromagnetic, fields, launchers

The necessity of solving the problems of modeling of electrodynamical accelerators arises from the needs of science and technology. In particular, such devices allow achieving a unique speed of macrobodies, exceeding the speed given by the conventional powder accelerators. It allows you to create new instruments and devices to study the behavior of matter at ultrahigh velocities, pressures, etc. Effective design of such devices, as well as research of phenomena taking place in them, without mathematical modeling is impossible. The report presents methods of mathematical modeling of quasi-stationary electromagnetic fields in inhomogeneous regions of the accelerator channel (including time-varying, incoherent and nonsmooth boundaries of the subdomains), built and implemented computational algorithms for the simulation of electromagnetic acceleration process in these areas, methods of computational experiment for study of the erosion of the metal contact, as well as qualitative features of the distributions of electromagnetic fields in the channel of the accelerator during starting.

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The work was executed under partial financial support of RFBR (project No. 15-01-03073).

## Matrix methods for fluid mechanics problems

*Michael Ermakov*

**Keywords:** supercomputing, matrix methods, Navier-Stokes equations, MUMPS, ARPACK

A matrix approach is used for modeling and stability analysis of axisymmetrical fluid flows for the Navier-Stokes equations in Boussinesq approximation. Advantages of the matrix approach consist in an unnecessity of equations splitting and an unnecessity of a partial method building for equations solution. For the solution of a system of discretized Navier-Stokes equations the matrix Newton method is employed. At each iterations a linear system for a vector of the full set of unknowns and for the Jacobian matrix is solved. For a flow stability analysis against 3-D disturbances, are being considered as a decomposition of normal modes in azimuthal direction, the inverse iterations and Arnoldi methods (ARPACK) are used. For a linear-system solution the direct method (MUMPS) is used. Due to application of matrix approach for numerical benchmark for Czochralski method of crystal growth, it was possible to get a solution for superfine mesh with 125M unknowns by use of 65 processors (24 GB) of the "Lomonosov" supercomputer.

## Method for reducing graph of communication delays in for visual analysis

*Alexey Salnikov and Nikolay Zhukov*

**Keywords:** weighted graphs, clustering algorithm, communications delays, compute cluster

There discussed methods for visualizing huge graphs where edges marked by distances between vertices. The goal is to reduce graph complexity of huge graph in context of visual analysis of delays. There we have used some methods of clusterization which save egde distances. This method usability has been tested on data about delays arrived in communications of Lomonosov supercomputer.

## Method of predicting the binding constants of steroids based on artificial neural networks

*Irina Fedyushkina, Ilacai Romero Reyes, Vladlen Skvortsov and Inna Levina*

**Keywords:** artificial neural networks, progesterone receptor, steroids, parallel computation, GPU

The system for prediction the values of binding constants of steroids with progesterone receptor on the basis of parameters, calculated from the ligand structures and from molecular modeling of protein/ligand complexes was developed. The original implementation of the artificial neural networks was used for correlated these values.

## Methods for increasing optimisation for large scale parallel computing experiments on unstructured grids

*Sergey Sukov*

**Keywords:** parallel algorithms, numerical simulation, unstructured grids

Methods are presenting for increasing optimisation for computing experiments on huge unstructured grids. Results of propositional algorhytmes testing are presented by the example of calculations using tetrahedral grids containing to 1.5 billion elements.

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## Microservices cloud applications testing approach

*Dmitry Savchenko and Gleb Radchenko*

**Keywords:** Cloud computing, Microservices, SOA, Fine-grained SOA

Microservice architecture is a cloud application design pattern that implies that the application is divided into a number of small independent services, each of which is responsible for implementing of a certain feature. The need for continuous integration of developed and/or modified microservices in the existing system requires a comprehensive validation of individual microservices and their co-operation as an ensemble with other microservices. In this paper, we would provide an analysis of existing methods of cloud applications testing and identify features that are specific to the microservice architecture. Based on this analysis, we will try to propose a validation methodology of the microservice systems.

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## Modeling distributed column indexes in the context of parallel database systems

*Stepan Prikazchikov and Pavel Kostenetskiy*

**Keywords:** DMM model, database multiprocessor, parallel data processing, multicore accelerators, distributed column indexes

The paper is devoted to extending of the mathematical model of database multiprocessor DMM [Kostenetskii P.S., Sokolinsky L.B. Simulation of Hierarchical Multiprocessor Database Systems // Programming and Computer Software. Vol. 39 No. 1. 2013. P. 10–24.] for parallel data processing using multicore accelerators and development on this basis of methods and algorithms for the simulation of processes in parallel processing of transactions. Extended model allows simulating and analyzing distributed column indexes in the context of parallel database systems.

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## Modeling the dynamics of the formation of clusters of radiation defects with the use of high-performance computing

*Alexsander Puzanov, Sergey Obolensky, Vladimir Kozlov, Ekaterina Volkova, Alexsander Potehin and Ilya Zabavichev*

**Keywords:** radiation defects, high-frequency response, high-performance computing

It is proposed to use a high-frequency response of semiconductor nano-meter diodes caused ionized electrons curent in the time of formation of clusters of radiation defects (CRD) for the

experimental study femtosecond and picosecond processes of formation of CRD. The results of the theoretical calculations obtained by high-performance computing and test experiments confirmed the feasibility of such an experiment.

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## Modern high-performance reconfigurable computer systems based on Xilinx Virtex-7 and Virtex UltraScale FPGAs

*Ilya Levin, Alexey Dordopulo, I. Kalyaev, Yu. Doronchenko and M. Raskladkin*

**Keywords:** Field programmable gate array, Reconfigurable computer systems, FPGA

The paper covers architectures and comparison characteristics of reconfigurable computer systems (RCS) based on field programmable gate arrays (FPGAs) of the Xilinx Virtex-7 family and technologies of task solving by means of software development tools. In the paper we also consider architecture and assembly of next-generation RCS with a liquid cooling system and give results of calculations and prototyping of principal technical solutions which provide the performance of 1 PFlops for a standard computational 47U rack with the power of 150 kWatt. This is promising approach because of RCS with a liquid cooling system have a considerable advantage for lot of engineering and economical parameters such as real and specific performance, power efficiency, mass and dimension characteristics, etc., in comparison with similar systems.

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## MPI implementation of dimension reduction multilevel scheme for parallel solving the global optimization problems

*Alexander Sysoyev, Konstantin Barkalov, Victor Gergel and Ilya Lebedev*

**Keywords:** global optimization, information-statistical algorithm, dimension reduction, multilevel scheme, synchronous scheme, asynchronous scheme, cluster

The paper presents the new approach to solve the global optimization problems that combines the information-statistical algorithm developed in the University of Nizhni Novgorod with multilevel scheme of dimension reduction. A parallel algorithm that implements such approach is suggested and its synchronous and asynchronous MPI implementation is presented. The advantage of asynchronous scheme is shown by comparing with synchronous one.

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## Multiscale modelling approach to property prediction: hypercrosslinked polystyrene

*Alexei Lazutin, Anna Glagoleva, Mikhail Glagolev and Valentina Vasilevskaya*

**Keywords:** multiscale modelling, hypercrosslinked polystyrene, mapping/reverse mapping

A multiscale modelling algorithm is suggested to simulate the crosslinking of the polystyrene dissolved in dichloroethane by monochlorodimethyl ether. The algorithm comprises consecutive stages: molecular dynamics atomistic simulation of a polystyrene solution, the mapping of atomistic structure onto coarse-grained model, the crosslink formation, the reverse mapping, and finally relaxation of the structure. The calculated values of the specific surface and the elastic modulus are in reasonable quantitative correspondence with experimental data.

# Numerical modeling of interacting galaxies on Intel Xeon Phi supercomputers

*Igor Kulikov, Igor Chernykh, Vladislav Nenashev and Eugenya Katysheva*

**Keywords:** Numerical modeling, parallel computing, parallel numerical method, computational astrophysics, interacting galaxies, Intel Xeon Phi accelerators

A new hydrodynamic numerical simulation of interacting galaxies on hybrid RSC PetaStream supercomputers by means Intel Xeon Phi accelerator was presented. The numerical model of interacting galaxies on systems of hyperbolic equations for hydrodynamical and collisionless components was based. The subgrid physics (star formation, supernovae feedback, molecular hydrogen formation, cooling/heating function) was included. The details of parallel development and efficiency co-design elements of numerical algorithm was described. A speed-up of 134 times was obtained within a single Intel Xeon Phi accelerator. The use of 64 Intel Xeon Phi accelerators resulted in 92 % parallel efficiency.

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# Numerical models of helical electron beams for cyclotron resonance-based masers

*Aleksey Kuntsevich and Vladimir Manuilov*

**Keywords:** parallel computing, cyclotron resonance maser, numerical models

The paper describes the hierarchy of numerical models used for calculation of properties of intense helical electron beams (HEBs) aimed to be used as a power source in powerful cyclotron resonance-based masers. Described set of numerical simulation models includes both static (for preliminary optimization of HEB properties) and dynamic models. The latter are based on method of big particles and allow simulate oscillatory processes in HEBs and thus determine the stability level of HEB. The possibility of using parallelization of calculations based on different approaches (Posix threads, OpenMP and TPL) to increase the calculation speed for the number of particles more than one million are discussed. The first implementation attempts of such approach are presented.

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# Numerical solution of kinetic equations for high-speed rarefied gas flows

*Vladimir Titarev*

**Keywords:** kinetic equations, unstructured mesh, parallel computing

Analysis of aerodynamics of re-entry vehicles of realistic shape requires the development of computational methods for rarefied gas flow modeling. The present work is devoted to the problem of creating efficient parallel method and parallel software to solve the kinetic equation with the model collision integral of E.M. Shakhov on modern multi-core CPU as applied to such problems. As a test calculation, the high speed rarefied gas flow over the reentry space vehicle model of TsAGI is considered.

## Octoshell: large supercomputer complex administration system

*Sergey Zhumatiy, Dmitry Nikitenko and Vladimir Voevodin*

**Keywords:** computing center, administration, user management, Octoshell

Managing and administering of modern supercomputer centers and HPC systems as a part is a complicated and complex task. The usage of numerous traditional stand-alone tools for administering and management of supercomputers becomes a bottleneck for efficient resource utilization in conditions of growing systems scale. The developed "Octoshell" system for support of running supercomputer centers is aimed at solving this problem. It implements essential tools for administering in a single interface and allows significant automatization of typical management tasks ensuring higher efficiency of large supercomputer complex output as a whole.

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## On parallel programming paradigms

*Lidia Gorodnyaya*

**Keywords:** educational programming languages, programming paradigms, functional models, parallel programming

The work describes research and specification of basic paradigms of programming. The author analyzes and compares special features of parallel programming languages. A functional model of comparative description of implementation semantics of basic paradigms is proposed. The author proposes a scheme of describing and defining paradigm features of programming languages.

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## On the experience of development and teaching the lecture course "Parallel numerical methods" in University of Nizhny Novgorod

*Konstantin Barkalov, Iosif Meyerov and Sergey Bastrakov*

**Keywords:** numerical methods, parallel algorithms, educational materials, lecture course

This work summarizes experience of the authors obtained during development of educational materials and teaching the lecture course "Parallel numerical methods" in Master's degree programme in Lobachevsky State University of Nizhny Novgorod. We demonstrate the relevance of developing the course on parallel numerical methods. General description of the Master's curriculum and the position of this course in the curriculum as well as main requirements to students are given. We present methods of organizing practice and laboratory works and evaluation of student performance. References to the website of the Volga Research and Education Center for Supercomputing Technologies that contains all presented materials in free access are given.

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## Operator library for solving of mathematical physics problems on locally adaptive grids using CUDA

*Michael Krasnov*

**Keywords:** Locally adaptive grids, Grid functions, Grid operators, Heterogeneous systems, CUDA

This paper describes a library of operators to work on grid functions defined on three dimentional locally adaptive grids. The functions is designed so that the details of its implementation are hidden from the user, allowing effective implementation on machines with different implementation (hybrid, parallel, etc.), including CUDA. The library creation raises several goals: the approximation of the appearance of the program to the theoretical formulas, the relative ease of use, including the work on the graphics card with CUDA architecture, computational efficiency.

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## Optimal checkpointing to the local storage device

*Aleksey Bondarenko and Mikhail Iakobovski*

**Keywords:** Parallel computation, checkpoints, fault tolerance

We consider the fault tolerance technique based on saving checkpoint files on the local node. We are proposing a division of failures into two kinds: light and heavy failures. For this separation we obtain the optimal checkpoint interval. Examples show that if MTBF is less than an hour then tools working with light and heavy failures reduce the computation time by more than 10%.

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## Optimized diamond photonic molecule for quantum communications

*Maxim Rogachev, Igor Kateev and Alexander Tsukanov*

**Keywords:** quantum communications, photonic molecule, microresonator

We propose the diamond structure, which can be used for an experimental study of spectral and dynamic properties of a photonic molecule formed by a chain of microresonators (disks or rings). The set of structure parameters that establishes an equally-weighted photonic mode is found. Spectroscopic modeling of photoluminescence is carried out in the weak driving regime.

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## Optimized implementation of HPCG benchmark on supercomputer with “Angara” interconnect

*Alexander Agarkov, Alexander Semenov and Alexey Simonov*

**Keywords:** HPCG, "Angara" interconnect, SHMEM, vectorization, OpenMP

The paper presents the optimized implementation of the HPCG benchmark on "Angara" interconnect developed by "NICEVT". HPCG implements conjugate gradient method with preconditioner to solve a sparse linear system. The proposed implementation includes compute node optimizations, such as new sparse matrix storage format, OpenMP-parallelization and vectorization, as well as interprocess communication optimizations targeted for "Angara" interconnect by using the SHMEM library instead of MPI. Compute node optimization includes changing the sparse matrix storage format, OpenMP-parallelization and vectorization. Obtained performance results on the cluster with "Angara" interconnect significantly exceed the results of the HPCG 2.4 reference implementation.

# Parallel algorithm for local-best-match time series subsequence similarity search on the Intel MIC architecture

*Aleksander Movchan and Mikhail Zymbler*

**Keywords:** time series data mining, subsequences similarity search, parallel algorithm, OpenMP, Intel Xeon Phi

The paper touches upon the problem of local-best-match time series subsequence similarity search that assumes that a query sequence and a longer time series are given, and the task is to find all the subsequences whose distance from the query is the minimal among their neighboring subsequences whose distance from the query is under specified threshold. The Dynamic Time Warping (DTW) is used as a distance metric, which currently is recognized as the best similarity measure for most time series applications. However, computation of DTW is an expensive operation, in spite of the existing sophisticated software approaches. Existing hardware approaches to DTW computation involve GPU and FPGA architectures and ignore the potential of Intel Many Integrated Core architecture. The paper proposes a parallel algorithm for solving this problem using both the CPU and Intel Xeon Phi many-core coprocessor. The implementation is based on the OpenMP parallel programming technology and offload execution mode, where part of the code and data is transmitted to the coprocessor. The algorithm utilizes a queue of subsequences on the processor side, which are uploaded to the coprocessor for the DTW computations. The results of experiments confirms the effectiveness of the algorithm.

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# Parallel algorithm for mathematical modeling of interaction of a strong shock wave with a molecular cloud

*Boris Rybakin, Valery Goryachev, Lyuben Stamov and Elena Mikhalchenko*

**Keywords:** parallel computing, shock waves, ablation, fragmentation MC

Results of numerical simulation of (SCI) interaction between strong (SW) shock wave generated after supernova explosion and molecular cloud (MC) have been presented in three-dimension gas-dynamical arrangement. Mach number of hypersonic SW is accepted by seven. Statement of problem: the compressed supernova remnants gas with plane frontal shock wave with hypersonic velocity runs into spherical cloud and interacts with more dense gas of the cloud. Developed computational code is based on numerical solution of the Euler equations for compressible flow. Gas flow equations were represented conservatively for velocities components, density and energy. The parallel in-house code using OpenMP for PC hybrid system was developed for modeling. The Intel Vtune Amplifier XE was used to profile the code using GPU. More than a quarter of billion cells mesh (1024x512x512) with effective resolution for cloud radius in 124 nodes was implemented. Peculiarities of molecular cloud forming and density fragmentation in time were analyzed during time-consuming simulation. Shock wave strikes the cloud, triggering weak reflected shock waves and transmitted shock that advances in to the cloud. Inner-cloud SW compresses and defragment MC media. Post-processing used allow to find out the circumstances of vortex transfer in MC, ablation and erosion phenomena.

## Parallel algorithm for solving large-scale dynamic general equilibrium models

*Nikolai Melnikov, Arseniy Gruzdev, Michael Dalton and Brian O'Neill*

**Keywords:** general equilibrium models, nonlinear systems of equations, iterative methods, parallel computing, OpenMP, MPI

We present a parallel algorithm for computing an equilibrium path in a large-scale economic growth model. We exploit the special block structure of the nonlinear systems of equations common in such models. Our algorithm is based on an iterative method of Gauss-Seidel type with prices of different time periods calculated simultaneously rather than recursively. We have implemented the parallel algorithm in OpenMP and MPI programming environments. The numerical results show that speedup improves almost linearly as number of nodes increases. Different methods for solving the individual block: Newton-type methods, Krylov methods and trust region methods, give similar results for the speedup.

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## Parallel algorithm for sparse QR decomposition of a rectangular upper quasi triangular matrix with ND-type sparsity

*Sergey Kharchenko*

**Keywords:** sparse rectangular matrix, upper quasi triangular matrix, nested dissection, volume partitioning, QR decomposition, Householder transformations, parallel algorithm, SLAE, least squares problem

The paper considers algorithm for computing sparse QR decomposition of a specially ordered rectangular matrix. Decomposition is based on block sparse Householder transformations. For ordering computations the ND-type ordering for sparsity of ATA matrix can be used, here A - original rectangular matrix. For mesh based problems the ordering can be constructed starting from appropriate volume partitioning of the computational mesh. Parallel computations are based on sparse QR decomposition for sets of rows with additional zero block at the beginning. The suggested algorithm is planned to be used as main computational kernel in the developed by the author parallel iterative algorithms for solving SLAEs and least squares problems. The corresponding algorithms will be based on composition of the subspaces represented by sparse bases.

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## Parallel clustering algorithm for Intel Xeon Phi coprocessor

*Timofey Rechkalov*

**Keywords:** clustering, PAM, Intel Xeon Phi, OpenMP

Article describes parallel version of Partitioning Around Medoids algorithm for Intel Xeon Phi coprocessor. It is based on OpenMP technology. Loop operations adopted for vectorization. Algorithm uses distance matrix in coprocessor memory. Experiment results show effectiveness of suggested approach.

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## Parallel computing in identification of steel corrosion processes

*Marat Enikeev and Irek Gubaydullin*

**Keywords:** Parallel computing, metal corrosion, computer vision, image processing

The purpose of this paper is investigation of corrosion process using method of computer vision. GPU using to process experiment.

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## Parallel implementation of extended Petri nets in the low-level modeling of traffic

*Nikolay Ershov*

**Keywords:** Petri nets, urban traffic simulation, graph partitioning, coarse-grained parallelism

This paper is devoted the problem of the microscopic simulation of urban road traffic by using extended Petri nets. The relevance of the microscopic approach to the modeling of road traffic is determined by the extensive development of parallel programming systems. This paper discusses the issues of coarse-grained parallel implementation of Petri nets on multiprocessor computer systems using MPI technology. This work was supported by RFBR (grant №14-07-00628 A).

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## Parallel implementation of the sparse QR decomposition for rectangular upper quasi triangular matrix with ND-type sparsity

*Sergey Kharchenko and Alexey Yushchenko*

**Keywords:** sparse rectangular matrix, upper quasi triangular matrix, nested dissection, QR decomposition, Householder transformations, MPI, multithreading, SIMD

The paper considers parallel MPI+threads+SIMD implementation of the algorithm for computing sparse QR decomposition of a specially ordered rectangular matrix. Decomposition is based on block sparse Householder transformations. The algorithm starts with independent parallel QR decompositions for sets of matrix rows; and then, according to the computations tree, the QR decomposition is performed for matrices, combined with elements of R factors of rows decompositions. The results of numerical experiments for test problems show efficiency of the parallel implementation. The algorithm can also be efficiently implemented on heterogeneous cluster architectures with GPGPU accelerators.

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## Parallel linear systems solution for multiphase flow problems in the INMOST framework

*Igor Konshin, Igor Kaporin, Kirill Nikitin and Yuri Vassilevski*

**Keywords:** INMOST, distributed meshes, linear systems, multiphase filtration

The solution on parallel computers of multiphase flow problems is considered. To store and operate with distributed mesh data on the problem discretization stage the INMOST program platform was exploited. The resulting linear systems were solved by the overlapping additive Schwarz method from PETSc package was well as by the developed linear solver on the base of BIILU2 method. The results of numerical experiments for different parallel computers were presented and analyzed. The efficiency of the INMOST platform and the involved linear solvers was demonstrated.

# Parallel partitioning tool GridSpiderPar for large mesh decomposition

*Evdokia Golovchenko and Mikhail Yakobovskiy*

**Keywords:** parallel programming, graph partitioning, mesh decomposition

The problem of load balancing arises in parallel mesh-based numerical solution of problems of continuum mechanics, energetics, electrodynamics etc. on high-performance computing systems. The number of processors to run a computational problem is often unknown. It makes sense, therefore, to partition a mesh into a great number of microdomains which then are used to create subdomains. Graph partitioning methods implemented in state-of-the-art parallel partitioning tools ParMETIS, Jostle, PT-Scotch and Zoltan are based on multilevel algorithms. That approach has a shortcoming of forming unconnected subdomains. Another shortcoming of present graph partitioning methods is generation of strongly imbalanced partitions. The program package for parallel large mesh decomposition GridSpiderPar was developed. We compared different partitions into microdomains, microdomain graph partitions and partitions into subdomains of several meshes (10^8 vertices, 10^9 elements) obtained by means of the partitioning tool GridSpiderPar and the packages ParMETIS, Zoltan and PT-Scotch. Balance of the partitions, edge-cut and number of unconnected subdomains in different partitions were compared as well as the computational performance of gas-dynamic problem simulations run on different partitions. The obtained results demonstrate advantages of the devised algorithms.

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# Parallel program complex for numerical weather prediction and climate modeling

*Mikhail Tolstykh, Rostislav Fadeev and Vassily Mizyak*

**Keywords:** Parallel implementation of the global atmosphere model, Global atmosphere model, Numerical weather prediction, Climate changes modelling

The global atmosphere SL-AV model (Semi-Lagrangian, based on Absolute Vorticity equation) has been introduced into the operational practice at Hydrometeorological center of Russia in 2010. This allowed to reduce considerably the gap between Russia and the leading group of world prediction centers in medium-range weather forecasts. The new version of the SL-AV model is developed. This version has the horizontal resolution about 20 km over the Russia territory for numerical weather prediction, and it can be applied to the atmosphere forecast at time scales about ten days. This version is certified by Roshydromet recently. The same model version having coarser resolution is validated with a problem of climate change modelling using the AMIP2 protocol. The program complex of the SL-AV model new version uses a combination of MPI and OpenMP parallel programming technologies and currently scales up to 1700 cores. To increase the file system efficiency, the parallel input-output system is developed that can be connected as a separate parallel program component. It can use if necessary some computing nodes for input/output operations. The parallel input-output system is introduced into the SL-AV model and observations data assimilation system based on the ensemble Kalman filter. Overall system performance is shown with the examples of numerical atmosphere modelling in various modes. Also, the work on memory access optimization is carried out in the model program complex. This increased the parallelization efficiency.

## Parallelization efficiency of model of joint implant with finite element software

*Razim Garipov, Polina Maximova, Aliya Gainetdinova and Alfiya Yamileva*

**Keywords:** Joint implant, finite element analysis, ANSYS, Abaqus

Joint implants simulation allows investigating the effect of implant's and bone's shape on stress-strain state of bony tissue. A simulation is resource-intensive due to the complex geometry and the large number of contacts in model. So it requires using supercomputer technologies actually on simplified simulation. A parallelization study with different software of finite element analysis is necessary for obtaining of resource efficient computer model. Comparison of computation results which obtained with Simulia/Abaqus and ANSYS Mechanical was performed.

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## Perspectives of exascale computing for novel energy technologies

*Vyacheslav Vecher, Nikolay Kondratyuk, Genri Norman, Nikita Orekhov, Vasiliy Pisarev, Grigory Smirnov and Vladimir Stegailov*

**Keywords:** energy technologies, multiscale models, molecular dynamics

The development of novel energy technologies essentially relies upon multiscale modelling and simulation which success crucially depends on the progress in supercomputing. In this talk we review several vivid examples of the problems that we solve using atomistic and multiscale models and the best supercomputers in Russia: properties gas hydrates and gas condensate, rheology of organic liquids and development of polymer materials. The wider context is presented as well with the corresponding examples from the DOE INCITE program. On the basis of the case studies considered we discuss the issues of hardware efficiency, software scalability, input-output problems and data processing.

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## “Programming and optimization for Intel Xeon Phi” course

*Alexey Linev, Iosif Meyerov, Alexander Sysoyev, Sergey Bastrakov, Anton Gorshkov and Alexey Svistunov*

**Keywords:** Intel Xeon Phi, Many Integrated Core Architecture, computer architecture courses, high performance computing, parallel programming, software optimization

In this work we discuss the problem of teaching programming for Intel Xeon Phi architecture. We present practice-oriented approach accompanied with extensive practical part. Our method has a distinctive feature of combined usage of classical teaching examples in the area parallel programming and real problems form areas of computational physics and financial mathematics. This work contains description of developed "Programming and Optimization for Intel Xeon Phi" course and it's approbation results. Russian language version of this course is freely available at www.intuit.ru.

# Quantum-chemical simulation of adsorption and catalytic properties of gold nanoparticles in the cluster approach

*Daria Pichugina, Sergey Nikolaev and Nikolay Kuzmenko*

**Keywords:** DFT calculation, gold clusters, hydrogen, adsorption, catalysis, hydrogenation of acetylene

The results of the theoretical simulation using density functional theory of the interaction of molecular hydrogen and gold clusters with various composition, structure and charge are presented. It is shown that the hydrogen dissociation occurs on the gold cluster if the cluster has: four-coordinated metal atoms, dynamic structure, and positive charge. The study of catalytic properties of gold nanoparticles is performed on the selective hydrogenation of acetylene (C2H2) to ethylene (C2H4) as an example. All stages have low activation energies. The recommendations about the way of increase the activity of gold based catalysts in partial acetylene hydrogenation are stated using the data obtained by the proposed approach of simulation of the catalytic reactions.

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# Research and development methods ensure acceptable thermal mode for teraflops supercomputers

*Alexsander Rymarchuk, Victor Maziuk, Nikolay Paramonov and Oleg Tchij*

**Keywords:** supercomputer, heat removal system, thermally conductive structure

The results of research promising methods (including decisions on the inside of the capillary-porous structure and pulse contour thermosiphons) removing heat from the heating elements of supercomputing hardware configurations.

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# Research of tomographic schemes of low-frequency ultrasonic diagnostics on supercomputers

*Sergey Romanov*

**Keywords:** Ultrasonics, 3D coefficient inverse problems, supercomputer, transmission and reflection tomography

Various ultrasonic tomography schemes are compared. Inverse problems of ultrasonic tomography are addressed as coefficient inverse problems for wave equation. The algorithms for solving inverse problems of ultrasonic tomography are based on direct computation of the gradient of the residual functional by solving the conjugate problem for the wave equation. The potentialities of different reflection and transmission tomographic schemes are compared. The results of the computation of model problems are analyzed in the 3D case and compared to those of modeling of common ultrasonic diagnostic schemes, where the image is taken from a single vantage point. Direct and inverse ultrasonic tomography problems are solved using a GPU-based supercomputer.

## Research on using trees to solve the knapsack problem by means of parallel computation

*Mikhail Kupriyashin*

**Keywords:** parallel algorithms, knapsack problem, packing tree

Algorithms for the knapsack problem are of interest due to extensive amount of various applications. In particular, knapsacks are used as a cryptographic primitive. The algorithm based on searching the knapsack packing tree is notable among the few exact algorithms for the knapsack problem. This paper states that the problems with load balancing make parallel implementations of the algorithm inefficient. One of the ways to solve this problem is to devise a feasible linear arrangement that represents the set of potential solutions as a numbered sequence and provides for splitting it into subsequences of equal lengths.

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## Serial-parallel method using for partial associative operation parallelizing

*Alexey Frolov*

**Keywords:** Serial-parallel method, associative operations, parallelizing

Serial-parallel method using for partial associative operations is discussed in this paper.

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## Simulation of unsteady processes in turbomachines based on non-linear harmonic NLH-method with the use of supercomputers

*Yuri Boldyrev, Alexander Rubtsov, Yuri Kozhukhov, Alexander Lebedev, Ivan Cheglakov and Aleksei Danilishin*

**Keywords:** non-linear harmonic method, Unsteady calculation, Turbomachines

The purpose of this work is to test the nonlinear harmonic method (NLH), intended for simulation of the unsteady aerodynamic interaction between the rotor and stator of the turbomachine, characterized by high speed of calculations in comparison with the fully unsteady flow calculation approach. Calculations of unsteady flows in turbomachines belong to the class of compute-intensive tasks and to solve real problems in a reasonable time requires the use of supercomputers. The Department of compressor, vacuum and refrigeration engineering for testing the obtained solution of two-dimensional and three-dimensional flows in Turbomachinery using this NLH method, implemented in the software package NUMECA Fine/Turbo. To date, a comparison of the behavior of unsteady flow with the steady solution. Obtained flow patterns and considered conservativeness of flow parameters.

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## Solution of problems of combustion gas dynamics on hybrid CPU/GPU computing system

*Lyuben Stamov and Elena Mikhalchenko*

**Keywords:** combustion, detonation, gas dynamics, parallel algorithms, GPU

In this paper an application of modern GPU containing computing system for computation of combustion problems is study. Some test problems of initiation of detonation in hydrogen-air

mixtures were considered. Several parallel algorithms based on GPU-computing were developed. High-order difference schemes for gas dynamics and chemistry equations were used. Good performance for a certain range of parameters was obtained.

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## Solving the global optimization problems on heterogeneous cluster systems

*Konstantin Barkalov, Victor Gergel, Ilya Lebedev and Alexander Sysoyev*

**Keywords:** global optimization, parallel algorithms, heterogeneous computing

The paper presents the results of investigation of parallel information-statistical algorithm of global optimization that developed in University of Nizhny Novgorod. This method is combined with multilevel scheme of dimension reduction. It allows us to solve multidimensional problems by reducing it to parallel solving a series of data-independent subtasks of lower dimension. New suggestion developed in the framework of current research is the method of using several graphics accelerators on different nodes of cluster. Results of solving a series of test problems on supercomputer Lobachevsky using tens of thousands GPU cores are given.

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## Solving unstable linear programming problems of high dimension on cluster computing systems

*Irina Sokolinskaya and Leonid Sokolinsky*

**Keywords:** linear programming, unstable problems of high dimension, cluster computing systems, Fejer mappings

Solving unstable linear programming problems of high dimension on cluster computing systems with multi-core accelerators

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## Some approaches to organizing of remote access to supercomputer resources

*Julia Dubenskaya, Alexander Kryukov and Andrey Demichev*

**Keywords:** supercomputer resources, remote access, grid, web services, REST

A progress of supercomputer technology poses a problem of user friendly access to such resources. Here we survey modern approaches to organizing of remote access to supercomputer such as direct access via secured protocol, access via RESTful web service, access via regular web interface, access via grid. In this paper we also consider prospective trends in remote access organizing. For each approach we discuss its features and case studies. We concentrate on comparative analysis of the approaches in terms of their functionality, information security and usability. Then we study their applicability for a range of computational problems.

# Supercomputer simulation of nanocomposites on the basis of carbon and silicon in new types of Li-Ion power sources

*Dmitry Varlamov, Vadim Volokhov, Tatiana Zyubina, Alexander Zyubin, Alexander Volokhov and Gennady Pokatovich*

**Keywords:** computer simulation, silicon-carbon nanocomposites, Li-ion power sources, VASP applied package, quantum chemistry

The results of a supercomputer simulation of nanocomposite materials based on carbon and silicon (pure silicon aggregates of various morphology and dimensionality, nanowires with a rod of silicon carbide and silicon coated, silicon nanorods with a core from silicon carbide, carbon nanotubes surrounded by a layer of silicon clusters) applied in case of creation of Li-ion sources of current of new types with the raised operational and cost characteristics are described. Are made the analysis of computational complexity and efficiency of parallelization, and also application of different methods of modeling.

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# Supercomputer simulations method of the coupled qubit and oscillator systems

*Marina Denisenko, Arkady Satanin, Alexey Liniov, Victor Gergel and Dmitry Pashin*

**Keywords:** qubit, non-destructive measurements, quantum trajectory technique(Monte Carlo wave-function method), GPU, CUDA

The algorithm based on quantum trajectory technique (Monte Carlo wave-function method) for modeling dissipative dynamics of multi-level quantum system was developed. The simulation of the interaction process a qubit with a quantum nonlinear oscillator based on the developed method has been conducted. It is shown that the measuring result for the average energy (number of photons) of the oscillator gives a possibility to carry out separation (tomography) of qubit states both as an average over an ensemble and as for a single trajectory. Monte Carlo wave-function method allows for effective parallelization on heterogeneous high performance computing clusters in calculation of experimentally observed values in multi-level quantum systems with relaxation processes. The basic principles of parallelism algorithm for solving stochastic Schrödinger equation, which were imple-mented by us in program complex, allowing to carry out high performance parallel calculations using GPU have been described. The efficiency of graphics accelerators, scalability of the method was demonstrated and possibility of interconnection of multiple graphics cards using MPI-technology was described.

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# Supercomputing in the context of the knowledge economy

*Yuri Zelenkov*

**Keywords:** knowledge economy, supercomputers, law of diminishing return, cloud manufacturing, product design

The main feature of the knowledge economy is the transition from mass market to satisfaction of individual needs. Herewith knowledge becomes a factor of production, in contrast to the "classic" factors, for which the law of diminishing returns is applied, marginal productivity of knowledge increases when the volume of used knowledge grows. This radically alters the mechanisms of development and competition. Under the new conditions, a number of activity

areas appears, which impossible to perform without the use of large computing resources. These are: the network platforms for the sharing of assets, the acceleration of new product's design, the establishment of dynamic relationships in the network of cloud manufacturing and etc. The article presents an analysis of the potential applications of supercomputers in the new economy. As example it is shown that investments in supercomputing in the design of new products ensure the rise in productivity.

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## The dependence of reverse micelles free energy from their size: a molecular dynamics simulation at “Lomonosov”

*Alexander Nevidimov, Sergey Tovstun and Vladimir Razumov*

**Keywords:** Molecular dynamics, reverse micelle, free energy, pressure

Molecular dynamics simulation of pressure into reverse micelles was conducted in our work. All calculations was carried out at "Lomonosov" supercomputer center. Free energy calculations we are going to provide by Laplace formula.

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## The development of basic GPU kernels for the new block AMG algorithms for solving SLE with explicitly calculated sparse basis

*Ilya Afanasyev and Yury Potapov*

**Keywords:** GPU, Sparse Matrix, Linear Algebra, Optimization, CUDA, High performance

The main purpose of this work is the development of basic kernels, which make it possible to transfer some computing functions of software package Flow Vision from CPU to GPU. It was necessary to implement a set of basic dense and sparse linear algebra operations, with the data specifics used in the package FlowVision. We could not use already-created by company NVidia library functions because they do not provide sufficiently effective algorithms of computing several small dimension tasks on a single GPU. As a result of this work acceleration from 2 to 20 times was obtained in comparison with the already mentioned library counterparts.

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## The efficiency of the implementation of iterative methods for the solution of elliptic equations in atmospheric general circulation models on massively parallel systems

*Evgeny Mortikov*

**Keywords:** atmospheric general circulation model, massively parallel systems, Intel Xeon Phi, Nvidia GPU

In this paper we study the possibility of the efficient implementation of atmospheric general circulation model and its particular components on modern massively parallel architectures. Main emphasis is placed on methods for solving elliptic equations, arising from applying semi-implicit in time approximations in thermo-hydrodynamic equations. Results are presented for computational architectures based on Intel Xeon Phi processors, as well as Nvidia graphic cards.

# The interdisciplinary course “Introduction to parallel evolutionary models and algorithms” - teaching experience

*Nikolay Ershov and Nina Popova*

**Keywords:** distributed models, evolutionary algorithms, natural computing, parallel computations

This work is devoted to describing the five-year experience of teaching an introductory course on parallel evolutionary computing at the Faculty of Computational Mathematics and Cybernetics, Moscow State University and the University "Dubna". The course covers such popular evolutionary models and algorithms as cellular automata, Lindenmayer systems, Petri nets, artificial neural networks, molecular computation, genetic algorithms, swarm optimization methods, etc. The presentation of theoretical material of the course is accompanied by a consideration of the possible schemes for parallel computing, in the practical part of the course the students supposed to perform a software implementation of evolutionary models using MPI technology and conducting numerical experiments to investigate the effectiveness of selected parallelizing schemes. This work was supported by RFBR (grant №14-07-00628 A).

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# The software platform of transmission of intense data streams on remote supercomputers

*Grigoriy Masich and Vladislav Shchapov*

**Keywords:** experimental stands, intense data streams, supercomputers, software platform, protocol, measurement

Many modern experimental stands generate intense data streams that must be processed and stored. High-speed data transmission network allow use to handle remote supercomputers and data centers. This requires a software infrastructure for efficient transmission and distribution data on the computing nodes or storage nodes. The article presents the results of research to develop the software platform of transmission of intense data streams on remote supercomputers for parallel processing.

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# The structure of INMOST program platform and its usage for numerical modeling problems

*Alexander Danilov, Kirill Terekhov, Igor Konshin and Yuri Vassilevski*

**Keywords:** INMOST, program platform, distributed meshes, numerical modeling

The INMOST program platform allows a user to work with distributed data on general meshes. The description of platform structure, the interrelation of mesh elements, the work with ghost cells, distribution and redistribution of mesh data is presented. Special aspects of the program platform implementation and usage as well as advantages over the analogous libraries are analyzed. For one of the specific tasks the exploiting of the INMOST program platform is demonstrated on the all stages of numerical modeling: distributed meshes construction, attachment of data to the mesh elements, the use of the mesh data for problem discretization, as well as the parallel solution of resulting linear systems.

## Topology reserves of flattened system networks

*Viktor Podlazov and Michail Karavay*

**Keywords:** Supercomputer interconnect, Flattened butterfly, Flattened system area networks, Hardware complexity, Power consuming, Number of network nodes

A method of modification the topology of double-hop system network type of Flattened Batterfly is considered. The method ensures diminution of component commutator sizes and as a consequence of that feature decrease in hardware complexity and power consuming, preserving number of network nodes (processors), network diameter and functional characteristics. In case of retain the original component commutator size the method gives a possibility to enhance number of network nodes dramatically with preservation of network diameter

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## Two-level parallel strategy for multifrontal sparse Cholesky factorization

*Sergey Lebedev, Dmitry Akhmedzhanov, Evgeniy Kozinov, Iosif Meyerov, Anna Pirova and Alexander Sysoyev*

**Keywords:** Sparse Algebra, Cholesky Factorization, Numerical Phase, Multifrontal Method, High Performance Computing, Dynamic Parallelization, Task-based Parallelism

In this paper we consider the problem of parallelization of Cholesky factorization numerical phase for sparse symmetric positive definite matrices. A new strategy for parallelization of the multifrontal method for shared-memory systems is suggested. This strategy combines two approaches to parallelism organization depending on the elimination tree level. At the bottom of the tree, parallel computing of nodes from a priority queue takes place. At the top levels of the tree, nodes are calculated sequentially, employing multithreaded BLAS procedures. Experimental results show that the implementation of the scheme described is commensurable with MUMPS and MKL PARDISO solvers.

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## Uncertainty in clouds: challenges of efficient resource provisioning

*Andrei Tchernykh, Uwe Schwiegelsohn, Vassil Alexandrov and El-Ghazali Talbi*

**Keywords:** Cloud computing, Uncertainty, Multi-objective Scheduling

We discuss the role of uncertainty in the resource/service provisioning, investment, operational cost, programming models, etc. that have not yet been adequately ad-dressed in the scientific literature.

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## Universal block Lanczos-Pade method for linear systems over large finite fields

*Nikolay Zamarashkin and Mihail Cherepnev*

In this paper we propose a universal algorithm designed for solving large sparse linear systems over finite fields with large prime number of elements. Such systems arise in the

solution of the discrete logarithm problem modulo a prime number. Parallel algorithms and effective data distributions are proposed.

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## Using Intel Xeon Phi coprocessor for execution of natural join on compressed data

*Leonid Sokolinsky and Elena Ivanova*

**Keywords:** columnar data representation, columnar indexes, database coprocessor, interval fragmentation, parallel database systems, cluster computing system with many-core accelerators, Intel Xeon Phi coprocessor

In the report describes a database coprocessor for high-performance cluster computing systems with many-core accelerators, which uses distributed columnar indexes with interval fragmentation. An activity of the coprocessor is considered by an example of natural join operation. The parallel decomposition of natural join operation is performed using distributed columnar indexes. The proposed approach allow to perform relational operators on cluster computing systems without massive data exchange. The results of computational experiments with using Intel Xeon Phi coprocessor confirm the effectiveness of the developed methods and algorithms.

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## Using multifrontal hierarchically solver and HPC systems for 3D Helmholtz problem

*Sergey Solovyev, Dmitry Vishnevsky and Hongwei Liu*

**Keywords:** HPS systems, optimal finite-difference scheme, low-rank approximation, HSS format, 3D Helmholtz problem

We present a multi-frontal hierarchically semi-separable solver to perform forward modeling of the 3D Helmholtz acoustic problem. Our frequency-domain solver combines two efficient approaches. First, it uses an optimal 27-point finite-difference scheme to decrease numerical dispersion and reduce required discretization of the model in terms of points per wavelength from 15 to about 4. Second, it uses a supernodal multi-frontal method based on low-rank approximation and hierarchically semi-separable (HSS) structure to improve performance, decrease memory usage and make it practical for realistic size 3D models required by full-waveform inversion. We perform validation and performance testing our new solver using a 3D synthetic model. Performance and OMP scalability of the solver were compared with the Intel MKL PARDISO.

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## Using of container virtualization to run tasks on a distributed supercomputer

*Vladislav Shchapov and Denis Chugunov*

**Keywords:** Distributed supercomputer, Container virtualization, Docker

This paper talks the launch of tasks on the compute nodes of the distributed supercomputer in isolated environments with the use of container virtualization technology. Using specially prepared containers will create virtual compute nodes over nodes of the distributed supercomputer that can have different pre-installed software and libraries. Virtual nodes have

a single set of software and settings that allow you to run computational tasks without the need for adaptation to the different versions of the system libraries, MPI and other settings.

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## Using of Lammps and Gromacs software packages for high-performance deposition simulation of nano-structured thin films

*A.N. Sharov, A.A. Gorokh, M.Y. Kozmin, A.V. Sulimov, D.V. Lukyanenko and S.A. Sharapova*

The paper presents an approach to molecular modeling of modern high-energy deposition processes of optical coatings of silicon dioxide and its implementation using the supercomputer "Lomonosov" and the software packages for molecular dynamics Lammps and Gromacs. In result layer were obtained with a thickness to a few tens of nano meters containing over one million atoms. The various structural characteristics of the resulting layer were calculated, such as density, radial distribution function, the number of point defects and other. Two models of deposition were considered using the same original force field. A comparison of the results for these two models as well as a comparison of the effectiveness of mentioned software packages in multiprocessor mode (both CPU and GPU) were performed. A good agreement of deposited layers characteristics obtained by the simulations to the experimental characteristics of quartz glass and nano silica was demonstrated.

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## Virtual prototyping technology is the key technology for analysis of results of supercomputer modeling

*Nikolay Shabrov, Vladislav Kiev and Aleksei Kuzin*

**Keywords:** Virtual Reality, Virtual Engineering, CAVE 3D environment, HPC, Tracking system, Display wall, Virtual prototyping

The major challenges of the 21st century can be attributed the problem of computing breakthrough technologies providing predictive modeling of multiscale and multi-disciplinary processes based on modern supercomputer computing systems (HPC). It is assumed that the volume of data generated by the peta/exaflops computing, reach the level of petabytes and exabytes. This means that to analyze the results of peta- exaflops simulation mode in real time virtual environment is almost the one and only effective tool for understanding of the huge amount of data, and will play a key role in the near future. The paper summarized and developed by the experience of creating and applying a multi screen virtual environment system to analyze the results of predictive modeling of complex objects of science and technology.

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## What is the fastest way to compute quantum and classical atomistic models using the latest software algorithms and supercomputing hardware?

*Grigory Smirnov and Vladimir Stegailov*

**Keywords:** atomistic models, efficiency, scalability, peak performance

Development of new HPC architectures proceeds faster than the corresponding adjustment of the algorithms for such fundamental mathematical models as quantum and classical and quantum molecular dynamics. Due to the abundance of hardware options there is the need for

clear guiding criteria for the computational efficiency of a particular model on a particular hardware. LINPACK benchmark alone can no longer serve this role. In this work we consider a practical metric of the time-to-solution versus the computational peak performance of a given hardware system. In this metric we compare different hardware (both legacy and modern) for the LAMMPS, GROMACS, NAMD and CP2K software packages widely used for atomistic modeling. The metric considered can serve as a universal unambiguous scale that ranges different combinations of CPUs, accelerators and interconnects.

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# Yet another tridiagonal matrix algorithm parallelizing method

*Alexey Frolov*

**Keywords:** Thomas algorithm, tridiagonal matrix algorithm, parallelizing

New tridiagonal matrix algorithm parallelizing method is described in this article. This method uses matrix multiplication associativity, and is stable for standard data of Thomas algorithm.