



**Joint U.S. Russia Conference  
on Advances in Materials Science  
Prague, August 30 - September 4, 2009**

**General survey of JIHT RAS team  
approach and results**

**Genri Norman**

***Joint Institute for High Temperatures  
of Russian Academy of Sciences***

***Moscow Institute of  
Physics and Technology***



# *My arguments*

- **Elite young perspective staff**
- **Multidisciplinary science**
- **Very active style of life**
- **Sustained funding**

**STAFF**

# Director of the JIHT RAS

Academician Vladimir V. Fortov



# Founder of the JIHT RAS

Academician Alexander E. Sheindlin

(celebrated 90 years on September 4, 2007)



# My Department

[www.ihed.ras.ru/norman](http://www.ihed.ras.ru/norman)

our site exists from **2003**

# Heads of laboratories



I.V. Morozov  
born **1978**,  
Ph.D. 2004



V.V. Stegailov  
born **1981**,  
Ph.D. 2005

# Task leaders



I.Yu. Skobelev, **born 1952**  
PhD, Dr.Sc.



I.A. Valuev, **born 1972**  
submitted PhD thesis



S.A. Pikuz, **born 1981**  
PhD 2006



S.V. Gasilov **born 1983**  
PhD 2008



A.Yu. Kuksin, **born 1983**  
submitted PhD thesis



S.V. Starikov, **born 1984**



A.V. Yanilkin, **born 1985**



A.V. Lanikin, **born 1985**

MIPT postgraduate students

# All-Russian awards



Two-year scholarship  
of the President of Russian Federation  
for young PhD's

***Morozov 2006***

***Pikuz 2008***

***Stegailov 2007***

# All-Russian awards



*Российская Академия Наук*

***Russian Academy of Sciences***

**Medals for**

**young researchers**

**and**

**students**

***Morozov 2004***

***Stegailov 2004***

***Yanilkin 2005***

***Lankin 2007***

# All-Russian awards



*Российская Академия Наук*



**Russian Academy of Sciences & RAO UES of  
Russia “New generation” award**

for students **and** **young scientists**

***Bazhirov 2004***

***Lankin 2006***

***Yanilkin 2007***

***Timofeev 2008***

***Pisarev 2008***

***Stegailov 2005***

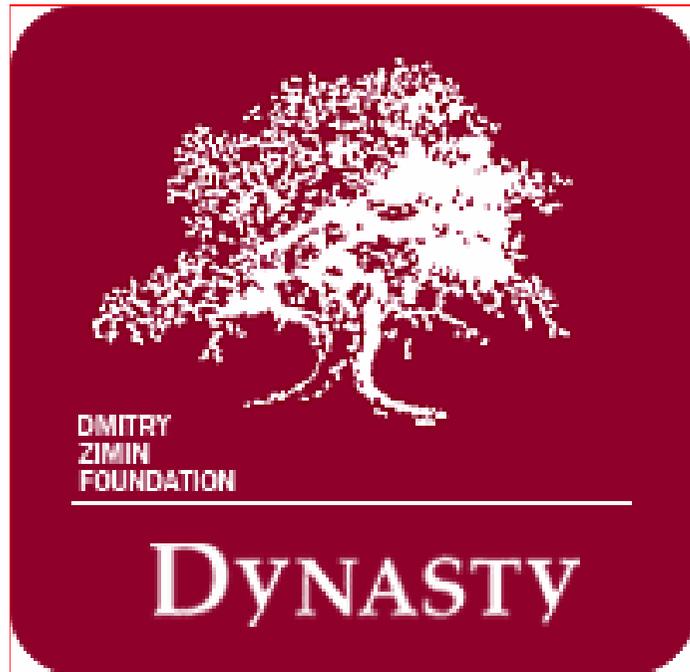
***Pikuz 2006***

***Morozov, Valuev, Kuksin 2007***

***Gasilov, Starikov 2008***



# All-Russian awards



Scholarship  
*in theoretical physics,*  
Dynasty Foundation and  
International Center of  
Fundamental Physics  
in Moscow for:

**students,**

***Stegailov 2003-2004***

***Kuksin 2004-2006***

***Lankin 2006-2008***

***Bazhirov 2007-2008***

***Yanilkin 2007-2008***

***Saitov, Timofeev 2009-2010***

***Pisarev 2009-2011***

**young scientists**

***Morozov 2004***

***Stegailov 2004-2007***

***Lankin 2009-2011***

**PhD's**

***Morozov 2008-2009***

# All-Russian awards



Award “Best PhD researcher of  
Russian Academy of Sciences”

*Morozov 2005-2006*

Award “Best PhD student of  
Russian Academy of Sciences”

*Pikuz 2005-2006*

# All-Russian awards



U.S. CIVILIAN RESEARCH & DEVELOPMENT FOUNDATION



МИНИСТЕРСТВО ОБРАЗОВАНИЯ И НАУКИ  
РОССИЙСКОЙ ФЕДЕРАЦИИ

CRDF & RF Ministry of Science and Education  
grants for young PhD's

*Morozov* 2006-2008

*Stegailov* 2007-2009

*Pikuz* 2008-2010

International award



**INTAS Young Scientists Fellowship**

*Pikuz 2005-2006*

# German awards

The logo for DAAD (Deutscher Akademischer Austauschdienst) consists of the letters 'DAAD' in a bold, black, sans-serif font. The letters are closely spaced, with the 'A's having a unique, slightly irregular shape.

Deutscher Akademischer Austauschdienst  
German Academic Exchange Service

Leonhard-Euler Scholarship

*Morozov* 1999

Scientific equipment support grant

*Valuev* 2001

# European award



Marie Curie Research Training Network "XTRA"

*Gasilov 2006-2007*

# All-Russian award



International Competition of  
Scientific Papers  
in Nanotechnology  
for Young Researchers

Section  
“Mathematical Simulation in  
Nanotechnology”

**1-st prize**

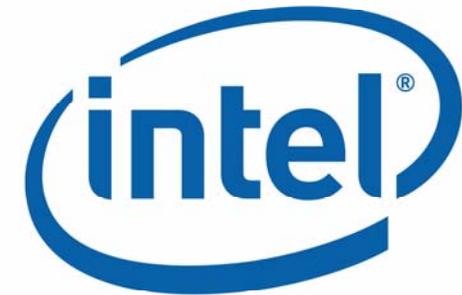
***Work “Deformation and  
strength of nanostructured  
engineering materials”***

V.V.Stegailov, A.Yu.Kuksin,  
S.V.Starikov, A.Yu.Yanilkin

# International award



**RUSNANO**  
Russian Corporation of Nanotechnologies



**Moscow, December 5, 2008**

The prize for the best project  
*in the field of high-performance computing*  
*for nanotechnology and nanoindustry*

«Modeling the properties of nanomaterials using the methods of classical and quantum dynamics»,  
*submitted by Vladimir Stegailov.*

The work was co-authored by members of JIHT RAS  
and Moscow Institute of Physics and Technology  
G.E. Norman, A.Yu. Kuksin, A.V. Yanilkin, S.V. Starikov, P.A.  
Zhil'aev, V.V. Pisarev, O.V. Sergeev.

**9**

**young persons**

**35**

All-Russian and International awards  
and many local awards

## Peer-reviewed publications 2006-2008

Phys. Rev., Phys. Rev. Lett.,  
Appl. Phys., Appl. Phys. Lett.,  
Laser and Particle Beams,  
J. Phys.: Condensed Matter,  
J. Phys. A: Math. Gen.,  
Optics Letters, Physica Scripta,  
Computer Physics Communications,  
Lecture Notes in Computer Science,  
J. Quantitative Spectroscopy and Radiative Transfer,  
Microscopy Research and Technique,  
Review of Scientific Instruments,  
Physics of Atomic Nuclei,  
Astrophysics and Space Science,  
Journal of Microscopy, Journal de Physique  
Totally – 47.

# Peer-reviewed publications and invited talks

**2006-2008**

## **Russian journals translated into English**

J. of Experim. and Theor. Physics,

Doklady Physics,

Physics of the Solid State,

High Temperature,

Russian Journal of Physical Chemistry,

Applied Physics,

Instruments and Experimental Techniques

totally – **19**

**Totally – **66** papers for **13** scientists** (*senior experimentalists Anatoly Faenov and Tatiana Pikuz included*)

**Invited talks – 21** (G.E.Norman, I.Yu.Skobelev, A.Ya. Faenov, *I.V.Morozov, V.V.Stegailov*).

# Learn-by-doing teaching & training

**Start - *Selection of 1 or 2 very gifted students at the lectures***

**18-19 years, 2<sup>nd</sup> year students are involved in the teaching & training process**

**21-22 years, 5th year student, key person,  
5 publications in peer-reviewed journals  
prizes, grants, stipends for students**

**23-24 years, post graduate student, task leader  
10 publications in peer-reviewed journals,  
individual publications included  
prizes, grants, stipends for post graduate students**

**24-25 years, PhD thesis  
senior researcher  
prizes, grants, stipends for PhD**

**about 30 years (expected), Dr. Sc. thesis  
25-30 publications in peer-reviewed journals**



# Lecture courses in MIPT

➤ **Prof. G.E.Norman:** *half-year courses*

«Molecular-dynamics and Monte Carlo methods»;

«Dynamics of chemical and biochemical reactions»;

«News and frontiers of quantum mechanics»;

«Foundations of condensed matter physics».

## **Assistant professors I.V.Morozov and V.V.Stegailov:**

*one year courses*

«Molecular modelling and simulation, parallel computations and Grid-technologies»

*at two different faculties*



## Next generation of MIPT students

*already 4 All-Russian awards and a number of local awards*



A.V. Timofeev, 6th year  
born 1987



I.M. Saitov, 6th year  
born 1987



V.V. Pisarev, 5th year  
born 1988



P.A. Zhilyaev, 5th year  
born 1988



O.V. Sergeev, 5th year  
born 1988



Yu.A. Nasretdinov, 5th year  
born 1988



A.M. Kazennov, 5th year  
born 1988

**SCIENCE**

# Main scientific directions

**Strategic directions, “tools”,  
“scientific weapon”**

Atomistic modeling&simulation  
(*our scientific brand*)

Theoretical physics

Computer or Computational Science

Connection to experiment

**Areas of our specific activity  
“targets”**

# Atomistic modeling&simulation

*It is one of the break-through branches of the fundamental and applied science*

It includes

- 1) Method of Molecular Dynamics
- 2) Monte-Carlo method
- 3) Quantum chemistry
- 4) Multi-scale and bridging the scales
- 5) Computer science

*Most of the High Performance Computing Systems are built for MD applications*

# Our “Corner stone” in modeling&simulation

*Molecular Simulation*, Vol. 31, No. 14–15, 15–30 December 2005, 1005–1017



## **Standards for molecular dynamics modelling and simulation of relaxation**

A. Y. KUKSIN, I. V. MOROZOV\*, G. E. NORMAN, V. V. STEGAILOV and I. A. VALUEV

Institute for High Energy Densities, Russian Academy of Sciences, Izhorskaya Street 13/19, Moscow 125412, Russia

*(Received October 2005; in final form October 2005)*

An attempt is made to formulate a set of requirements for simulation and modelling of relaxation in dense media. Each requirement is illustrated by examples of numerical simulation of particles with different types of interaction given by soft-sphere, Lennard–Jones, embedded atom method or Coulomb potential. The approaches developed are expected to be universal for some classes of relaxation processes in liquids, fluids, crystals and plasmas.

*Keywords:* Modelling of relaxation; Numerical simulation; Lennard–Jones potential; Coulomb potential; Molecular dynamics; Metastable states; Dynamical memory time

# Theoretical Physics

RUSSIAN ACADEMY OF SCIENCES

*L. D Landau*  
INSTITUTE FOR  
THEORETICAL  
PHYSICS



We presented our results in  
Landau institute for **theoretical physics** RAS (Chernogolovka),  
Bogolubov laboratory of **theoretical physics** JINR (Dubna),  
Steklov **mathematical** institute RAS,  
MGU faculty of **mathematics and mechanics**  
and some others

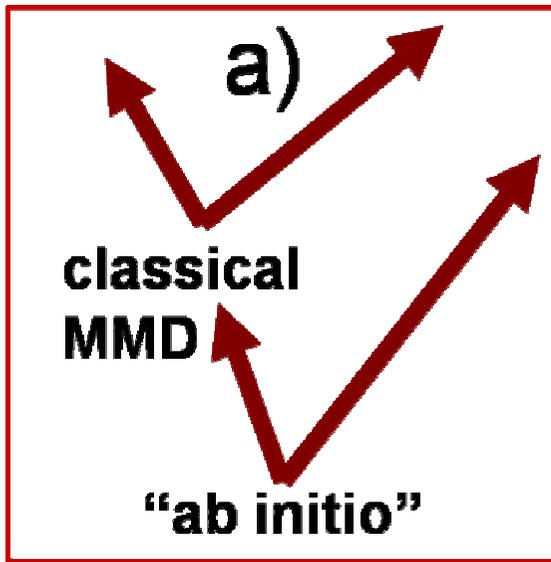
Scholarship of the Dynasty Foundation  
for students, young scientists and PhDs  
in **theoretical physics**

# Computational Science

# Software - 1

## ***Classical MD with diverse interatomic interaction potentials***

- metals, semiconductors, organics,
- strongly coupled Coulomb systems,
- high performance parallel computations up to  $10^8$  atoms and  $10^4$  processors,
- original algorithms and codes,
- using open source packages LAMMPS, GROMACS, NAMD, Accelrys DS



surface geometry

plasticity of nanocrystalline materials

composite with nanotubes

plasticity and fracture of single crystal

single dislocation

nucleation of voids and dislocations

nanotubes

EOS

number of processing elements

$10^0$   $10^1$   $10^2$   $10^3$   $10^4$   $10^5$   $10^6$

number of atoms

$10^2$   $10^3$   $10^4$   $10^5$   $10^6$   $10^7$   $10^8$   $10^9$   $10^{10}$   $10^{11}$   $10^{12}$

**b)**

## Software - 2

### ***Quantum MD using electron density functional theory:***

Carr-Parinello and Born-Oppenheimer

different bases

pseudopotential library and its extension

finite temperatures

excited states and nonadiabatic transitions

high parallelization and scaling

using open source packages VASP, CPMD, SeqQuest

# Computer facilities: cluster in MIPT



**Since December 2001**

16 dual AMD Athlon 2GHz

6 dual Pentium III 866MHz

RAM per node: 512M6

2 frontends

Storage: 1.12Tb

Network:

Fast Ethernet, Gigabit Ethernet

# Computer facilities: **cluster in JIHT**



**Since April 2005**

13 dual CPU nodes

Intel Xeon **3.0 GHz x 2**

RAM: 2 Gb x 13 = **26 Gb**

Storage: 160 Gb x 13 = **2 Tb**

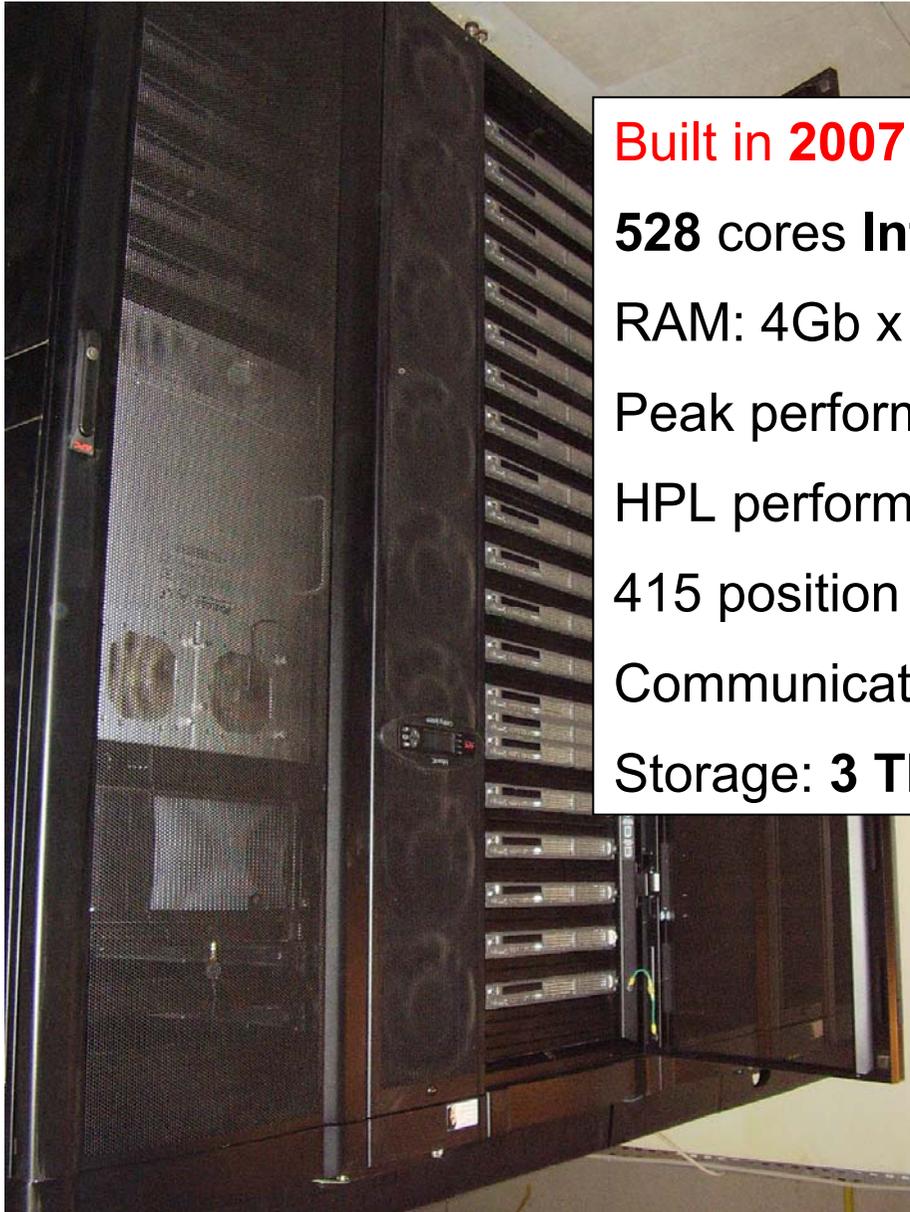
Network:

Fast Ethernet, **Gigabit Ethernet**

CrossGRID



# Computer facilities: cluster «MIPT-60»



Built in **2007**

**528** cores Intel Xeon 5160 3GHz

RAM: 4Gb x 132 = **528Gb**

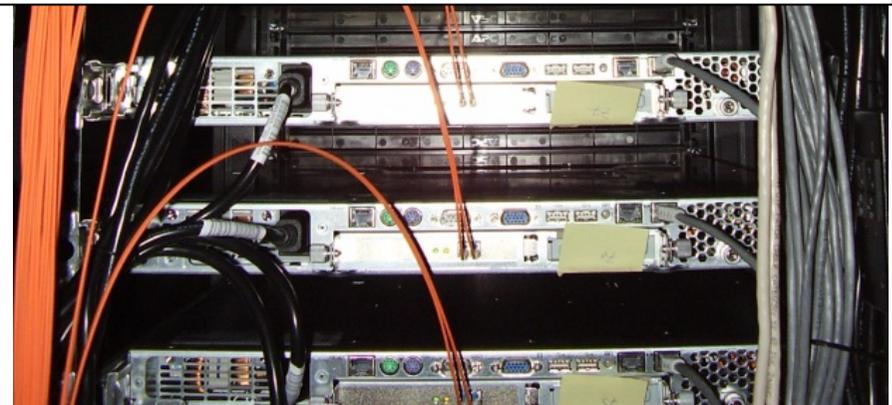
Peak performance: **6.5 TFlop/s**

HPL performance test  $\geq$  **4.5 TFlop/s**

415 position in Top-500 (June 2007)

Communication: **Myrinet 2000**/Gigabit Ethernet

Storage: **3 Tb**



# Computer facilities include Joint Super Computer Center of RAS



The cluster **MVS-100K** is the most powerful supercomputer in Russia for civil applications with the peak performance 75 Teraflops.

The cluster MVS-15000BM consists of

- \* 782 base blocks
- \* each block is a HP Proliant server with 2 quad-core Intel Xeon 3GHz processors, 4Gbyte DDR2 RAM, 36 Gbyte disk storage
- \* Infiniband DDR Communication network;
- \* Gigabit Ethernet system and data networks.

# Hybrid system: PC + NVIDIA GPUs

## Video cards: 2 x NVIDIA GeForce GTX 260

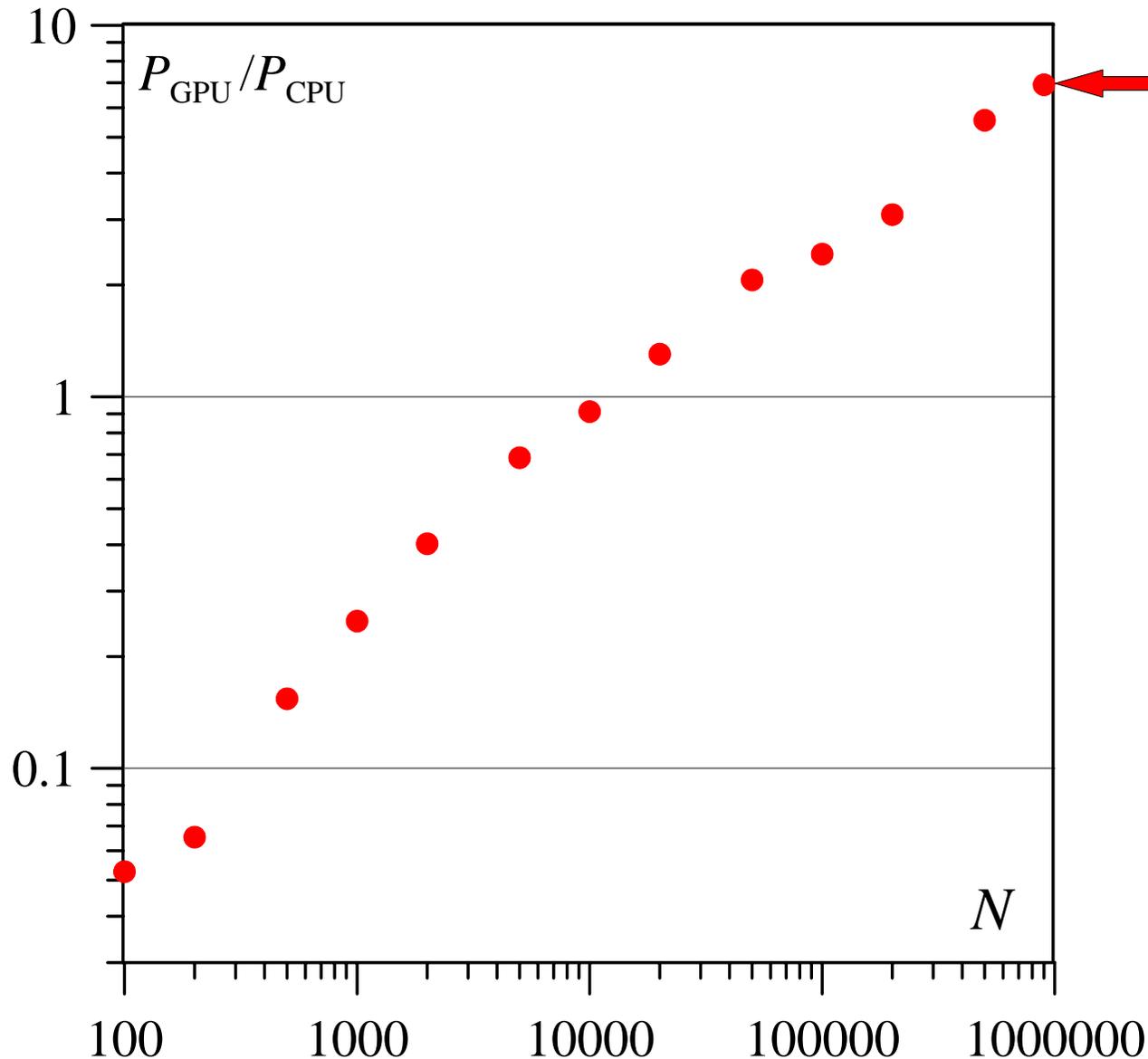
Processor cores	<b>192</b>
Processor clock	<b>1242 MHz</b>
Memory clock	<b>999 MHz</b>
RAM	<b>896 MB</b>
Memory bandwidth	<b>111.9 GB/sec</b>
Input power	<b>182 W</b>

## Host system

CPU	<b>Core 2 Quad Q6600 2.4GHz/8Mb/1066</b>
RAM	<b>4GB DDR2 800</b>
MB	<b>ASUS P5Q pro</b>



# Ratio between GPU and CPU performance depending on the number of particles



**GPU (192 cores):**  
HOOMD (ver. 0.8.1)  
runs on NVIDIA  
GeForce GTX 260

**CPU (8 cores):**  
LAMMPS (ver. June  
6, 2009) runs on Intel  
Xeon X5570  
(Nehalem), 2.93GHz,  
8MB L3

**Interactions:**  
Lennard-Jones  
(non-bonded)

## Areas of our specific activity, “targets”

- **Non-ideal plasma.**
- **Phase transitions, stability boundaries of solids and liquids.**
- **Plasticity and fracture at high rate deformation.**
- **Cavitation in metastable liquids.**
- **Scientific foundations of nanotechnologies.**
- **Creation of new interatomic potentials.**
- **Modeling of biomolecules**
- X-ray plasma spectroscopy.
- X-ray diagnostics of micro- and nano-objects.
- Data base on spectroscopic properties of atoms and ions.

Multidisciplinary approach

**Plasma, solids and liquids,  
biomolecules, nanotechnologies,  
material science etc**

It corresponds to the general trend  
of the world science  
which is on the eve of the  
Renaissance of the natural philosophy

# STANDARD OF LIFE

**We really work hard**

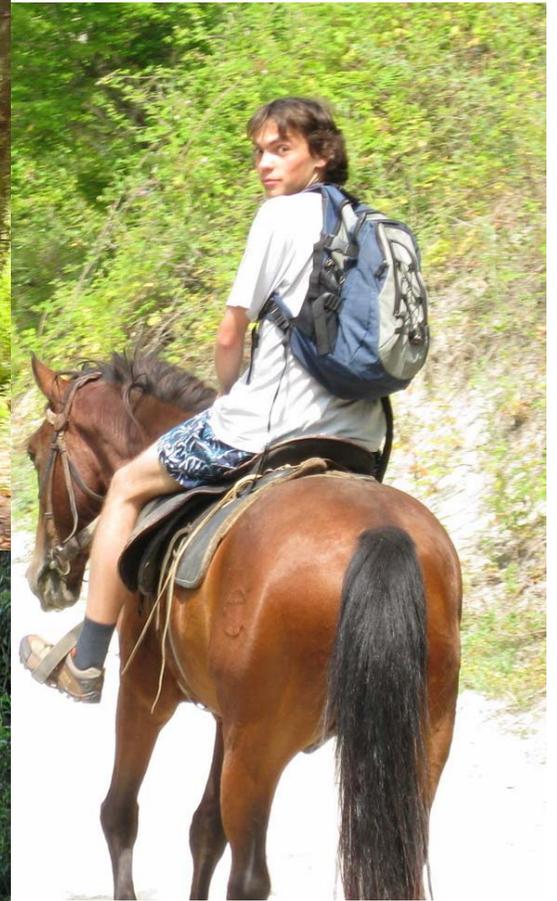
**we are young,  
enjoy life,  
have various hobbies....**



# Hobbies



# Hobbies



# Hobbies



# Banquets



Hawaii, 2007



Elbrus



New Athos

**We enjoy business trips and  
scientific conferences  
in interesting places**

# Great Rally 2002



Hoover Dam

TM Headquarters  
Rancho Santa-Margarita



Monument Valley



Grand Canyon

**Problem: 4 days, 2000 km**

**Solution: Rental Car**

# Great Journey 2003



Moscow

**Boulder, CO**  
**June 22-27**  
**15th STP**

**July 6-11**  
**Key Stone Resort**  
**FOMMS2003**

rafting along Colorado river,  
hiking in Rocky Mountains

**Albuquerque**  
**June 28 – July 5**  
**Sandia Nat. Labs,**



**Chicago, July 13-19**  
**Argonne Nat. Lab,**  
**University of Illinois**  
**at Urbana-Champaign**



# Great Journey 2007



**Chicago**  
Argonne Nat. Lab.  
July 5-7



**Albuquerque**  
Sandia Nat. Labs  
July 1-3



**Hawaii's Big Island**  
July 1-3

**APS SCCM**  
June 23-29



# Great Journey 2008

# Camerino, SCCS2008 July 24 – August 2



**Rome**  
**August 12**  
**sightseeing**

**Ouro Preto**

**Belo Horizonte**

**CCP 2008**

**August 5-9**

**August 3-4**  
**sightseeing**

**Rio de Janeiro**

## Other conferences

***Asia:*** Pune, India, Fukuoka, Tokyo, Japan  
Kuala Lumpur, Malaysia, Beijing, China

***Australia,*** Great Barrier Reef included  
***USA,*** Tallahassee, FL

***Europe:*** Germany, France, Spain, Italy  
United Kingdom, Portugal, Netherlands,  
Belgium, Greece, Poland

***Russia:*** Elbrus, S.Petersburg, Tomsk,  
Ekaterinburg, Novosibirsk,

Elbrus,  
March 1-6,  
every year





*last decade  
of July,  
every year  
in New Athos,  
Abkhazia*

annual All-Russian  
symposium  
*Physics problems of  
ultrafast processes in  
non-equilibrium media*



# Task Leaders in New Athos, *Abkhazia*

organizers of the 2003 All-Russian symposium

*Physics problems of ultrafast processes in non-equilibrium media*



# Local Organizing Committee 2009

organizers of the annual All-Russian symposium

*Physics problems of ultrafast processes in non-equilibrium media*



# Local Organizing Committee 2009



**2008:** 55 business trips – 55 scientific reports

Elbrus – 10  
Petersburg – 6  
Tomsk – 3  
Ekaterinburg – 2  
Novosibirsk – 1  
Dubna – 3

***totally* – 25**

Abkhazia – 9

*Moscow – 34 scientific talks*

Brasil – 4

USA – 2

Japan – 1

India – 1

Italy – 4

England – 3

Portugal – 3

Germany – 2

France – 1

***totally* – 21**

## Key person travel expenses in 2008

<i>post-graduate</i>	Yanilkin (1985)	<b>\$15 000</b>
<i>post-graduate</i>	Kuksin (1983)	<b>\$10 700</b>
<i>laboratory head</i>	Morozov (1978)	<b>\$8 000</b>
<i>post-graduate</i>	Lankin (1985)	<b>\$7 900</b>
<i>department head</i>	<i>Norman (1936)</i>	<b>\$7 700</b>
<i>laboratory head</i>	Stegailov (1981)	<b>\$6 900</b>
<i>senior researcher</i>	Pikuz (1981)	<b>\$6 000</b>
department travel expenses		<b>\$80 000</b>

# **COOPERATION AND FUNDING**

# Cooperation

- **Moscow Institute of Steel and Alloys**
- **Institute of Problems in Mechanics RAS**
- **Lomonosov Moscow State University**
- **St. Petersburg Institute of High Performance Computations and Databases**
- **Orenburg State University**
- **Sandia National Laboratories, USA**
- **Hebrew University Jerusalem**
- **Centre for Development of Advanced Computing, Pune, India**

# Funding (2006-2008)

***Programs of Fundamental  
Research of the Presidium  
of the Russian Academy  
of Sciences***



*Российская Академия Наук*

**#3 Quantum macrophysics**

**#9 Extreme state of matter research**

#14 Fundamental problems of computer science and information technologies

#15 Development of fundamental principles of data-processing GRID-oriented frameworks construction.

*And three others*

# Funding (2008)

## The Russian Ministry of Education and Science projects

- RNP2.1. 1.712 “Computer simulation of metals in the region of phase transitions and under extreme conditions”
- “Mathematical modeling methods in nanotechnology”



## The Russian Foundation for Basic Research grants

- 07-08-00738 “Relaxation in latent tracks of fast single heavy ions”
- 06-02-16174 “Investigation of non-linear effects caused by interaction of laser fields with clusters”,
- 06-02-72005 **Russian-Israeli** project “Investigations of non-linear effects caused by interaction of high intensity laser fields with clusters and microdroplets”
- 08-01-91306 **Russian-Indian** project “Mathematical modeling and continuum mechanics fundamental problem study using multi-processor systems”



## Project funded by Sandia National Laboratories under the «U.S. DOE/NNSA Advanced Simulation and Computing»



“Extending Non-Equilibrium Molecular Dynamics Simulation Methods”

## International Science and Technology Center

3504 Atomic database SPECTR-W3 for plasma spectroscopy and other application



# Conclusions: present status

*Dynamically developing* and *ambitious*  
scientific team

**Strategy:** Atomistic modeling & simulation  
(our *break-through* scientific brand),  
Theoretical physics, Computational science  
Connection to experiment

*Funding* from various research projects in a  
number of specific scientific areas

*Advanced* selection and *learn-by-doing*  
teaching & training system

# Outlook: future plans

***To extend areas*** of our scientific activity  
using our “scientific weapons”

***To apply the multidisciplinary*** approach in selection  
new specific problems, targets for our “weapons”

***To increase and strengthen*** our scientific team using  
our learn-by-doing teaching & training system

***TO DEVELOP*** OUR COOPERATION NET

***TO LOOK FOR*** NEW SOURCES OF FUNDING

***To enjoy life***