Educational Landscape of the Exascale Future

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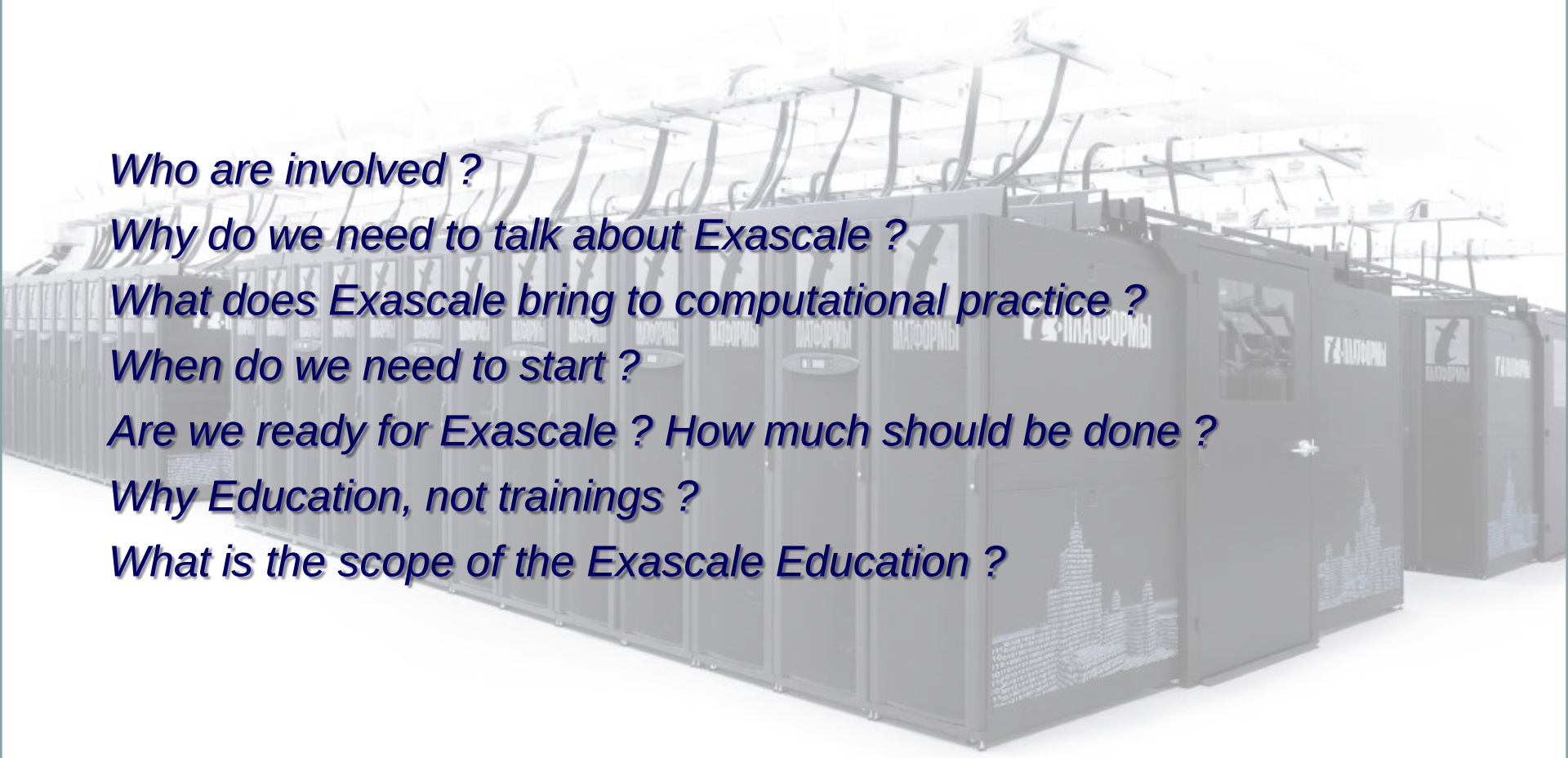
SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

Educational Landscape of the Exascale Future

(different facets of the title)



Who are involved ?

Why do we need to talk about Exascale ?

What does Exascale bring to computational practice ?

When do we need to start ?

Are we ready for Exascale ? How much should be done ?

Why Education, not trainings ?

What is the scope of the Exascale Education ?

Moscow State University

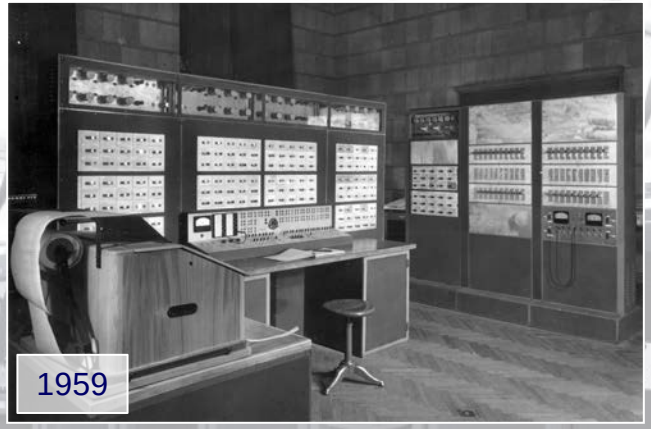
(established in 1755)

40+ Faculties
350+ Departments
5 major Research Institutes

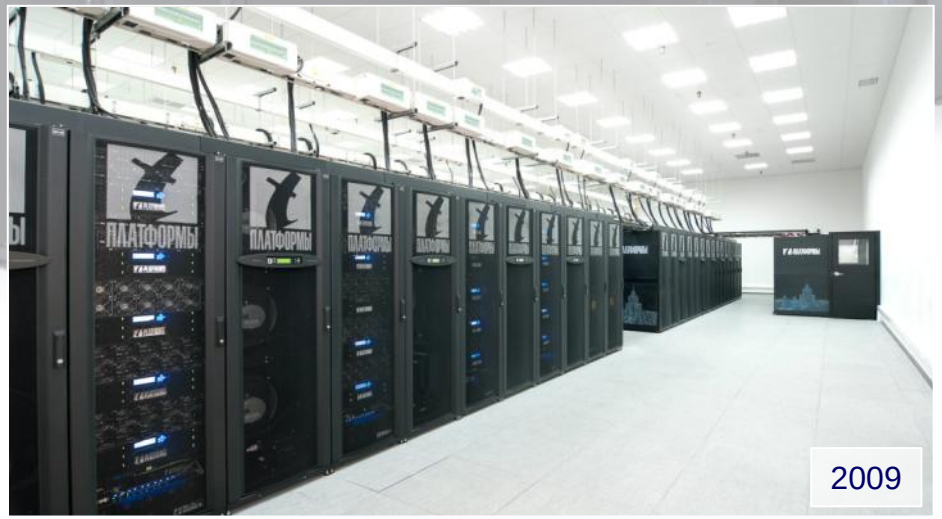
More than 40 000 students,
2500 full doctors, 6000 PhDs,
1000+ full professors,
5000 researchers.

Computing Facilities of Moscow State University

(from 1956 up to now)



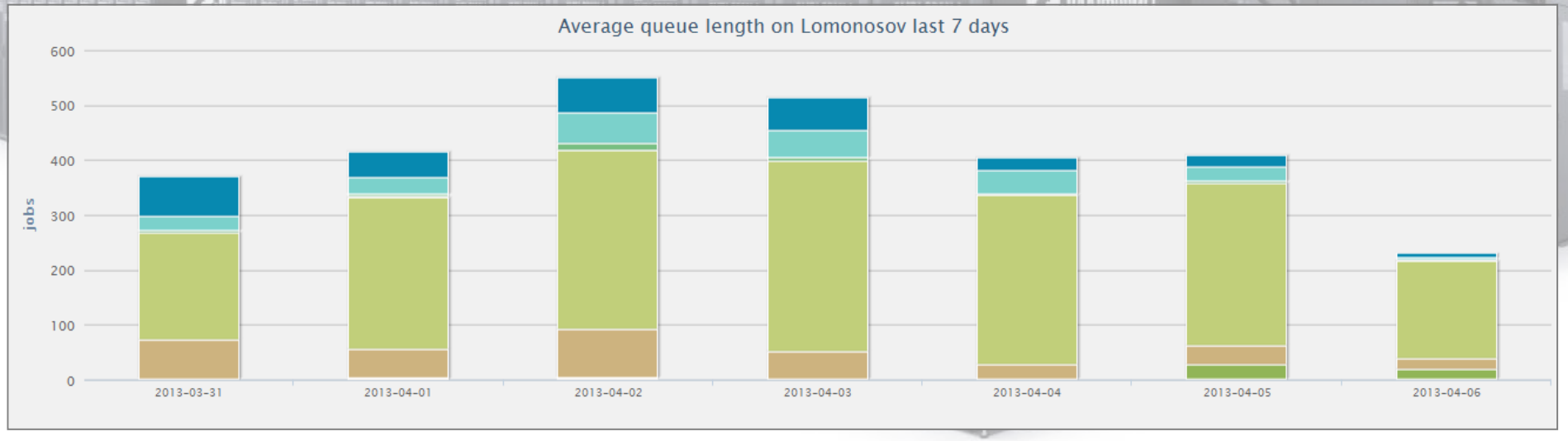
MSU: from Kflops to Petascale



MSU Petaflops Computing Facilities: "Lomonosov" Supercomputer

M.V.Lomonosov
1711 – 1765

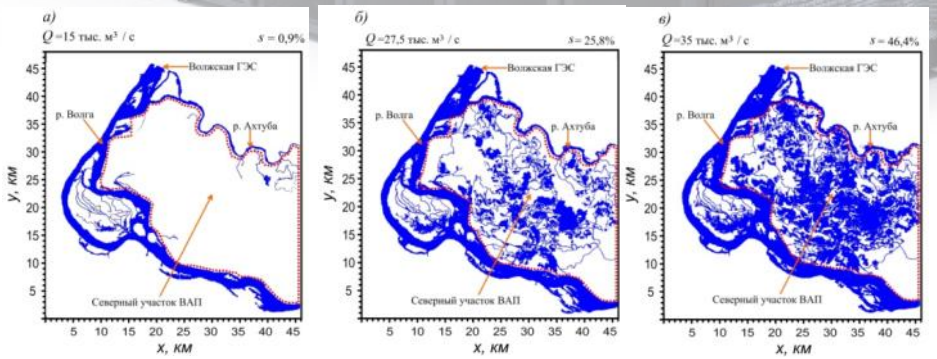
Stats on “Lomonosov” Supercomputer
(Average queue length)

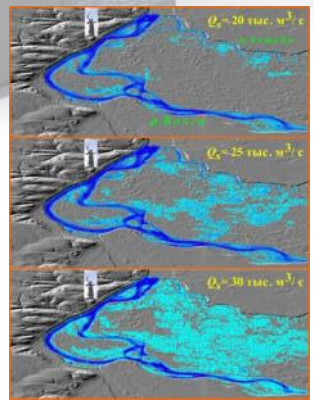


Modeling of the dynamics of shallow waters on the northern part of Volga-Akhtuba floodplain

Khoperskov A., Khrapov S., Agafonnikova E., Pisarev A.

AREA. Mechanics, Geography and Land Hydrology
DRIVER. We solve the problem of software package creating for the seasonal flooding modeling on the northern part of the Volga-Akhtuba floodplain with the main physical and meteorological factors on the basis of parallel technologies.
STRATEGY. Model is based on numerical integration of Saint-Venant equations using a combined SPH-TVD method.
OBJECTIVE. The main goal of the project is to create a tool to predict of hydrological regime in the territory of northern part of the Volga-Akhtuba floodplain and the subsequent construction of the optimal hydrograph for the Volga Hydroelectric Power Station.
IMPACT. The method of constructing an optimal hydrograph will allow us to increase the flooding of area considering various features of the landscape.
USAGE. Analytical tool for environmental organizations and agencies, the Ministry of Emergency Situations.

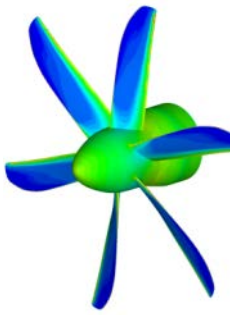


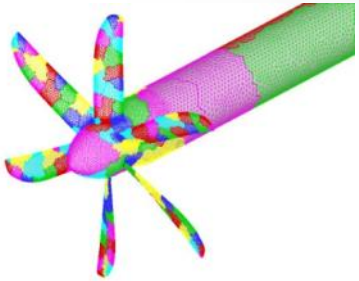


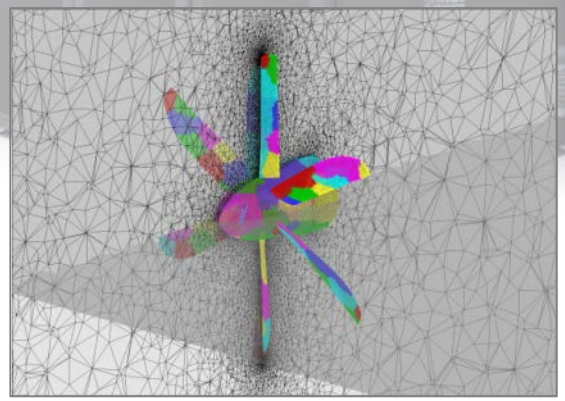
Modeling of acoustics of open rotors

Titarev V., Kopiev F., Belyaev I.

AREA. Mathematics, Informatics
DRIVER. Modeling of open rotors.
STRATEGY. Our approach is based on the combined use of computational physics, aeroacoustics as well as high-performance computing.
OBJECTIVE. The goal is to develop efficient computational tools for analyzing the aerodynamics and noise of open rotors.
IMPACT. The main expected result is the capability to given an expert opinion regarding perspective transport aircraft using open rotors.
USAGE. Main beneficiaries of the project will be aerospace industry as well as TsAGI.



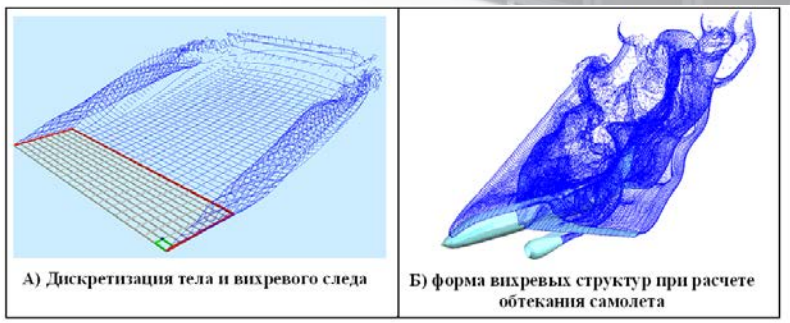




Numerical modeling of separated flows based on vortex approach

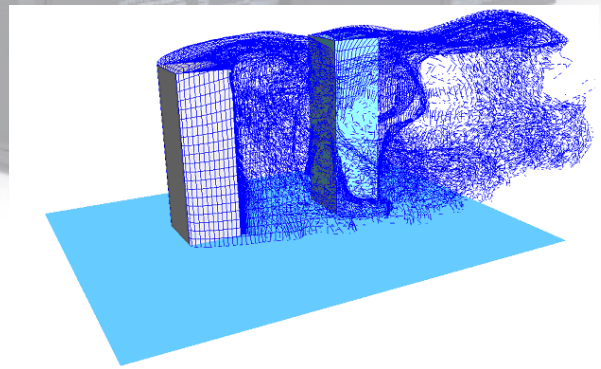
Setukha A.: Research Computer Center, Moscow State University;
Aparinov A.: NII Parachutostroeniya

AREA. Mathematics, Mechanics
DRIVER. Development and testing of parallel numerical algorithm for solving aerodynamic problems with vortex method.
STRATEGY. Applying efficient methods of big-size matrix approximation with paralleling of numerical algorithms at the same time.
OBJECTIVE. To analyse increased opportunities of aerodynamic vortex methods provided by supercomputer technologies.
IMPACT. The solution of complex aerodynamic and dynamic problems for air vehicles, modeling of non-stationary separated flows past group of objects with complicated geometry, for example, building and constructions or multi-cupolas parachute systems.
USAGE. Aerodynamics of air vehicles, aerodynamics and aeroelastics of parachutes, constructing aerodynamics.



А) Дискретизация тела и вихревого следа

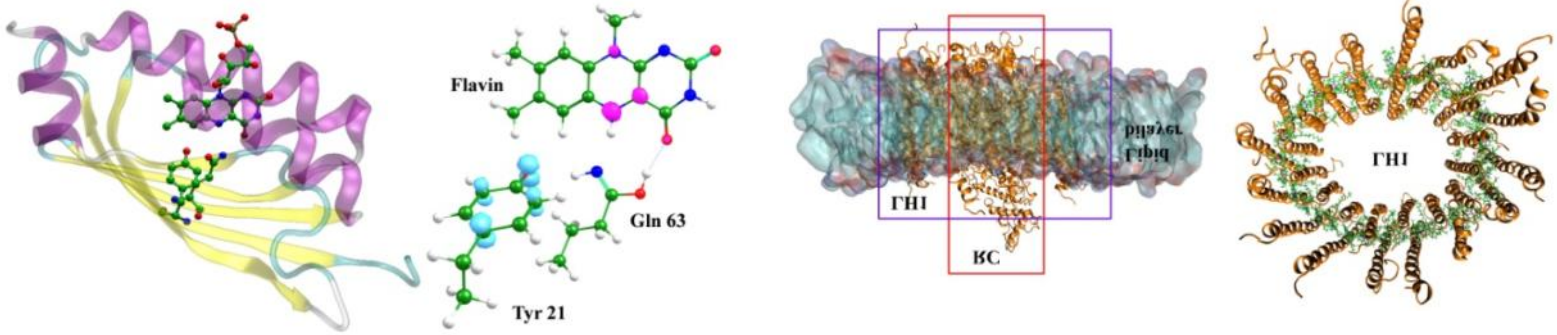
Б) форма вихревых структур при расчете обтекания самолета



Modeling mechanisms of photochemical processes in photoreceptor and fluorescent proteins

Khrenova M., Bochenkova A., Mironov V., Andrijchenko N., Nikiforov A., Vasilevskaya T.:
M.V. Lomonosov Moscow State University, Chemistry Department

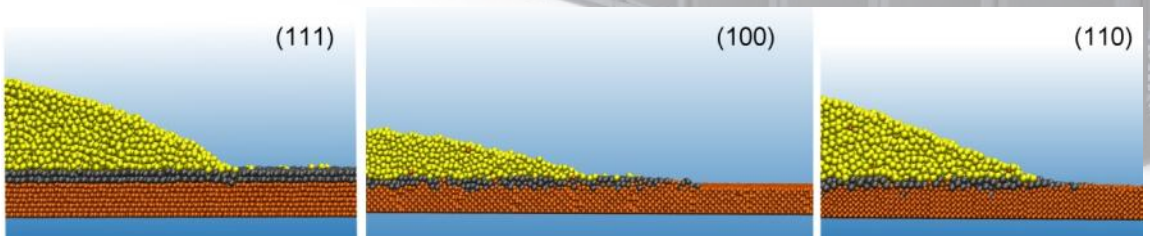
AREA. Structure and Dynamics of Atomic-Molecular Systems, Physicochemical Biology
DRIVER. Studying mechanisms of functioning of fluorescent proteins, flavin containing photoreceptor proteins and bacterial photosystem.
STRATEGY. Development and application of methods of computer molecular modeling for properties calculations of photoreceptor proteins and their chromophores.
OBJECTIVE. Establishment of mechanisms of functioning of fluorescent proteins, flavin containing photoreceptor proteins and bacterial using combined method of quantum mechanics/ molecular mechanics and modern methods of quantum chemistry of high level of accuracy.
IMPACT. Prediction of new fluorescent and photoreceptor proteins with the suggested properties, on the basis of mechanisms established in the project.
USAGE. Biosensor technologies, life sciences.

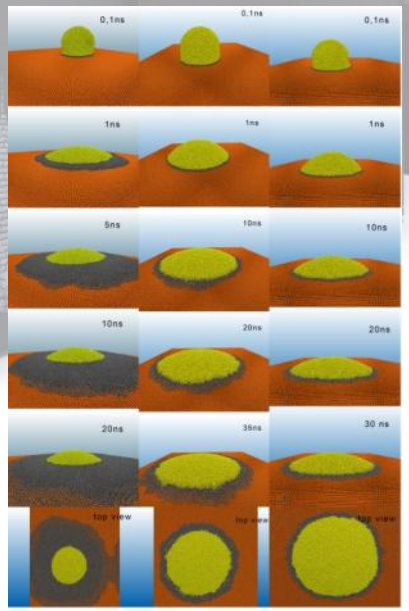


The kinetics of spreading of lead nanodroplets on monocrystalline copper surface

Timoshenko V., Protsenko P.

AREA. Physical Chemistry
DRIVER. The project aims to study the wetting characteristics of single-crystal metal surfaces using molecular dynamics simulation.
STRATEGY. Method of molecular dynamics is used to analyze the process of spreading droplets of lead on the surface of copper.
OBJECTIVE. The aim is to determine the effect of substrate orientation on the kinetics of the spreading melt of lead on the surface of single-crystal copper
IMPACT. Development of new and improvement of existing solders for microelectronic devices.
USAGE. Soldering processes.

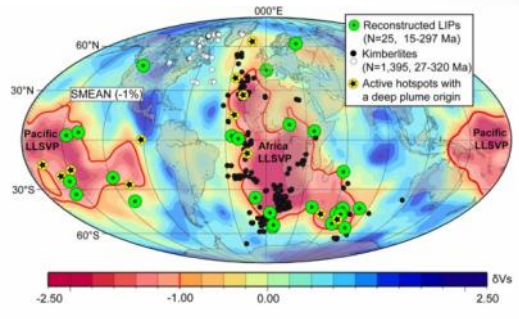


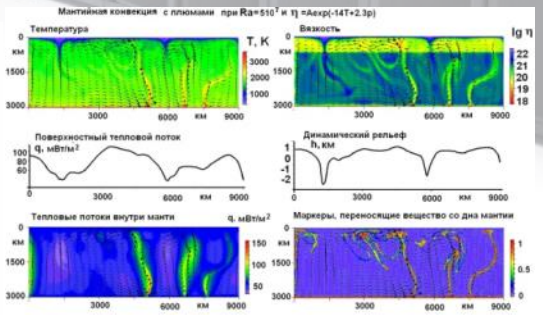


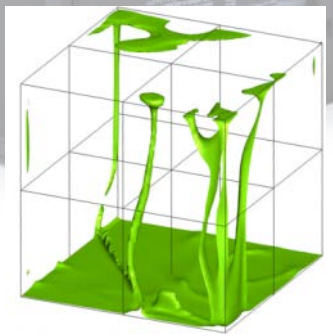
Mantle plumes in the models of quasi turbulent thermal convection

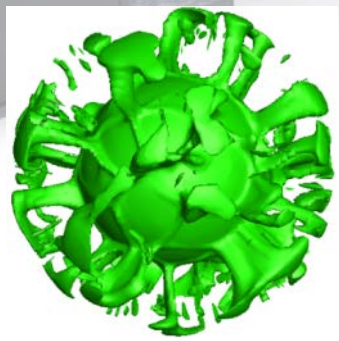
Evseev A., Trubitsyn V.: IPE RAS

AREA. Geophysics
DRIVER. Development of methods of numerical modeling of thermo-compositional convection in multi-component fluid with large viscosity variations.
STRATEGY. On the basis of numerical models of thermal convection in mantle a process of spontaneous multiple creation and lifting of hot plumes, generating volcanoes and ore fields, is investigated.
OBJECTIVE. Mantle convection modeling allows to recognize places of plumes origin and their lifting, and then to predict global volcanic disasters and ore deposit.
IMPACT. Prediction of possible large ore deposits, created during last billion years and future volcanic catastrophes.
USAGE. Prediction of possible large ore deposits, created during last billion years and future volcanic catastrophes.





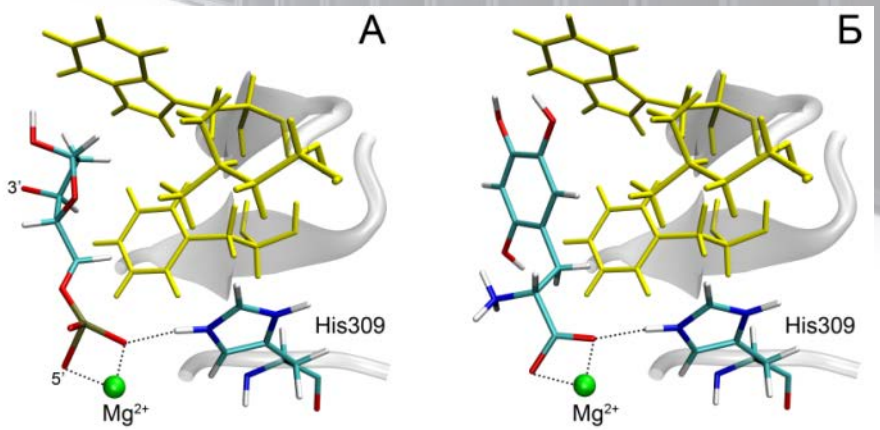


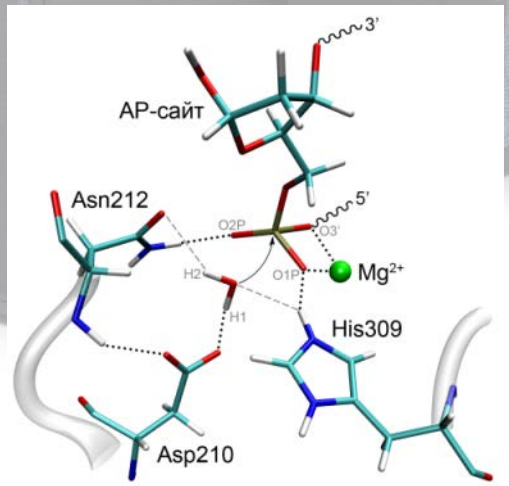


Molecular model of human apurinic/apyrimidinic endonuclease

Nilov D., Khaliullin I.: Belozersky Institute of Physicochemical Biology, MSU

AREA. Informatics, Fundamental Medicine and Physiology
DRIVER. Construct a full-atomic model of human apurinic/apyrimidinic endonuclease.
STRATEGY. Apply hybrid quantum mechanics/molecular mechanics simulation technique to calculate a full-atomic structure of an enzyme.
OBJECTIVE. Create a model of human apurinic/apyrimidinic endonuclease for virtual screening of novel inhibitors (potent anti-cancer drugs).
IMPACT. Development of novel inhibitors of human apurinic/apyrimidinic endonuclease using constructed enzyme model.
USAGE. Application of developed apurinic/apyrimidinic endonuclease inhibitors as anti-cancer drugs in medicine.

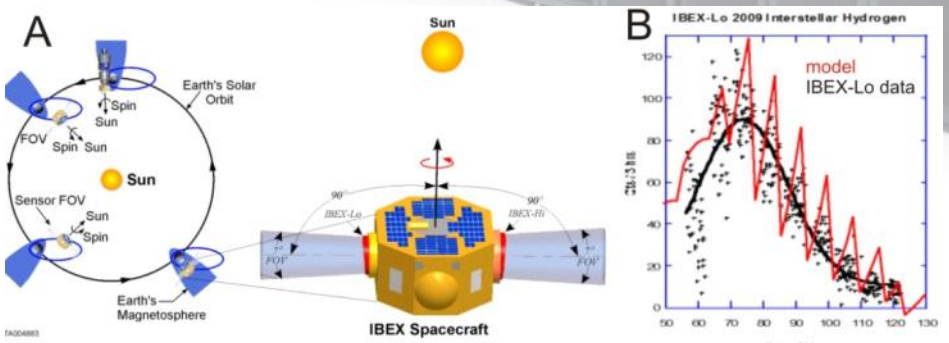


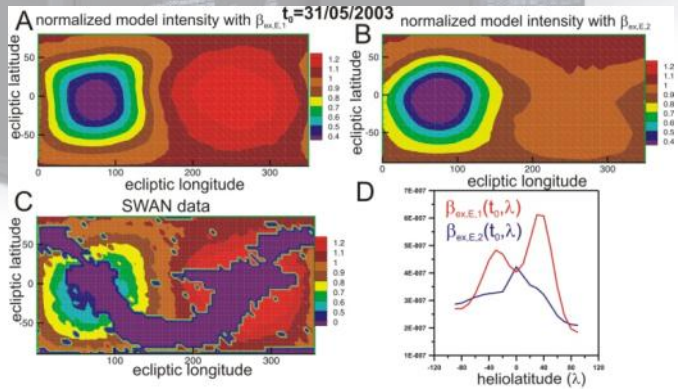


Investigation of the interstellar neutrals in the heliosphere

Katushkina O., Izmodenov V.: MSU, IKI RAN; Taghirova R.: IKI RAN

AREA. Mechanics, Astronomy
DRIVER. To develop a model of the interstellar hydrogen distribution in the heliosphere. To apply this model for the analysis of experimental data from different spacecraft.
STRATEGY. The main idea for the solving of this problem is to use the kinetic approach for the modeling of interstellar hydrogen distribution. To do this, we solve the 7-dimension kinetic equation in 3D time-dependent case.
OBJECTIVE. To develop the model of the interstellar hydrogen distribution inside the heliosphere. It is needed for explanation and interpretation of different experimental data. From this we can obtain additional restrictions for the parameters of the Local Interstellar Medium and properties of the heliospheric boundaries.
IMPACT. Scientific effect is the following: we are going to explain.
USAGE. The field of view - the investigation of the solar wind and the heliosphere.

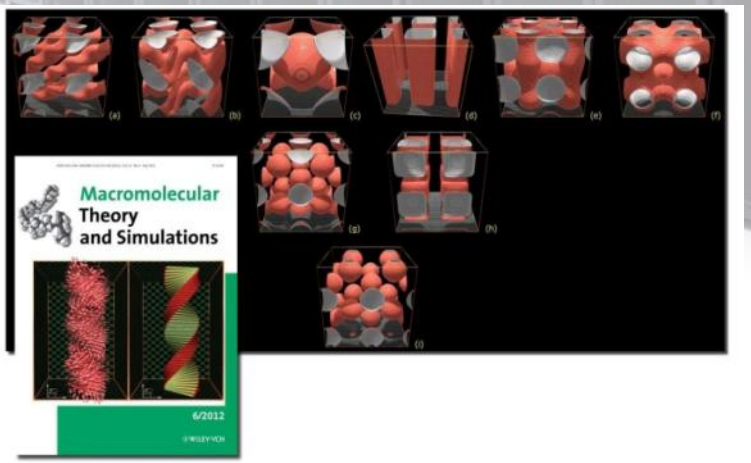


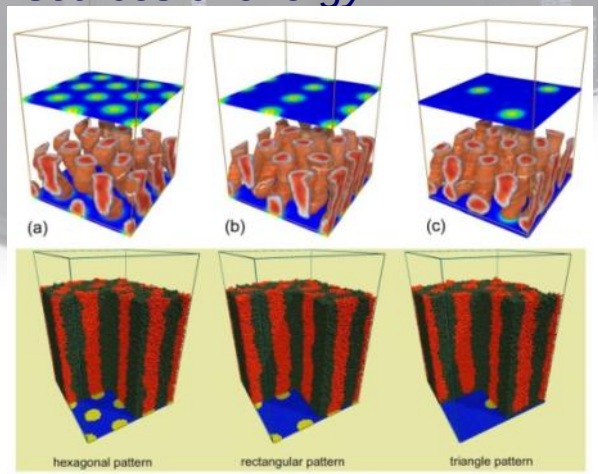


Selforganization of copolymers in nanosized films: Field-theoretic methods and computer simulation

Khalatur P.: INEOS RAS; Khokhlov A., Ivanov V.: MSU; Neratova I.: TSU

AREA. Condensed Matter Physics, High Molecular Weight Compounds
DRIVER. Development of new scientific and technological principles for designing the thin-film functional materials with controlled nanostructure, based on self-organizing polymers.
STRATEGY. The prediction of the structure and properties of ordered nanoscale polymer films using computer modeling techniques.
OBJECTIVE. A theoretical study of the fundamentals related to the formation of copolymer nanostructures in a situation when the system self-organizes in ultra-thin polymer films with a thickness of several tens of nanometers.
IMPACT. New strategies for designing block copolymer films and membranes for solar cells, fuel cells, and other advanced technologies.
USAGE. Nanosystems, molecular microelectronics, new sources of energy.

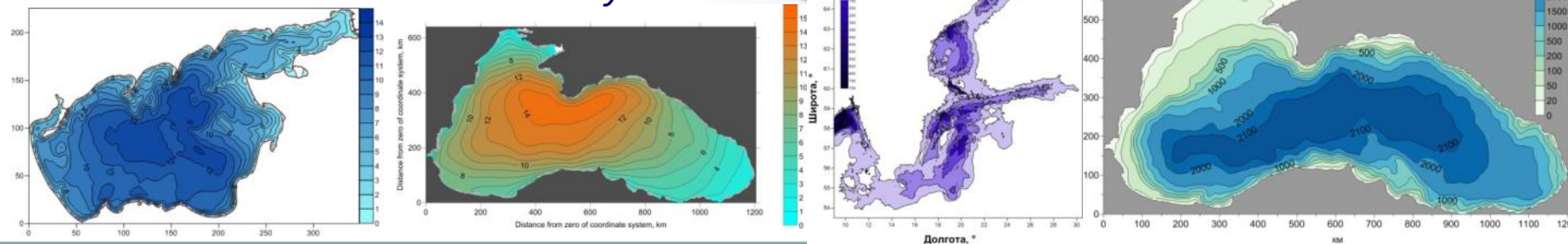




Retrospective forecast of high resolution storm waves and surges in coastal areas of European Russia

Arkhipkin V., Myslenkov S., Gippius F.: faculty of geography Lomonosov Moscow State University

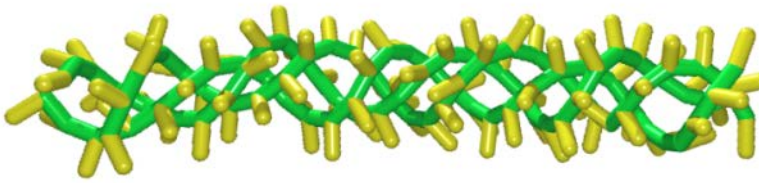
AREA. Marine Sciences, Aerophysics
DRIVER. Statistics and analysis of parameters of storm waves and surges in coastal areas of the Caspian, Black, Azov and Baltic Seas, based on the results of numerical modeling.
STRATEGY. To calculate the parameters of wind waves was applied spectral model wind-wave third-generation SWAN.
OBJECTIVE. Estimation of extreme values of regime characteristics of waves and surges in the coastal areas of the European Russia.
IMPACT. The project contributes to reduction of environmental risks in coastal areas of Russia. Long-term forecast of probable dangerous of hydrometeorological events and their intensity in the regional and macro-scale is important for risk assessment of storm surges and extreme waves and develop ways to minimize it.
USAGE. The results of the project can be used by the Ministry of Natural Resources, Ministry of Emergencies, Fisheries, Hydrometeorology, the Ministry of Transport, as well as in the tourism and recreation industry.

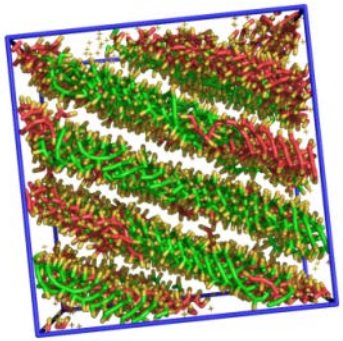


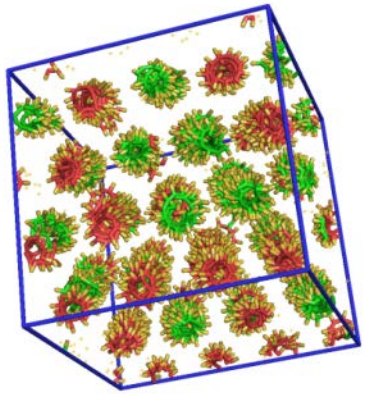
Self-Organization of Amphiphilic Macromolecules with Local Helix Structure in Concentrated Solutions

Khokhlov A.: Moscow State University, INEOS RAS; Vasilevskaya V., Glagolev M.: INEOS RAS

AREA. High Molecular Weight Compounds
DRIVER. Demand for understanding the interactions of helical macromolecules.
STRATEGY. We introduce a coarse-grained model of a polymer with helical secondary structure, and study self-organization of the polymer in concentrated solutions.
OBJECTIVE. The objective is to obtain the properties of the structure formed by helical polymer in concentrated solutions.
IMPACT. Understanding the interactions between helical macromolecules.
USAGE. Theory development, macromolecule design, fabrication of nanofibers.



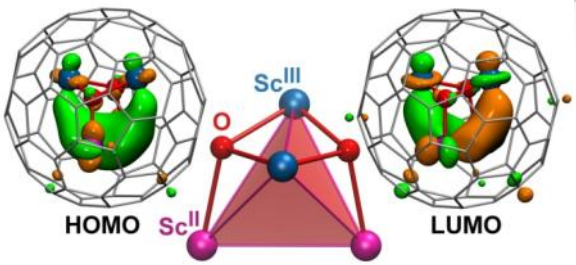


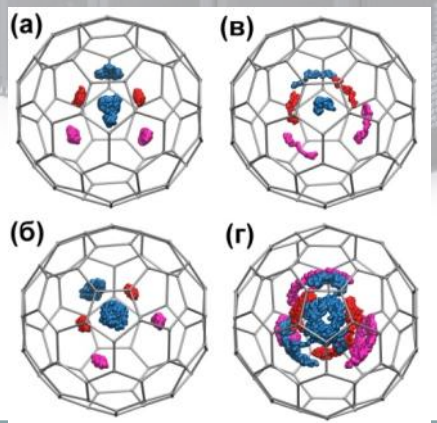


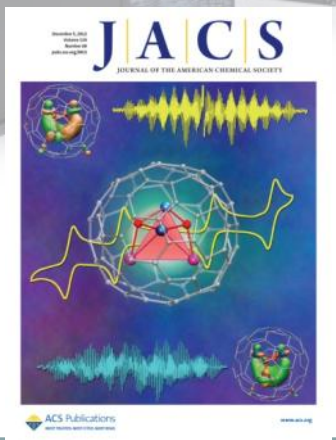
Molecular structure and internal dynamics of endohedral metallofullerenes in different charge states

Popov A.: Moscow State University and IFW Dresden

AREA. Structure and Dynamics of Atomic-Molecular Systems
DRIVER. Search of the stable isomers of endohedral metallofullerenes and their chemical derivatives.
STRATEGY. Optimization of the molecular structures of endohedral metallofullerenes (EMFs) and their derivatives in different charges states using density functional theory.
OBJECTIVE. Endohedral metallofullerenes exhibit unique electronic and magnetic properties, therefore, prediction of the possible products is important task which can be solved by means of computational studies.
IMPACT. Prediction of the most stable and hence experimentally accessible structure of EMFs.
USAGE. Further development of the molecular nanostructures based on EMFs



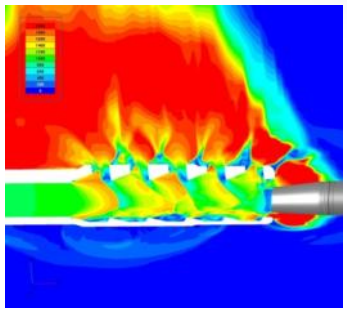


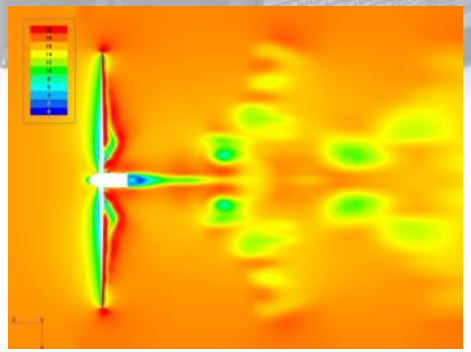


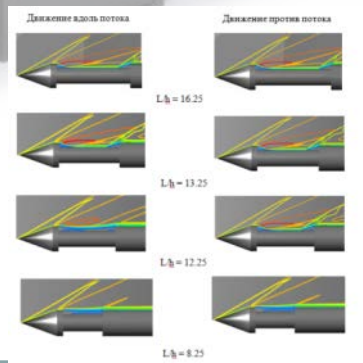
Development of FlowVision CFD Software

Aksenov A., Kharchenko S., Moskalev I., Dyadkin A., Pohilko V., Zhluktov S., Kutin V., Sazonova M., Kuznetsov K., Markova T., Karasev P., Shishaeva A.

AREA. Heat and Mass Transfer Processes, Matter Properties, Other
DRIVER. Need for simulating large industrial problems with multiphase and multi-physics phenomena in computational domains with arbitrary complex shape and moving/deformable bodies.
STRATEGY. Automatic mesh generation with dynamic local adaptation, high accuracy implicit numerical schemes.
OBJECTIVE. Create powerful and extendable CFD computing platform for virtual fluid engineering of large and complex industrial design projects in areas of automotive, shipbuilding, atomic energy and aerospace.
IMPACT. Reduced simulation time and increased accuracy result in reducing design time and increasing design reliability.
USAGE. it is a base technology for design in industries: automotive, shipbuilding, nuclear power, wind turbines, etc.



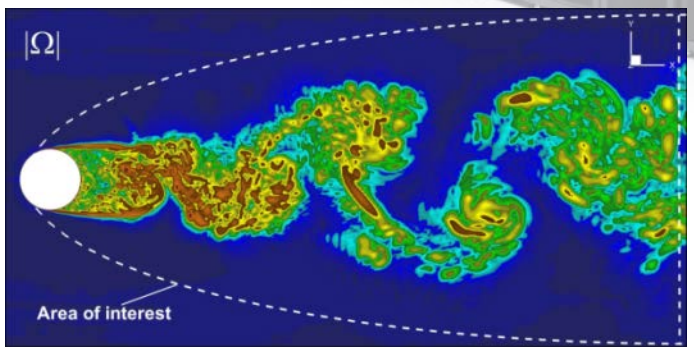


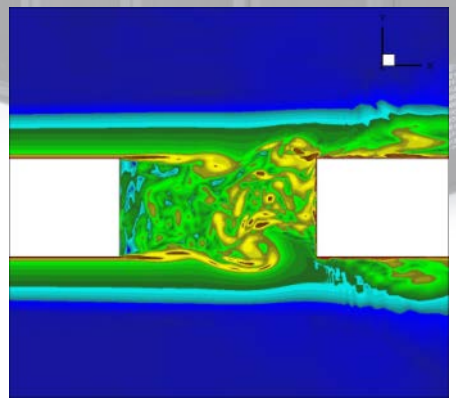


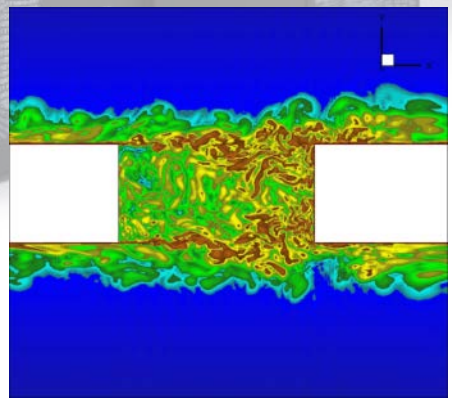
Simulation of complex turbulent flows using unstructured meshes

Duben A., Abalakin I., Gorobets A., Kozubskaya T., Lukianov N.: KIAM RAS; Bahvalov P.: MIPT.

AREA. Mathematics, Aerophysics
DRIVER. Numerical investigation of aerodynamic and aeroacoustic charateristics of bluff aircraft elements and complex turbulent flows.
STRATEGY. Identification of optimal configurations in aerodynamic and aeroacoustic characteristics, design of better noise prediction tools for development of quieter aircrafts.
OBJECTIVE. Investigation and improvement of aerodynamic and aeroacoustic characteristics of aircraft elements and complex turbulent flows.
IMPACT. Improvement of aircraft aerodynamic characteristics; reduce of airframe noise in near and far field.
USAGE. Aircraft industry; computational mathematics; computer science.



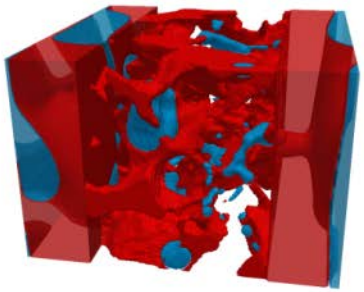
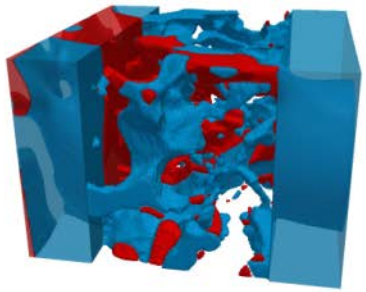
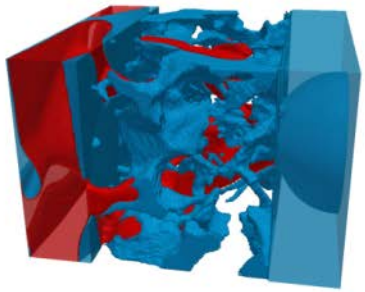
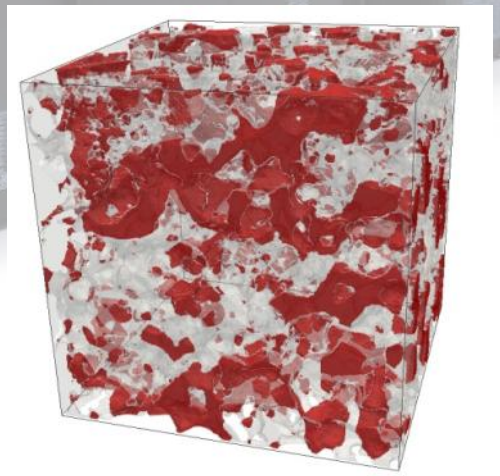




Modeling of single- and multi-component fluid flows using Lattice-Boltzmann Method on hybrid multi-GPU supercomputers

Bikulov D., Senin D.: Moscow State University Physics Faculty

AREA. Geology, Geophysics
DRIVER. Modeling of single- and multi-component filtration in porous medium using Lattice Boltzmann Method on hybrid Multi-GPU supercomputers.
STRATEGY. We use Lattice-Boltzmann method for modeling of single- and two-component fluids in complex geometries.
OBJECTIVE. Objective is to obtain filtration parameters of geological samples (cores) in numerical experiment using computer tomography of them.
IMPACT. Replacement of expensive and time-consuming laboratory experiments on hydrodynamic studies of geological samples by computational experiments in order to reduce costs and time for research.
USAGE. Oil Gas sector, Hydrodynamics.

Development of DISLIB Library

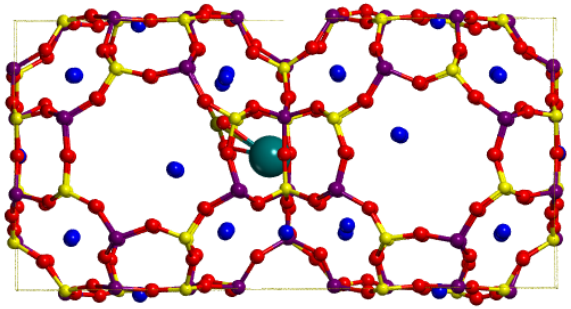
Korzh A., T-Platforms

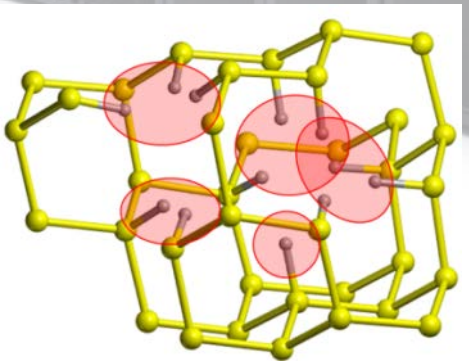
AREA. Networking Technologies, Fundamental Principles of Information and Communication Technologies and Computing Systems
DRIVER. Development and optimizing of DISLIB library.
STRATEGY. Using ideas of efficient message coalescing and active messages. Using MPI3 and other communication layers.
OBJECTIVE. Creating productive and robust approach to parallelizing DIS applications.
IMPACT. Easing programmers task, and green energy use due to better scaling and performance.
USAGE. DIS applications: graph problems, irregular meshes.

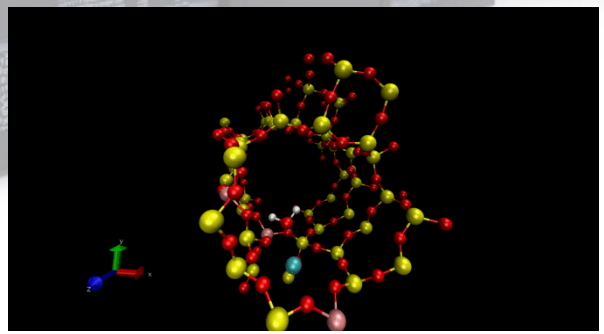
Modeling of molecular systems containing d-metals

Larin A., Bryukhanov I., Rybakov A., Buchachenko A., Bezrukov D.: Moscow State University

AREA. Inorganic Chemistry, Physical Chemistry
DRIVER. Optimal choice of cationic and zeolite framework for methanol carbonylation, definition of optimal regime of ALD techniques for achieving available passivation of Si and hydrogenated Si.
STRATEGY. Quantum chemical approaches using isolated clusters and periodic boundaries.
OBJECTIVE. Development of catalytic cycle for CO2 utilization from atmosphere on the basis of alkali earth and transition metals, modeling of oxide deposition on the surface of Si and hydrogenated Si, control over the extent of Si passivation.
IMPACT. Scientific and commercial.
USAGE. Development of catalytic cycle for CO2 utilization from atmosphere on the basis of alkali earth and transition metals, modeling of oxide deposition on the surface of Si and hydrogenated Si, control over the extent of Si passivation.



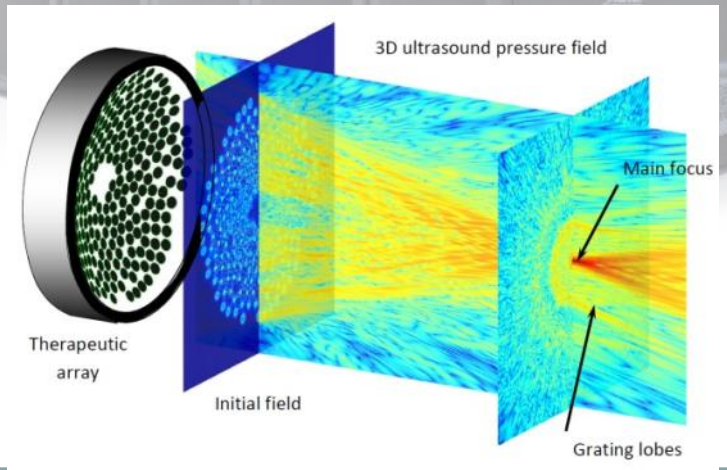


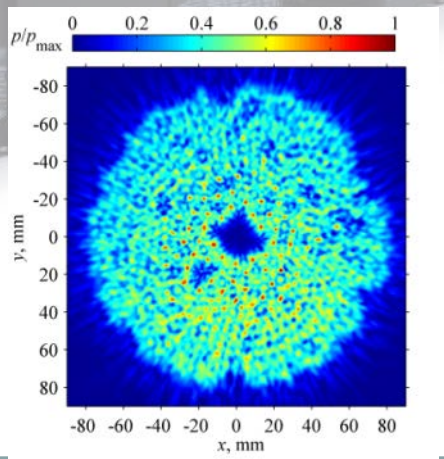


Calibration of nonlinear acoustic fields of therapeutic multi-element arrays of modern ultrasound surgery systems

Sapozhnikov O., Yuldashev P., Ilyin S., Annenkova E.

AREA. Radiophysics, Electronics and Acoustics
DRIVER. Development of a combined method to evaluate characteristic of acoustic fields produced by modern therapeutic ultrasound arrays.
STRATEGY. At a low power output level of the array, measure the pressure field over a plane near the source to construct initial conditions for a numerical model.
OBJECTIVE. Develop original numerical algorithms to simulate the effects of nonlinearity, diffraction, and absorption in the three-dimensional focused fields produced by multi element arrays used in noninvasive ultrasound surgery.
IMPACT. Development of high power multi-element transducers for ultrasound surgery systems, calculation of the characteristics of their fields, assessment of the impact of nonlinear effects in instrument calibration, quality control and planning of treatment protocols.
USAGE. Application of high intensity ultrasound in medicine and bioengineering.

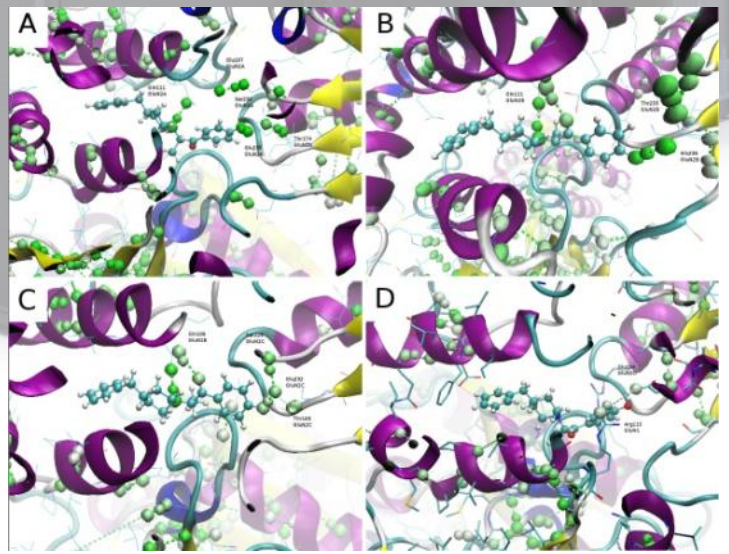




Investigation of GluN1/GluN2B aminoterminal domain allosteric modulators' binding features

Karlov D., Radchenko E., Palyulin V.: Lomonosov Moscow State University, Chemistry Department

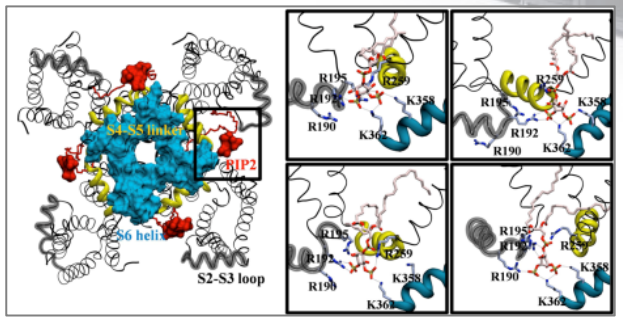
AREA. Organic Chemistry, Physicochemical Biology
DRIVER. Examination of conformational transformation in aminoterminal domains during molecular dynamics.
STRATEGY. Molecular dynamics modeling of GluN1/GluN2B complex; ifenprodil molecular docking in structure of GluN1/GluN2A, GluN1/GluN2C, GluN1/GluN2D.
OBJECTIVE. Assessment of per residue contribution values in modulators' binding enthalpy. Rationalize the essence of conformational transformation occurred without bound ligand.
IMPACT. Development of new scaffolds in design of NMDA receptor aminoterminal domain modulators.
USAGE. Medicine, Pharmacology.

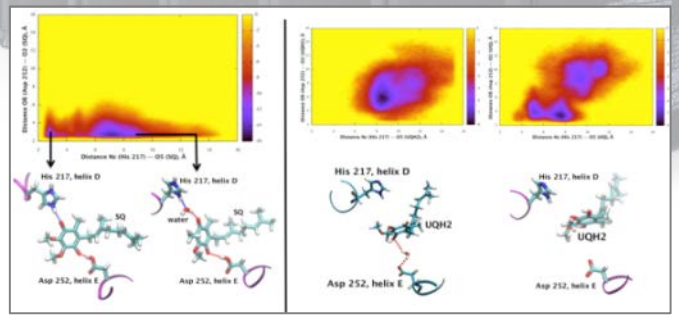


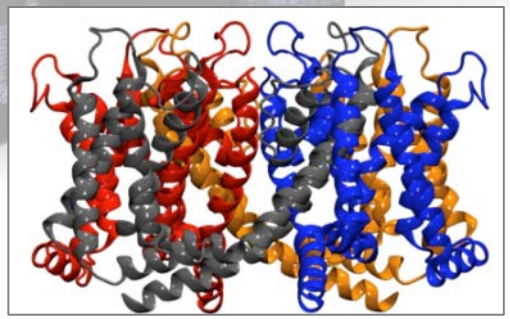
Multi-scale molecular simulations of membrane proteins

Shaitan K., Shaytan A., Kasimova M., Orekhov P.: Moscow State University, Biology Faculty

AREA: Biology, Medicine
DRIVER: Understanding functioning of membrane proteins at molecular level.
STRATEGY: Use multi-scale molecular modeling techniques.
OBJECTIVE: Study of membrane protein dynamics and its dependence on internal and external factors.
IMPACT: Understanding the fundamentals of living systems, drug design.
USAGE: Pharmacology, Medicine.

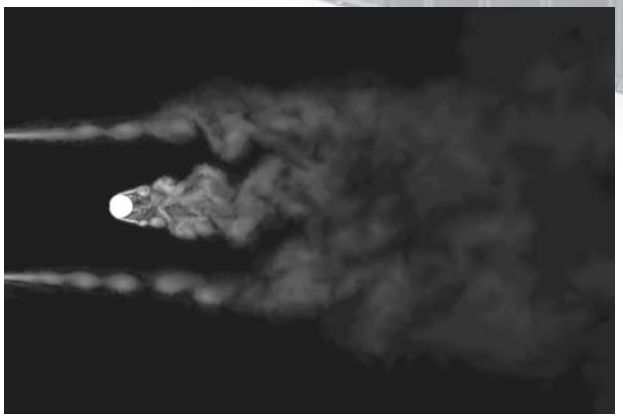


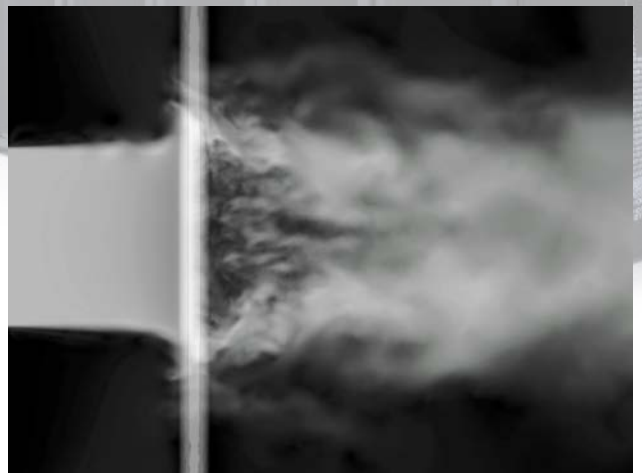


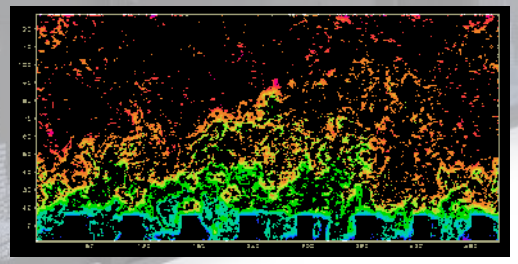


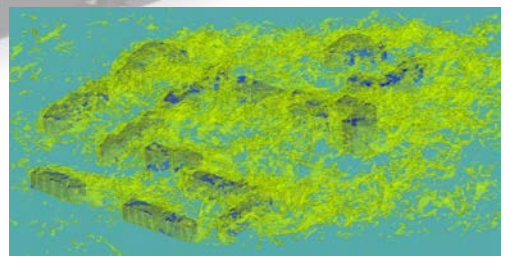
Turbulence Modeling

DRIVER. Find a new way to reduce turbulent friction drag in gas or liquid flows near solid surface.
STRATEGY. Use direct numerical simulation for fundamental studies of the microphysics of turbulent flows with different boundary conditions.
OBJECTIVE. Make an assumption about mechanism of turbulent energy production in wall-bounded flows.
IMPACT. Better and more clear understanding of mysterious phenomenon - turbulence.
USAGE: Aerospace, Construction industry



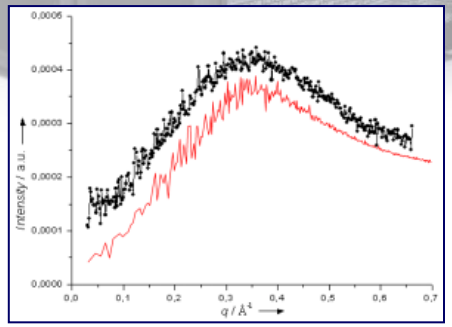


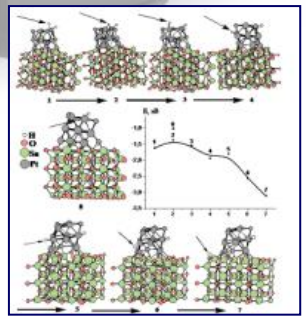




Hydrogen Energy

DRIVER: Improve electrochemical fuel cells efficiency and reduce costs.
STRATEGY: Understand of elementary steps of processes in electrochemical fuel cells. Elucidate factors determining efficiency and stability of composite catalysts based on nano-sized metal particles on proton-conducting oxide substrates.
OBJECTIVE: Use ab initio DFT-based techniques to model interactions of oxygen and fuel molecules with metal surfaces up to dissociation, moving of atoms and functional groups from metal to substrate (spillover-effect), migration of atoms along catalyst and substrate surfaces, interaction between metal particles and substrate. Elucidate factors determining molecule activation on catalyst particles, proton conductivity trough the composite system and fastening of metal particles on substrate.
IMPACT: Design of electrochemical fuel cells with high stability and low content of platinum metals.
USAGE: Automotive industry.

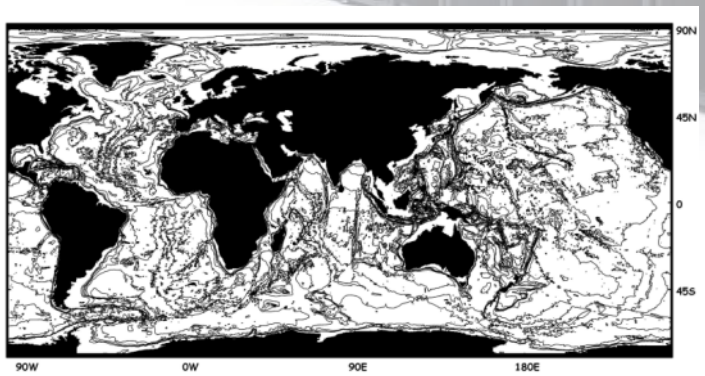


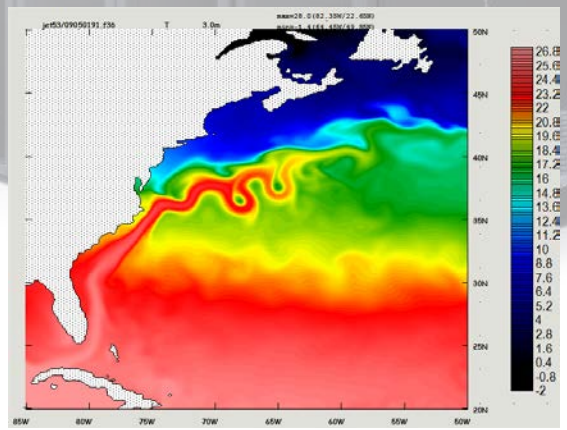


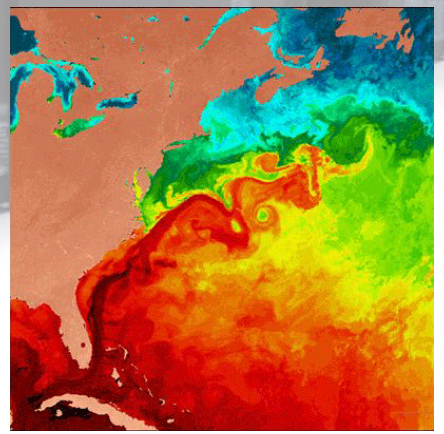
World Ocean modeling

Ibrayev R.: INM RAS; Ushakov K., Khabeev R., Orekhova M.: IO RAS, Kalmykov V.: MSU

AREA. Marine Sciences
DRIVER. Study of 3-dimensional variability of water circulation, heat and salt fluxes of the World Ocean during the second half of the XX'th century by means of a high resolution numerical model.
STRATEGY. Model calibration according to the CORE-I data, numerical experiments with CORE-II and ERA-40 atmospheric conditions.
OBJECTIVE. Reproduction of interannual variability of ocean parameters known from observational data.
IMPACT. Gain of knowledge about the mechanisms of the Earth climate system.
USAGE. Weather forecasts and assesses of climate change for the coming decades.





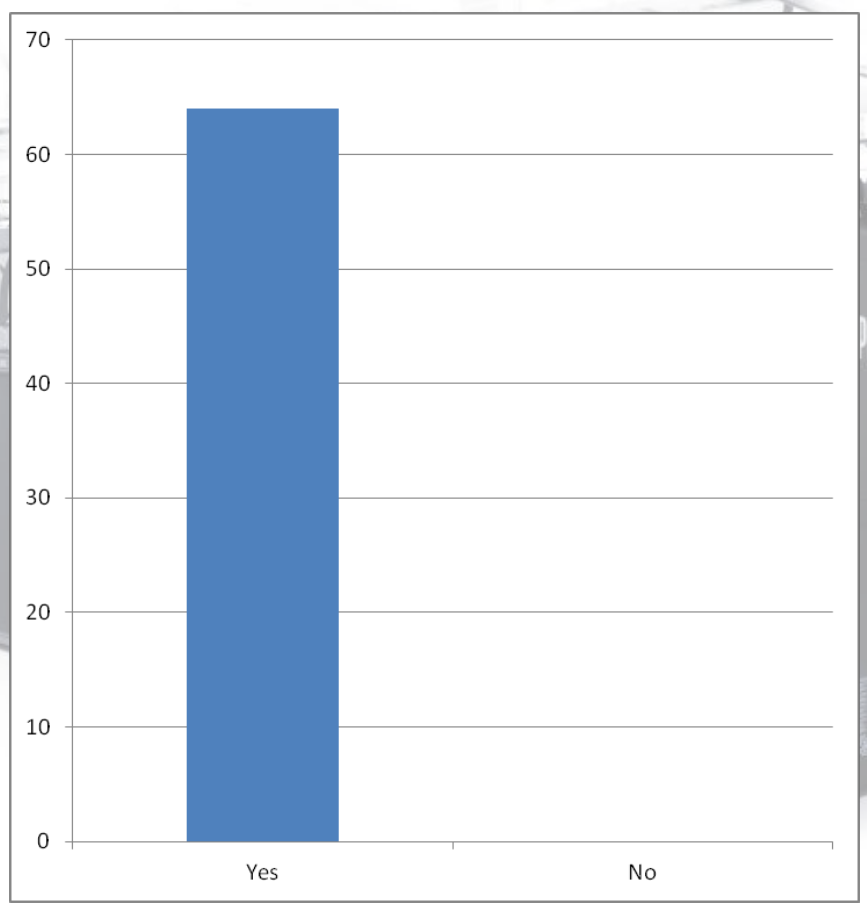


MSU Supercomputing Center
(users & organizations)

	2009	2010	2011	2012
User groups, total:	241	369	545	610
including:				
from Moscow University:	155	241	359	406
from Institutes of RAS:	53	77	110	121
from other organizations:	33	51	76	83
Faculties / Institutes of MSU:	15	21	24	24
Institutes of RAS:	20	28	35	39
Others:	19	24	34	39

Computational science is everywhere. This is a very serious argument for Supercomputing Education!

Informatics Europe: a survey on needs for Supercomputing education



Is "Parallel Computing & Supercomputing" a strategically important area?

What does Exascale bring to computational practice?

Answer: incredible degree of parallelism.

June 02, 2013

Full Details Uncovered on Chinese Top Supercomputer

HPC wire

Nicole Hemsoth

At the end of May, an international group of high performance computing researchers gathered at the International HPC Forum in Changsha, China. One of the talks detailed the specs for the new Tianhe-2 system, which as we reported last week, is expected to rather dramatically top the Top500 list of the world's fastest supercomputers.

Artist's rendering of the system as it will look once finally implemented at its final destination.

As noted previously, the system will be housed at the National Supercomputer Center in Guangzhou and has been aimed at providing an open platform for research and education and to provide a high performance computing service for southern China.

Dr. Jack Dongarra from Oak Ridge National Lab, one of the founders of the Top500, was on hand for the event in China and shared a draft document that offers deep detail on the full scope of the Tianhe-2, which will, barring any completely unexpected surprises, far surpass the Cray-built Titan.

Newborn giant: Tianhe-2

16 000 compute nodes

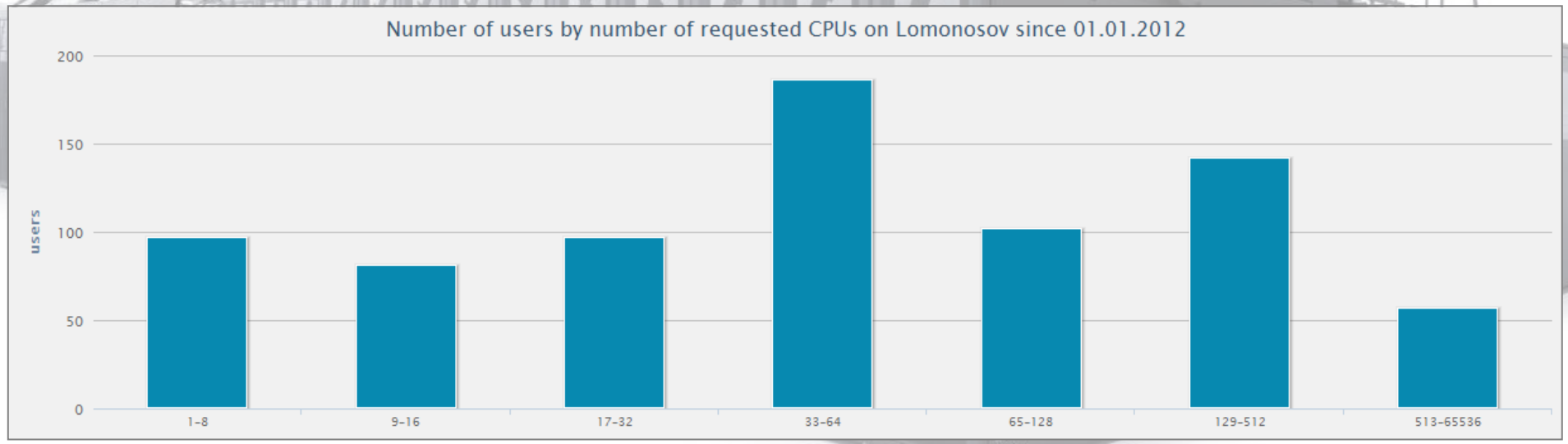
32 000 Intel Ivy Xeon

48 000 Intel Xeon Phi

3 120 000 cores

54.9 Pflop/s (peak)

Stats on "Lomonosov" Supercomputer
(Number of users by number of requested CPUs)



What does Exascale bring to the computer world ?

Exascale (at 2019-2020)

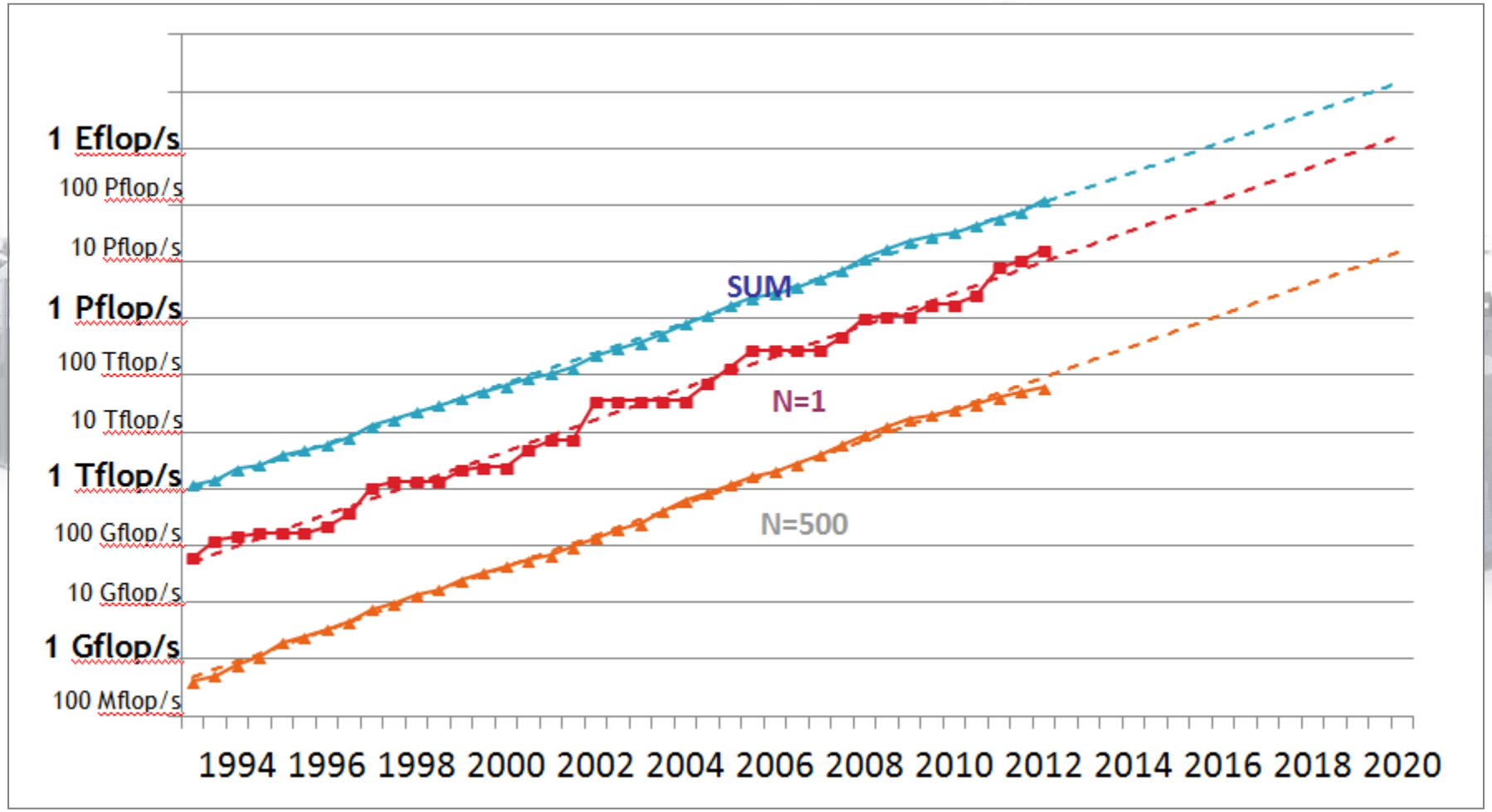
- *Supercomputers – billions cores,*
- *Laptops – thousands cores,*
- *Mobile devices – dozens/hundreds cores.*

Parallelism will be everywhere… And what does it mean ?

All software developers need to be fluent in the concept of parallelism.

When Do We Need to Start ?

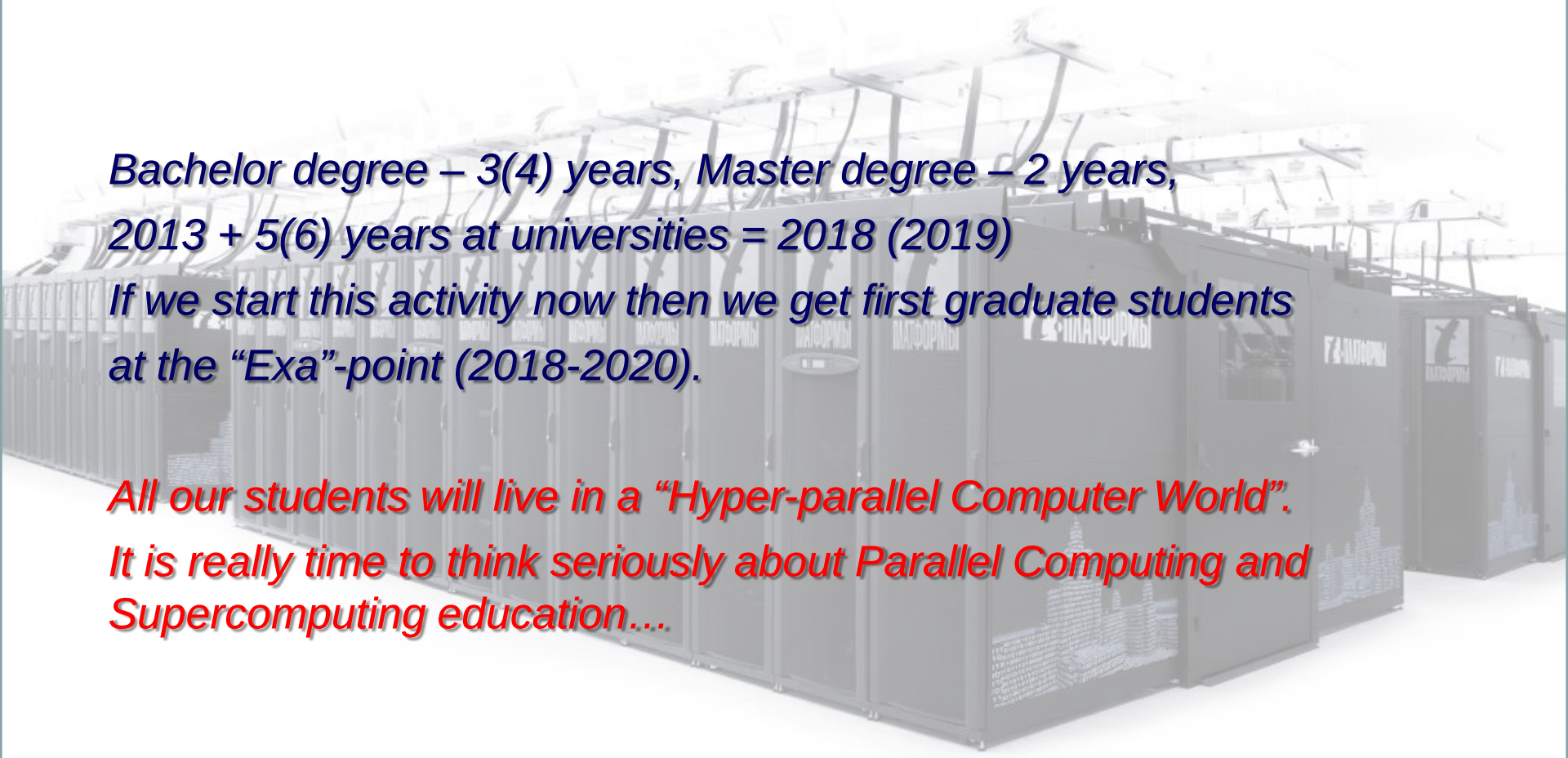
(Exascale is far away...)



Courtesy of E.Strohmaier, top500.org

It is Time to Act !

(Exascale is NOT far away…)



Bachelor degree – 3(4) years, Master degree – 2 years,

2013 + 5(6) years at universities = 2018 (2019)

If we start this activity now then we get first graduate students at the "Exa"-point (2018-2020).

All our students will live in a "Hyper-parallel Computer World".

It is really time to think seriously about Parallel Computing and Supercomputing education….

Simple questions ?

(ask students from your faculties…)

- *What is complexity of a parallel algorithm? Why do we need to know a critical path of an informational graph (data dependency graph)?*
- *Is it possible to construct a communication free algorithm for a particular method?*
- *How to detect and describe potential parallelism of an algorithm? How to extract potential parallelism from codes or algorithms?*
- *What is co-design?*
- *What is data locality?*
- *How to estimate data locality in my application?*
- *How to estimate scalability of an algorithm and/or application? How to improve scalability of an application?*
- *How to express my problem in terms of MapReduce model?*
- *What is efficiency of a particular application?*
- *What parallel programming technology should I use for SMP/GPU/FPGA/vector/cluster/heterogeneous computers? …*

How many software developers will be able to use easily these notions?

Simple questions ?

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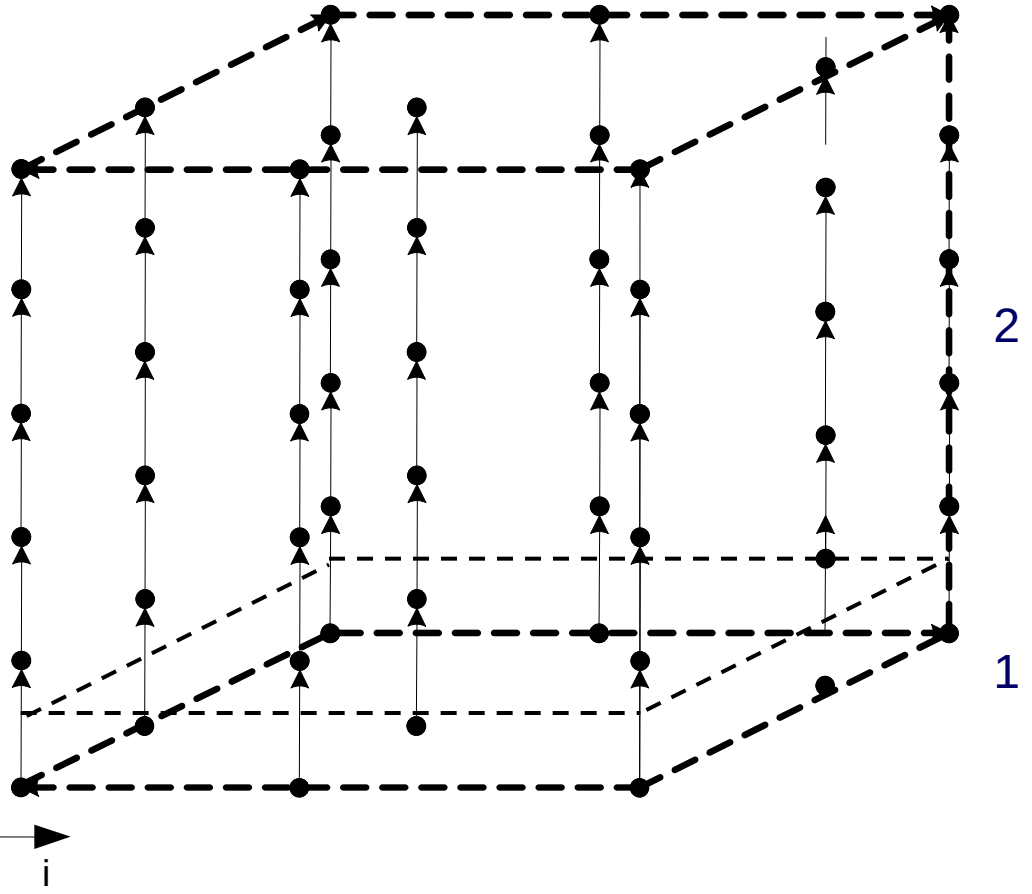
Informational Structure is a Key Notion

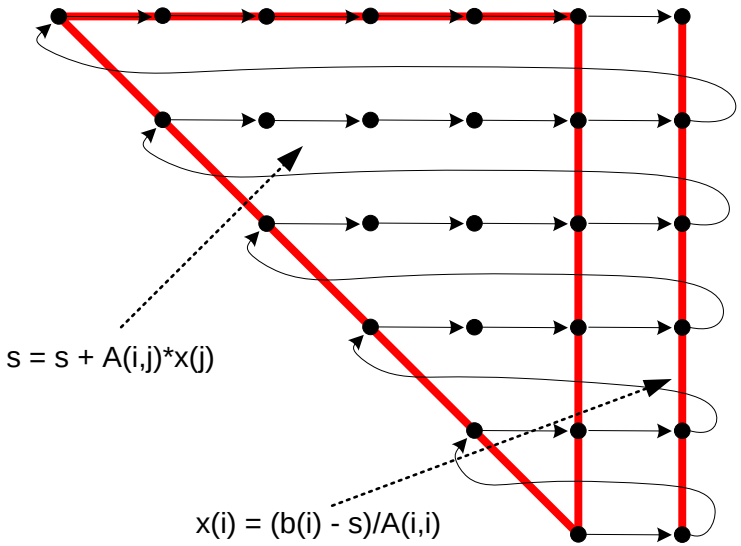
(matrix multiplication as an example)

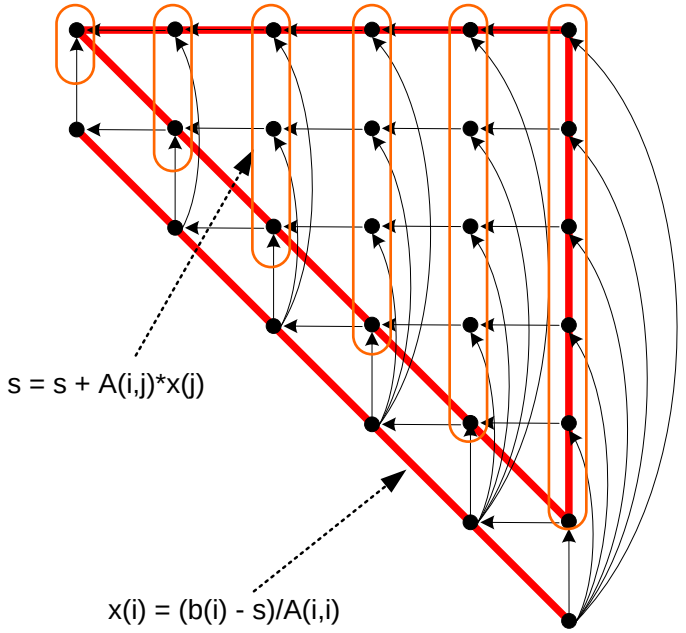
```
      Do i = 1, n
        Do j = 1, n
1         A(i,j) = 0
          Do k = 1, n
2           A(i,j) = A(i,j) + B(i,k)*C(k,j)
```

$$\begin{cases} 1 \le i \le n \\ 1 \le j \le n \\ k = 1 \\ \begin{cases} i_1 = i \\ j_1 = j \end{cases} \\ из\ (1) \end{cases} \qquad \begin{cases} 1 \le i \le n \\ 1 \le j \le n \\ 2 \le k \le n \\ \begin{cases} i_1 = i \\ j_1 = j \\ k_1 = k - 1 \end{cases} \\ из\ (2) \end{cases}$$



GAUSS elimination method
(informational structure)






```
do i = n, 1, -1
   s = 0
   do j = i+1, n
      s = s + A(i,j)*x(j)
   end do
   x(i) = (b(i) - s)/A(i,i)
end do
```

```
do i = n, 1, -1
   s = 0
   do j = n, i+1, -1
      s = s + A(i,j)*x(j)
   end do
   x(i) = (b(i) - s)/A(i,i)
end do
```

Simple questions ?

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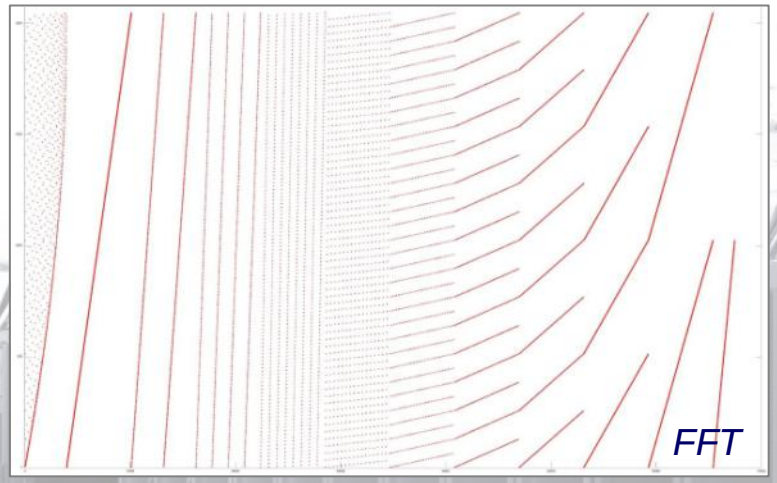
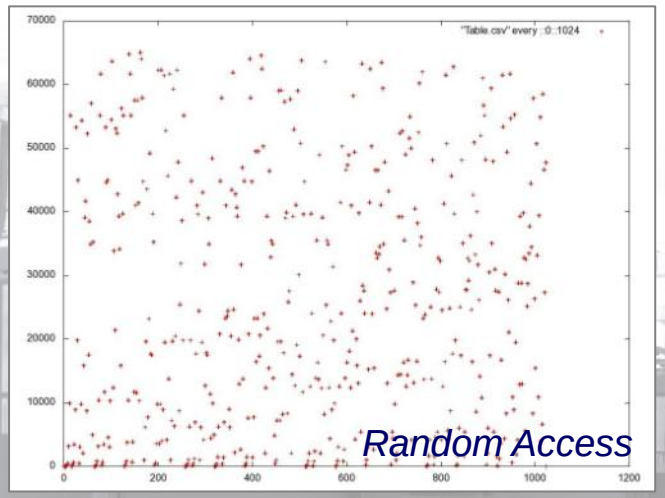
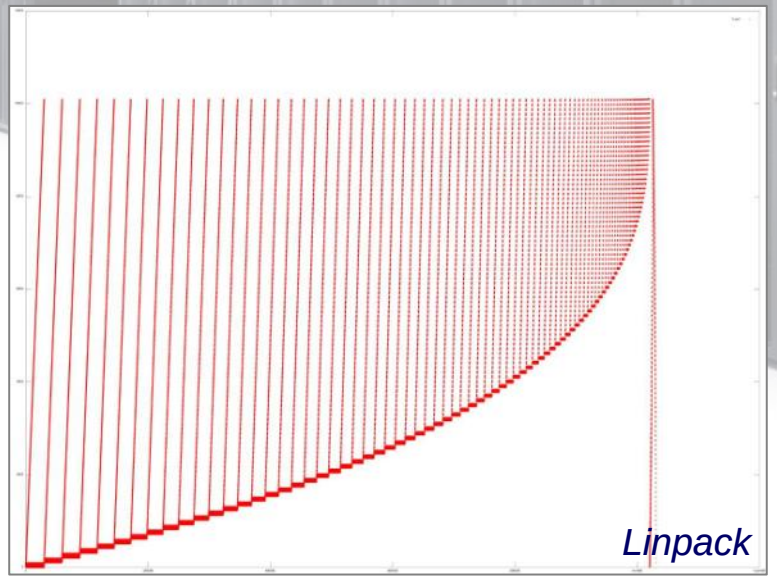
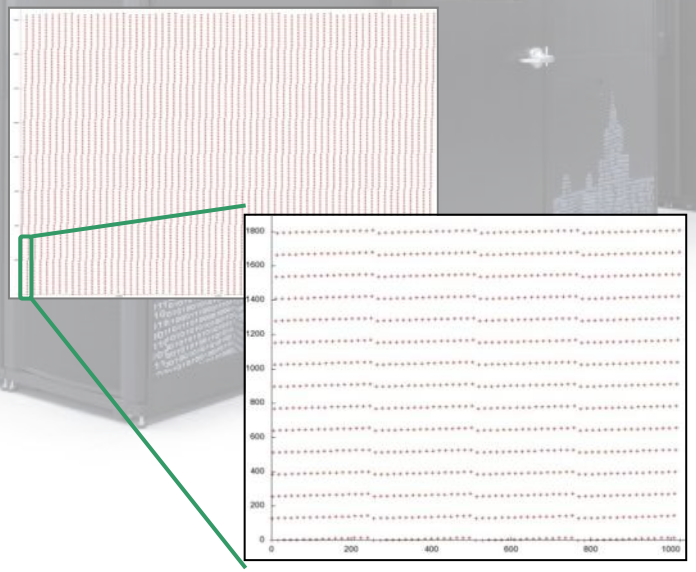
Data Locality in Applications

(profiles of memory usage)



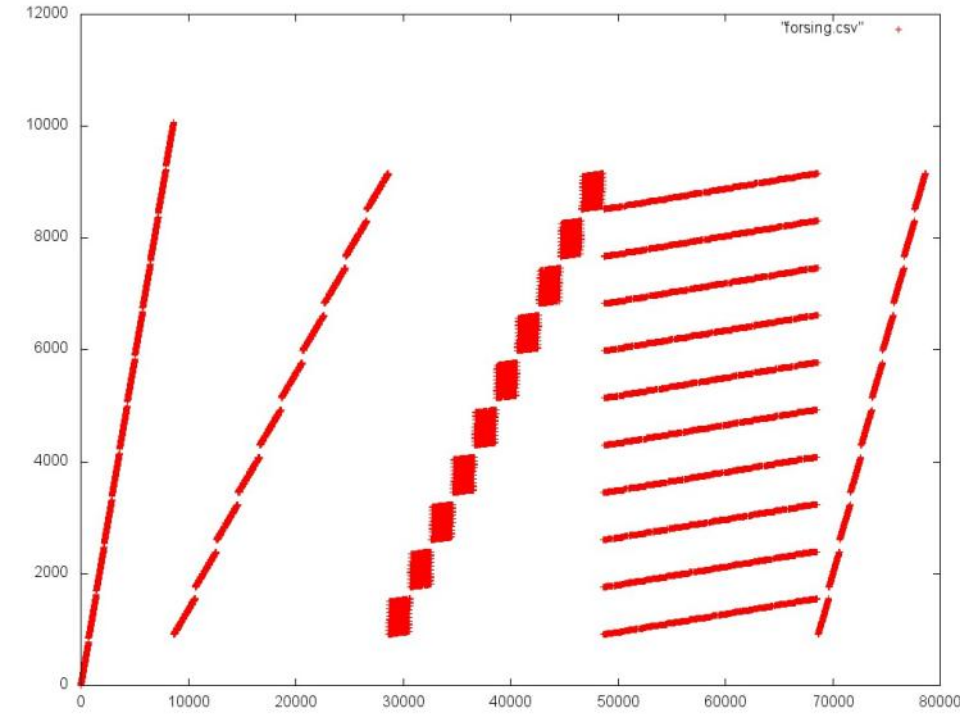


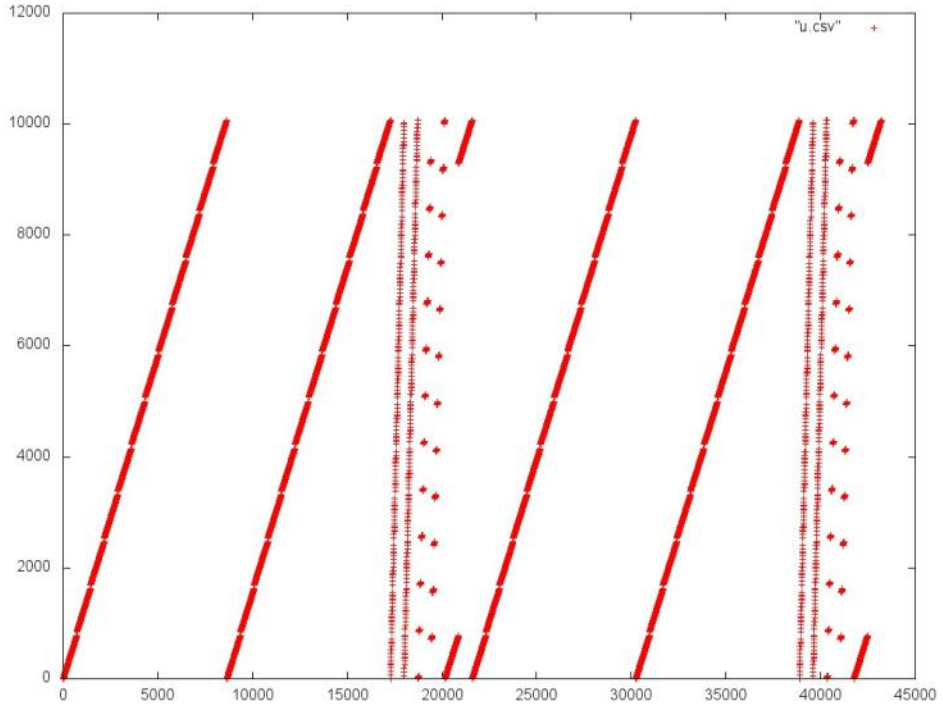




Courtesy of Vad.Voevodin, MSU

Data Locality in Applications
(profiles of memory usage)





NPB - BT

Courtesy of Vad.Voevodin, MSU

Simple questions ?

(ask students from your faculties…)

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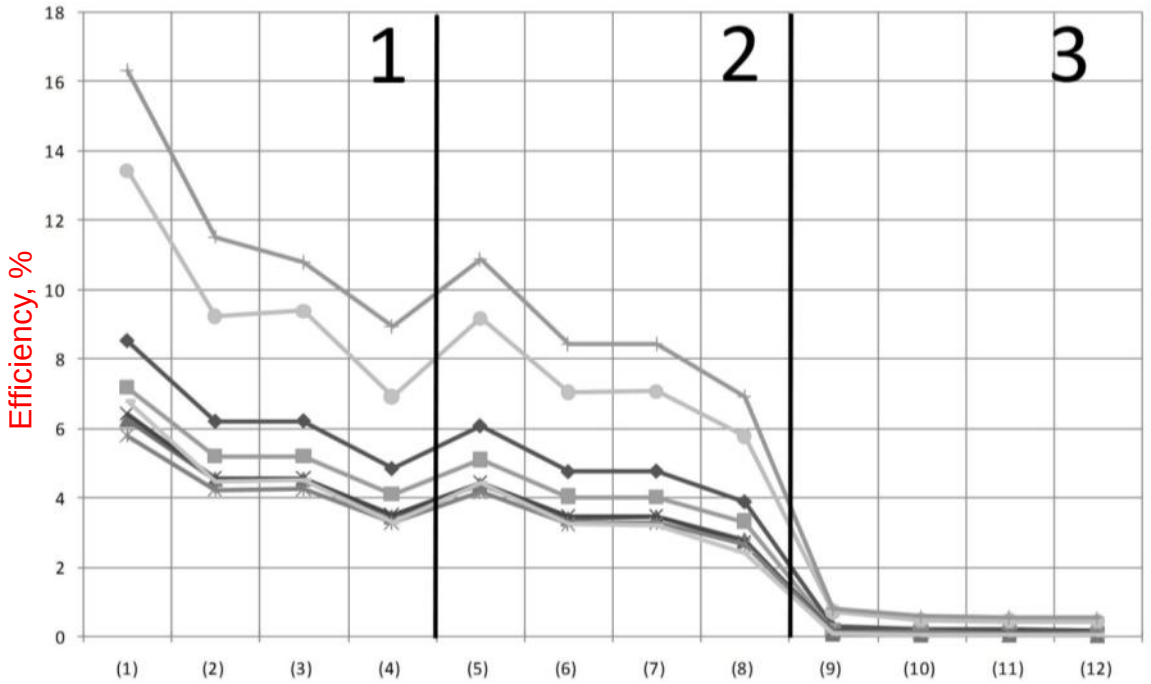
Efficiency of Applications
(variants of TRIAD operation)



1) A[i] = B[i]*X + C
2) A[i] = B[i]*X[i] + C
3) A[i] = B[i]*X + C[i]
4) A[i] = B[i]*X[i] + C[i]

5) A[ind1[i]] = B[ind1[i]]*X + C
6) A[ind1[i]] = B[ind1[i]]*X[ind1[i]] + C
7) A[ind1[i]] = B[ind1[i]]*X + C[ind1[i]]
8) A[ind1[i]] = B[ind1[i]]*X[ind1[i]] + C[ind1[i]]
ind1[i] = i

9) A[ind2[i]] = B[ind2[i]]*X + C
10) A[ind2[i]] = B[ind2[i]]*X[ind2[i]] + C
11) A[ind2[i]] = B[ind2[i]]*X + C[ind2[i]]
12) A[ind2[i]] = B[ind2[i]]*X[ind2[i]] + C[ind2[i]]
ind2[i] = random_access

1 2 3

Courtesy of Vad.Voevodin, MSU

Simple questions ?

(ask students of your faculties...)

- *What is complexity of a parallel algorithm? Why do we need to know a critical path of an informational graph (data dependency graph)?*
- *Is it possible to construct a communication free algorithm for a particular method?*
- *How to detect and describe potential parallelism of an algorithm? How to extract potential parallelism from codes of algorithms?*
- *What is co-design?*
- *What is data locality?*
- *How to estimate data locality in my application?*
- *How to estimate scalability of an algorithm and/or application? How to improve scalability of an application?*
- *How to express my problem in terms of MapReduce model?*
- *What is efficiency of a particular application?*
- *What parallel programming technology should I use for SMP/GPU/FPGA/vector/cluster/heterogeneous computers? ...*

We really need a systematic approach to be able to answer similar questions…

How many software developers will be able to use easily these notions?

What could be a solution ?

Trainings ?!

MSU: Trainings and Schools

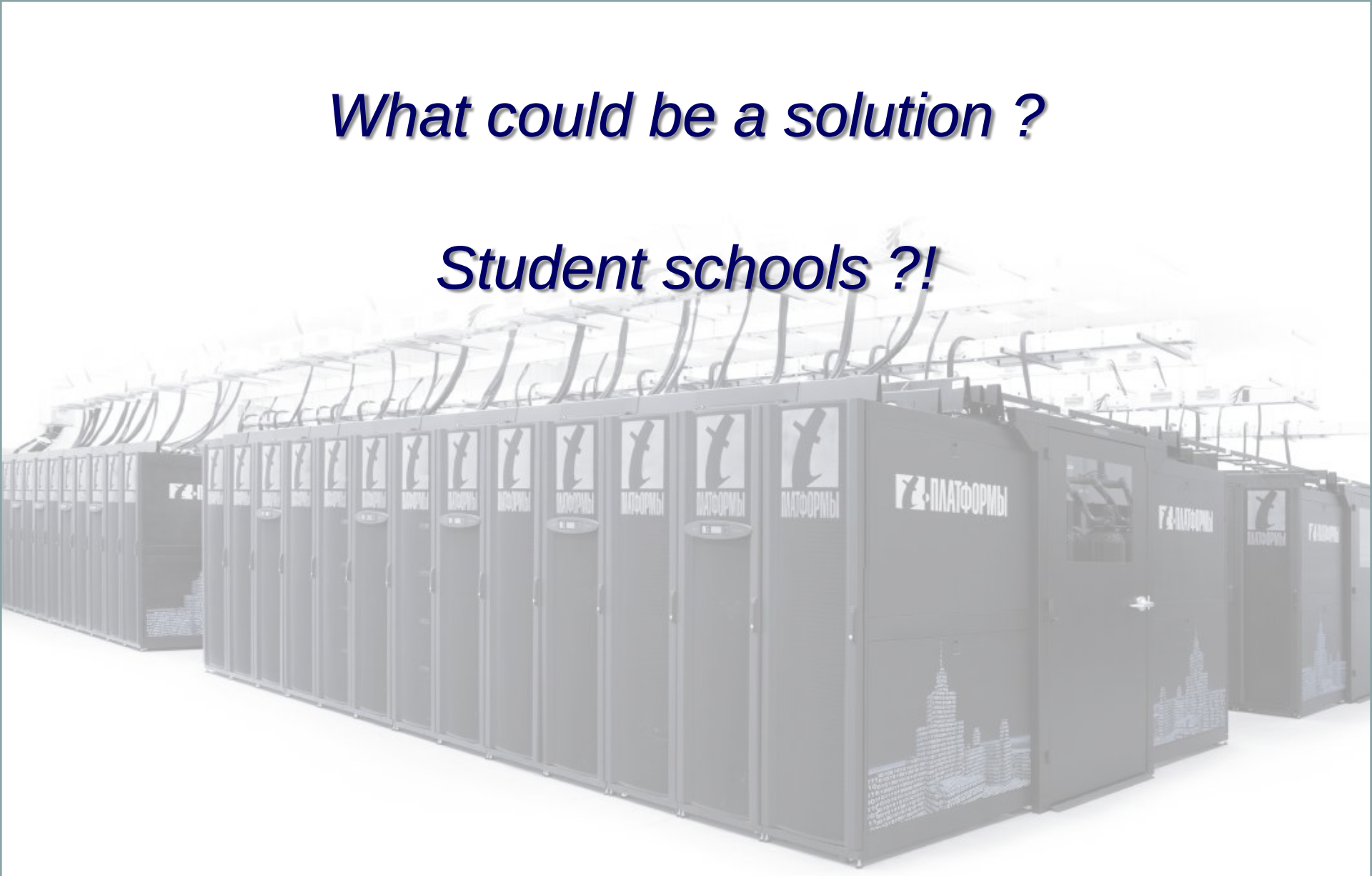
Trainings on Intel programming tools. Optimization and tuning of user's applications.

Student summer schools on parallel programming technologies

Trainings on Accelrys Material Studio

What could be a solution ?

Student schools ?!

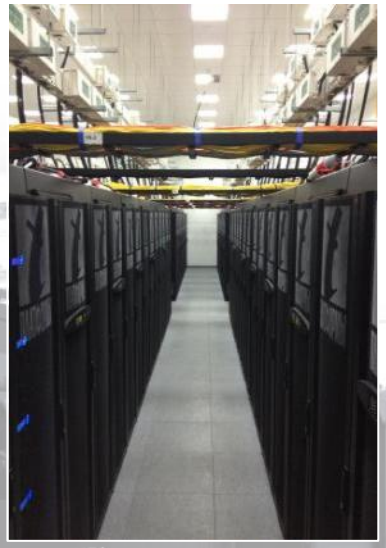


GPU Technology Schools at MSU

Major topics at schools:

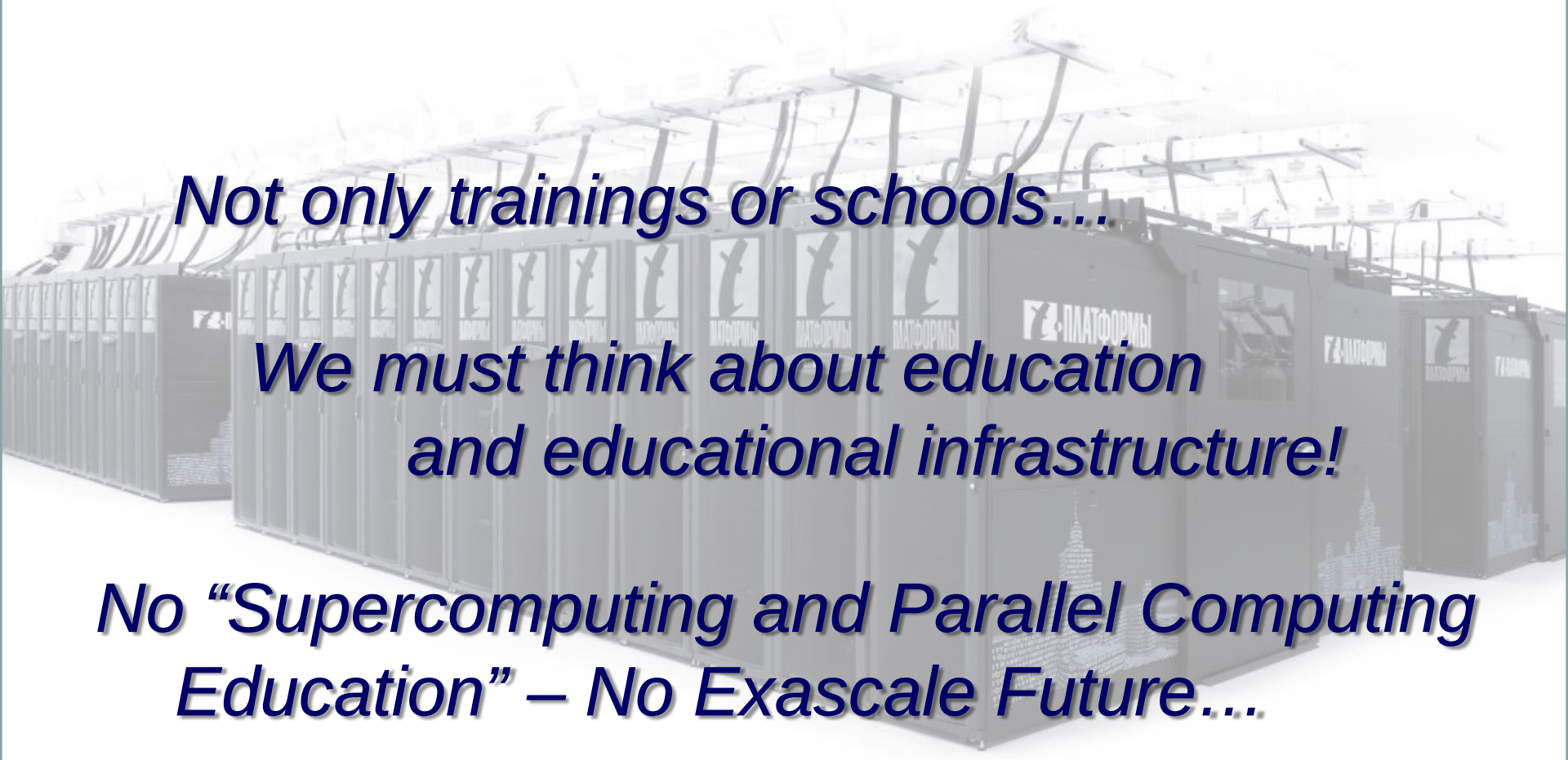
- *Massively Parallel Processing*
- *GPGPU Evolution*
- *Architecture of NVIDIA GPUs*
- *CUDA Programming Model*
- *CPU-GPU Interaction*
- *CUDA Memory Types*
- *Standard Algorithms on GPU: Matrix Multiplication, Reduction*
- *CUDA application libraries: CURAND, CUBLAS, CUSPARSE, CUFFT, MAGMA, Thrust*
- *Program Profiling, Performance Analysis, Debugging and Optimization*
- *Asynchronous Execution and CUDA Streams*
- *Multi-GPU Systems: Programming and Debugging*
- *nvcc Compiler Driver, cuda-gdb Debugger*
- *Kernel Configuration and Paralleling of Loops*
- *OpenACC Directives*

January, 2012
July, 2012
October, 2012
February, 2013
July, 2013



In collaboration with NVIDIA and Applied Parallel Computing

What could be a solution ?



Not only trainings or schools….

We must think about education and educational infrastructure!

No “Supercomputing and Parallel Computing Education” – No Exascale Future….

HPC Educational Infrastructure

- *Interaction with government, ministries, funding agencies.*
- *Close contacts with leading IT companies and research institutes.*
- *Strong interuniversity collaboration.*
- *Body of knowledge on HPC & Parallel Computing.*
- *All target groups: researchers, students, teachers, schoolchildren.*
- *Courses, textbooks, intensive practice, trainings on HPC.*
- *Individual research projects of students.*
- *Bank of exercises and tests on HPC & Parallel Computing.*
- *Internet-university on supercomputing technology.*
- *National scientific conferences and student schools.*
- *Research on advanced computing techniques, HW, SW, apps….*
- *HPC and Industry.*
- *International collaboration.*
- *PR, mass-media, Internet resources on HPC.*

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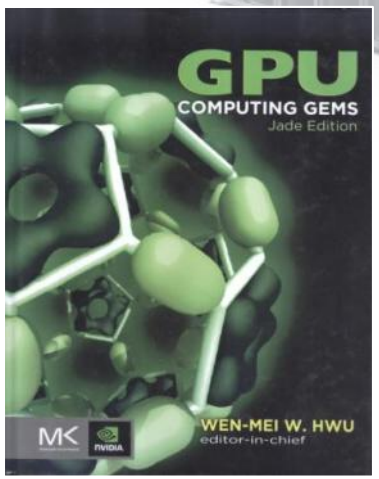
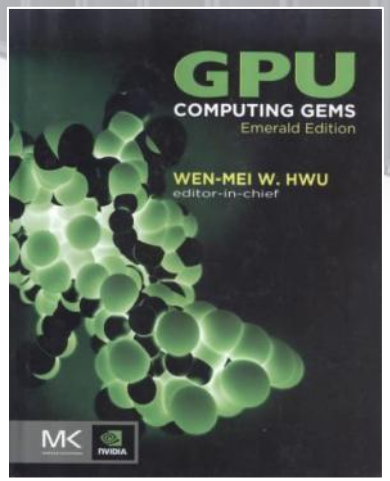
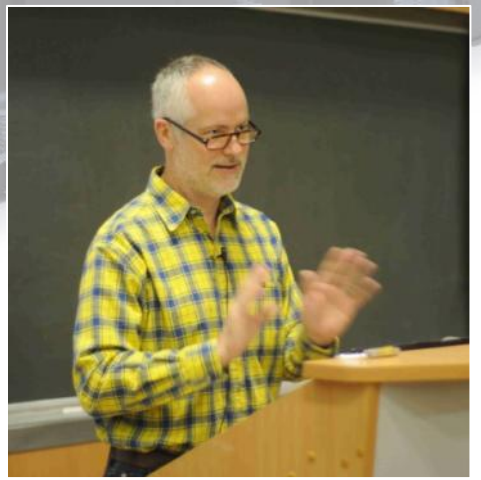
Joint MSU – Intel
Student Lab and Center on HPC

CUDA Center of Excellence at MSU

- *Hardware Platforms and Software Infrastructure*
- *GPU Applications: Regular and Superscalable*
- *Contacts with Leading Experts in the Area*
- *GPU HPC and Industry*
- *GPU Programming Technologies*
- *Broad GPU Education*
- *GPU Research Contests*
- *Dissemination and Popularization*







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MSU Petaflops Computing Facilities: "Lomonosov" Supercomputer

M.V.Lomonosov
1711 – 1765

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MINISTRY OF EDUCATION AND SCIENCE
OF THE RUSSIAN FEDERATION

Project "Supercomputing Education"
Presidential Commission for Modernization and Technological Development of Russia's Economy

Duration: 2010-2012

Coordinator of the project: M.V.Lomonosov Moscow State University

Wide collaboration of universities:

- *Nizhny Novgorod State University*
- *Tomsk State University*
- *South Ural State University*
- *St. Petersburg State University of IT, Mechanics and Optics*
- *Southern Federal University*
- *Far Eastern Federal University*
- *Moscow Institute of Physics and Technology (State University)*
- *members of Supercomputing Consortium of Russian Universities*

More than 600 people from 75 universities were involved in the project .
Budget: 236,42 million rubles (about $8M)

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

National System of Research and Education Centers on Supercomputing Technologies in Federal Districts of Russia

8 centers were established in 7 federal districts of Russia during 2010-2012

Entry-Level Training on Supercomputing Technologies

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

3269 people passed trainings, *60+* universities from *35* cities of Russia
All Federal Districts of Russia

Series of Books "Supercomputing Education"

"Computational Mathematics and Algorithm`s Structure"
V.V. Voevodin

"High-Performance Computations for Multiprocessor Multi-Core Systems"
V.P. Gergel

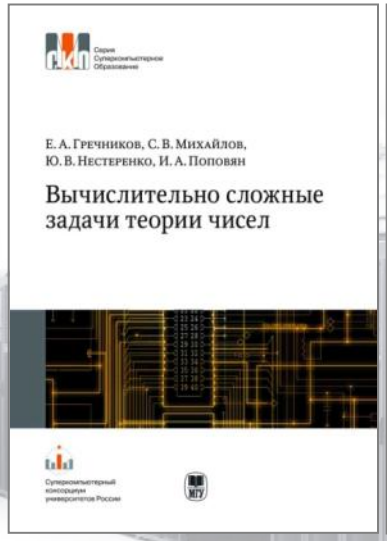
"Practical Course on Parallel Computing Techniques"
A.V. Starchenko, E.A. Danilkin, V.I. Laeva, S.A. Prokhanov

"Parallel Programming Tools in Shared-Memory Systems"
K.V. Kornyakov, V.D. Kustikova, I.B. Meyerov, A.A. Sydnev, A.V. Sysoev, A.V. Shishkov

"Parallel Programming Technologies for New Architecture Processors"
A.V. Linev, D.K. Bogolepov, S.I. Bastrakov

There are 21 books in the "Supercomputing Education" series.

Series of Books "Supercomputing Education"



"Computationally Intensive Problems of Numbers Theory"
E.A. Grechnikov, S.V. Michailov, Y.V. Nesterenko, I.A. Popovyan

"Supercomputing Modeling in Climate System Physics"
V.N. Lykosov, A.V. Glazunov, D.V. Kulyamin, E.V. Mortikov, V.M. Stepanenko

"Parallel Computing on GPU: Architecture and Programming Models"

"New Computational Fluid Dynamics Algorithms for Parallel Computers"
V.M. Goloviznin, M.A. Zaitsev, S.A.Karabasov, I.A. Korotkin

"Parallel Programming Technologies MPI and OpenMP"
A.S. Antonov

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

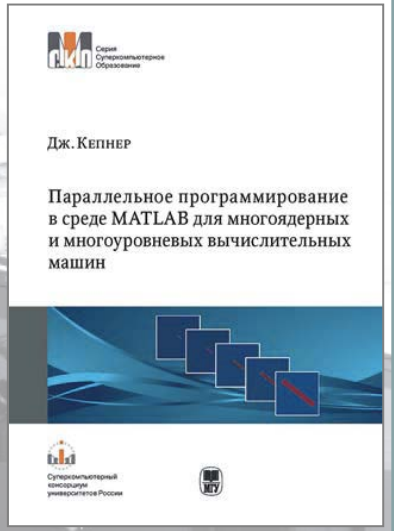
Series of Books
“Supercomputing Education”

“Introduction to Parallel Methods”
M.V.Jakobovsky

“Principles of Parallel Programming”
C.Lin, L. Snyder,

“Iterative Methods for Sparse Linear Systems”
Y.Saad

“Models of Global Atmosphere and Ocean. Algorithms and Supercomputing Technologies”

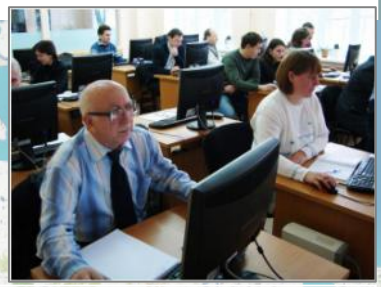


“Parallel MATLAB for Multicore and Multinode Computers”
J. Kepner

***31.500** books of the series will be delivered to **43** Russian universities.*

Retraining Programs for Faculty Staff

СУПЕРКОМПЬЮТЕРНЫЙ
КОНСОРЦИУМ УНИВЕРСИТЕТОВ РОССИИ



453 faculty staff passed trainings, *50* organisations, *29* cities, *10* education programs.
All Federal districts of Russia.

Education Courses on Supercomputing Technologies

Development of new courses and extension of existing ones…

50 courses covering all major parts of the Body of Knowledge in SC…

- *"Parallel Computing",*
- *"High Performance Computing for Multiprocessing Multi-Core Systems",*
- *"Parallel Database Systems",*
- *"Practical Training on MPI and OpenMP",*
- *"Parallel Programming Tools for Shared Memory Systems",*
- *"Distributed Object Technologies",*
- *"Scientific Data Visualization on Supercomputers",*
- *"Natural Models of Parallel Computing",*
- *"Solution of Aero- and Hydrodynamic problems by Flow Vision",*
- *"Algorithms and Complexity Analysis",*
- *"History and Methodology of Parallel Programming",*
- *"Parallel Numerical Methods",*
- *"Parallel Computations in Tomography",*
- *"Final-Element Modeling with Distributed Computations",*
- *"Parallel Computing on CUDA and OpenCL Technologies",*
- *"Biological System Modeling on GPU“,*
- *"High Performance Computing System: Architecture and Software",*
- *…*

Intensive Trainings in Special Groups

40 special groups of trainees were formed,

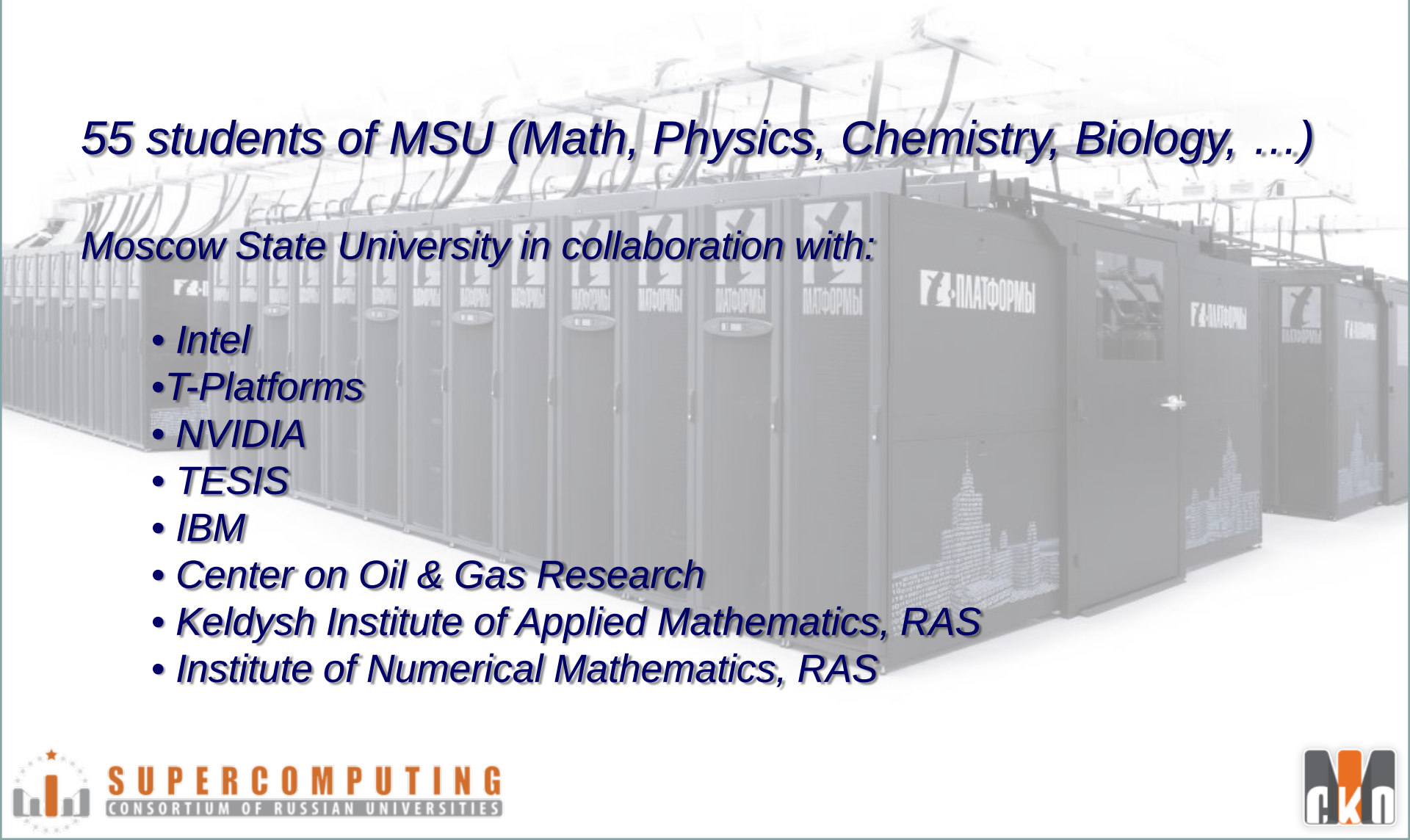
790 trainees successfully passed advanced training,

15 educational programs,

All Federal districts of Russia.

IT-Companies + Research Institutes & Edu

(special group of students on Parallel Software Development)



55 students of MSU (Math, Physics, Chemistry, Biology, …)

Moscow State University in collaboration with:

- *Intel*
- *T-Platforms*
- *NVIDIA*
- *TESIS*
- *IBM*
- *Center on Oil & Gas Research*
- *Keldysh Institute of Applied Mathematics, RAS*
- *Institute of Numerical Mathematics, RAS*

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

"Supercomputing Education" Project

(key results for 2010-2012)

- *National system of research and education centers on supercomputing technologies: 8 centers in 7 Federal districts of Russia,*
- *Body of Knowledge on parallel computing and supercomputing,*
- *Russian universities involved in supercomputing education – 75,*
- *Entry-level trainings: 3269 people, 60+ universities, 34 Russian cities,*
- *Intensive training in special groups – 790 people, 40 special groups,*
- *Retrained faculty staff on HPC technologies – 453 people, 50 organizations,*
- *New and modified curriculum and courses of lectures – 50,*
- *Using distant learning technology – 731 people, 100 cities,*
- *Partners from science, education and industry – 120 Russian and 65 foreign organizations,*
- *Series of books and textbooks "Supercomputing Education" – 21 books, 31500 books were delivered to 43 Russian universities,*
- *National system of scientific conferences and students schools on HPC,*
- *...*

Summer Supercomputing Academy

at Moscow State University
June,24 – July,6, 2013

- *Plenary lectures by prominent scientists, academicians, CEO/CTO's from Russia and abroad,*
- *6 parallel educational tracks,*
- *Trainings on a variety of topics,*
- *Attendees: from students up to professors.*

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

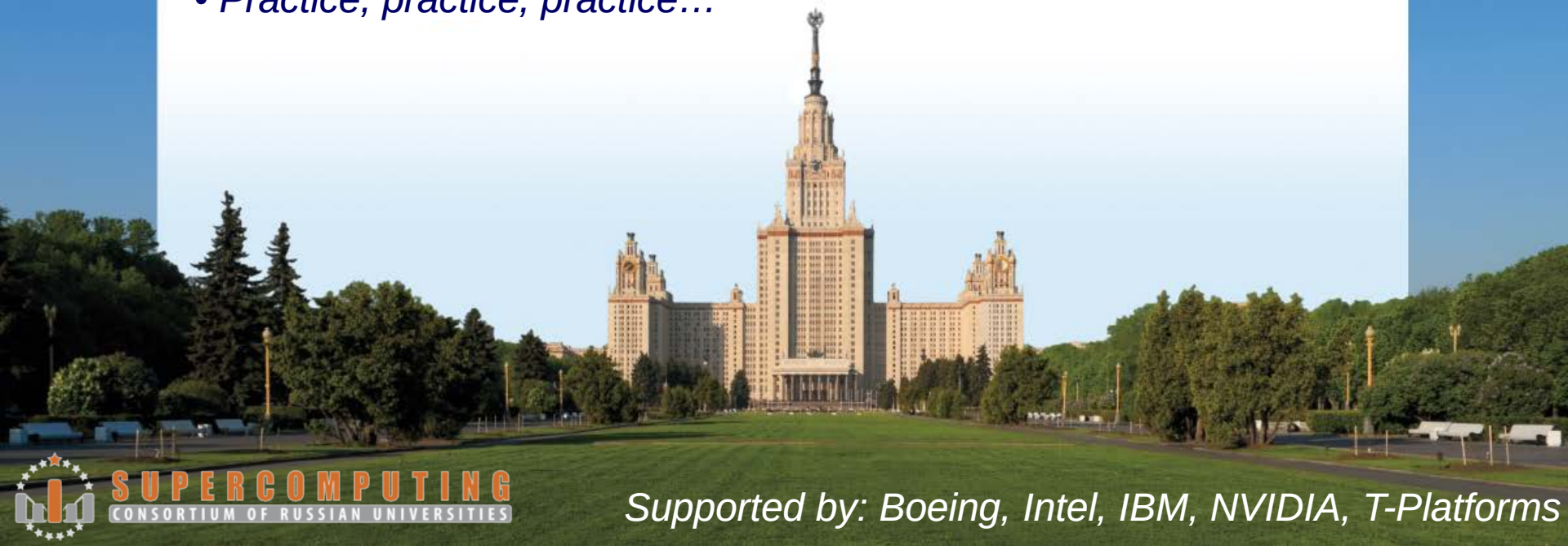
Supported by: Boeing, Intel, IBM, NVIDIA, T-Platforms

Summer Supercomputing Academy

at Moscow State University
June,24 – July,6, 2013

Track for school teachers of informatics:

- *Large problems and basics of supercomputing,*
- *Parallel methods: structure, parallelism, complexity*
- *Introduction to parallel programming*
- *Mathematical modeling, supercomputer simulation*
- *Practice, practice, practice…*



SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

Supported by: Boeing, Intel, IBM, NVIDIA, T-Platforms

Supercomputing Consortium of Russian Universities

(http://hpc-russia.ru)

2013: 57 full and associated members

Body of Knowledge: Parallel Computing and Supercomputing

(what is inside "Parallel Computing / HPC" area?)

Major 5 sections on the upper level:

1. Mathematical foundations of parallel computing,
2. Parallel computing systems (computer system foundations),
3. Technologies of parallel programming (parallel software engineering foundations),
4. Parallel methods and algorithms,
5. Parallel computing, large-scale problems and problem-oriented applications.

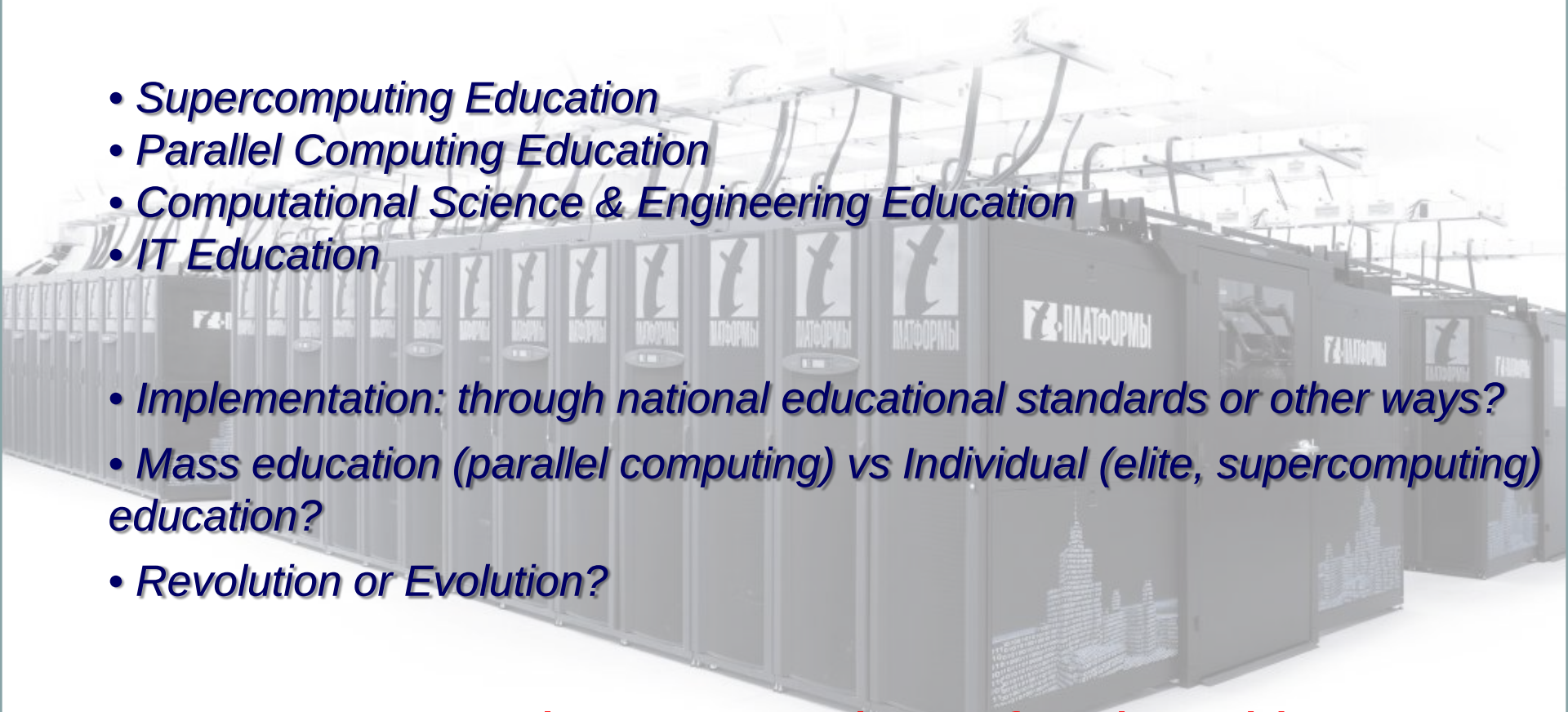
Certification of Curricula and Educational Courses
(by Consortium through the Body of Knowledge)

- *Structure*
- *Completeness*
- *Quality of materials*
- *…*

Moscow State University. High quality. Certification passed.
Northern (Arctic) Federal University. Good quality. Corrections are needed.
Voronezh State University. Good quality. Corrections are needed.

SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES

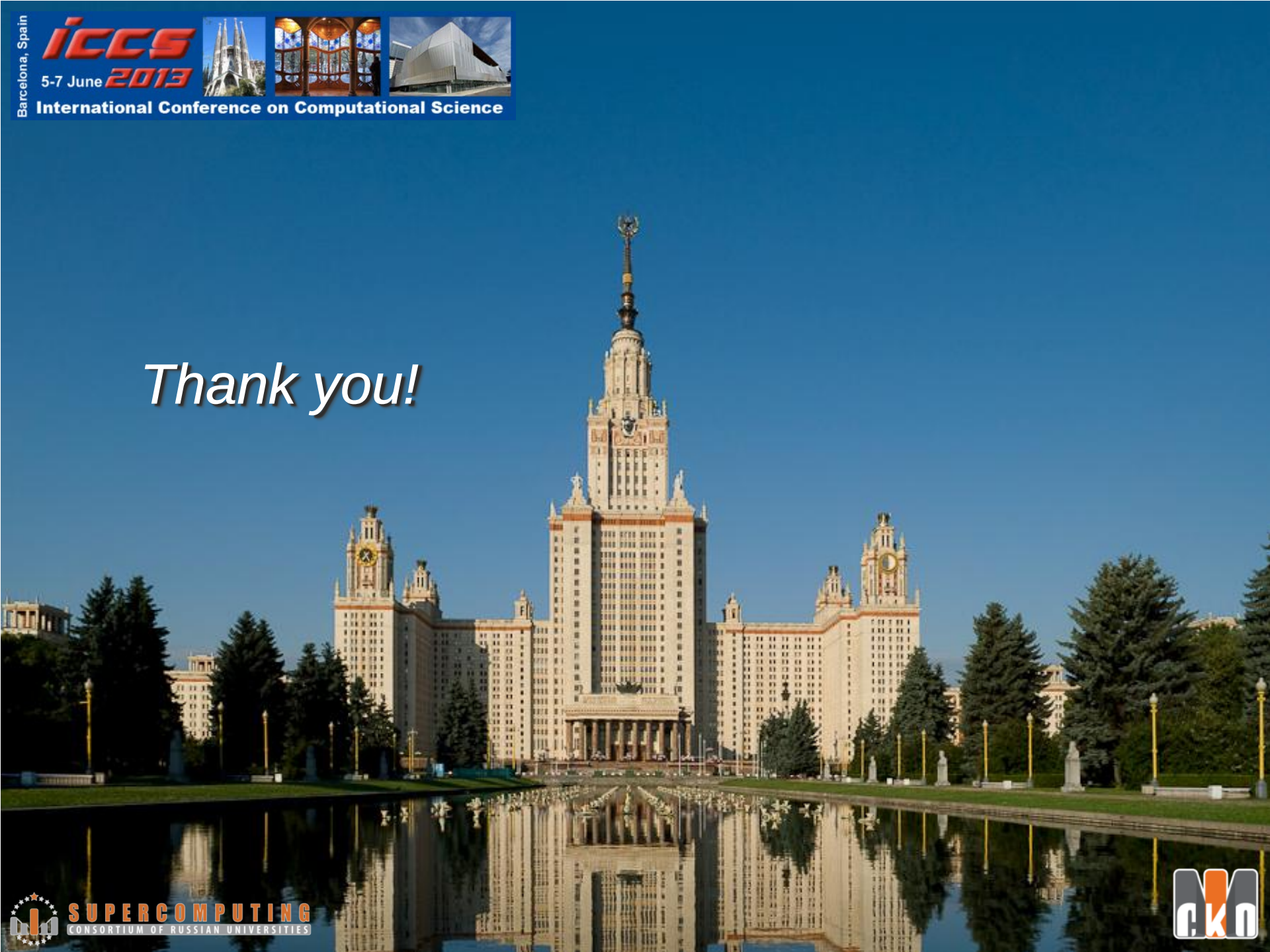
To Discuss, to Think about…



- *Supercomputing Education*
- *Parallel Computing Education*
- *Computational Science & Engineering Education*
- *IT Education*

- *Implementation: through national educational standards or other ways?*
- *Mass education (parallel computing) vs Individual (elite, supercomputing) education?*
- *Revolution or Evolution?*

Supercomputing Consortium of Universities ?


Barcelona, Spain
ICCS
5-7 June 2013
International Conference on Computational Science
Thank you!
SUPERCOMPUTING
CONSORTIUM OF RUSSIAN UNIVERSITIES