

# Supercomputing Support of the Researches and Education

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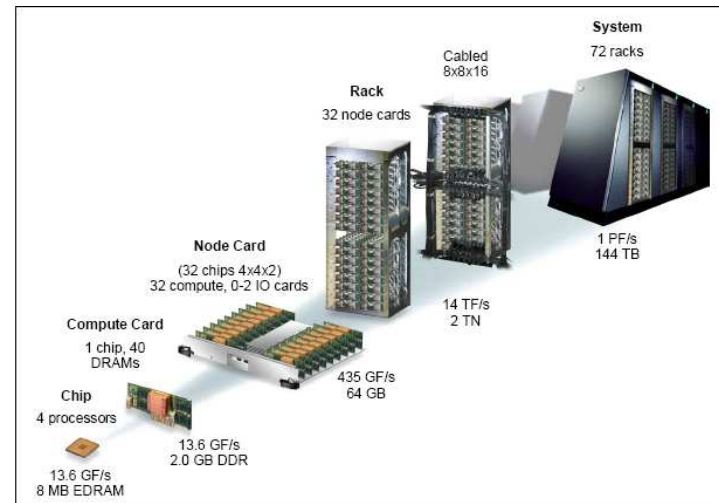
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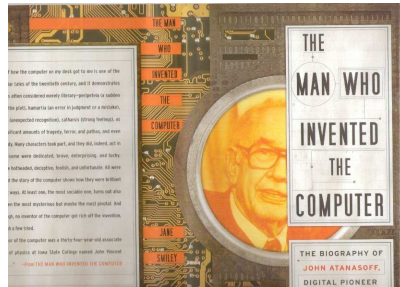
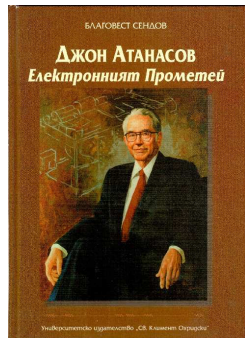


# 1. Introduction

- 1961 - The first computer center in Bulgaria is established
- 2007 - Blue Gene/P is installed at the Bulgarian Supercomputing Centre



# From Ritz to advanced SuperCA



- Atanasoff has been familiar with the numerical **method of Ritz** leading for his problem to a system of **29 linear algebraic equations**.
- Such computations have required many weeks efforts using the Monroe manual rotary Calculator.
- Atanasoff has tried to run several Monroe machines in parallel rotated by a common handle.
- Finally, with a grant of \$650 Atanasoff and Berry have created the prototype of the ABC computer in 1939.

B. Sendov, John Atanasoff, The Electronic Prometheus, St. Kliment Ohridski University Press, 2003

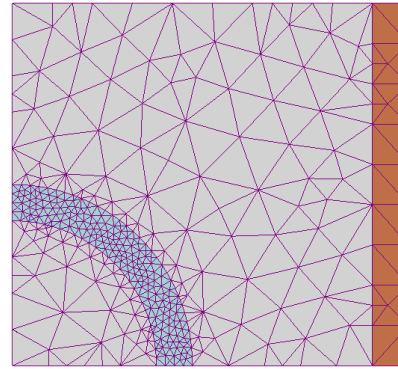




# Ritz method



Walter Ritz (1878-1909)



FEM discretization

- The Ritz method (1909) is a direct method to find an approximate solution of boundary value problems.
- The Ritz method is described in terms of minimizing the "energy functional" or Hamiltonian of the system.
- In the language of mathematics, it is exactly the **finite element method**.
- Not so well known is that in 1908 Ritz has published a lengthy criticism of Maxwell-Lorentz electromagnetic theory.

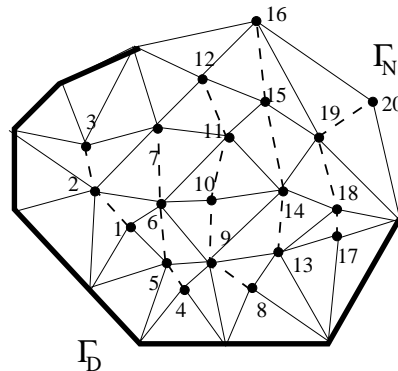


Consider the weak formulation of a given elliptic b.v.p. in the form

$$a(u, v) = \mathcal{F}(v), \quad \forall v \in \mathcal{V},$$

and the related FEM problem

$$a_h(u_h, v_h) = \mathcal{F}_h(v_h), \quad \forall v_h \in \mathcal{V}_h.$$



We are interested in the efficient solution of the resulting large-scale FEM linear systems

$$Au = f.$$



# PCG scalability

- For large-scale problems, the iterative methods have advantages due to their better/optimal computational complexity and storage requirements.
- The Conjugate Gradient (CG) method is the best iterative solution framework for large scale FEM systems.
- The development of robust Preconditioned Conjugate Gradient (PCG) methods and their parallel implementation is a hot topic in SuperCA.

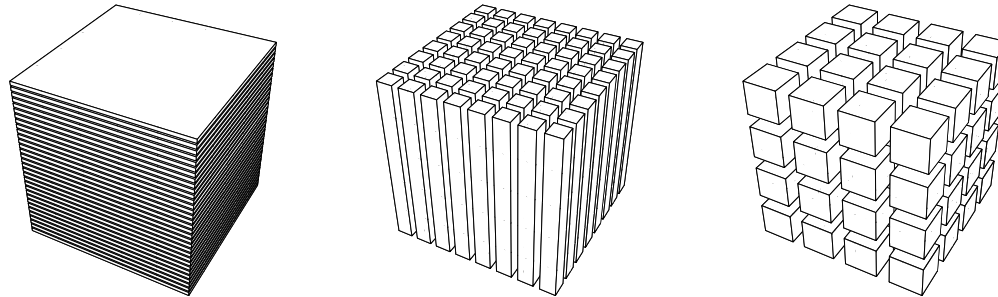
| $h^{-2} \approx N$ | DIRECT   | CG           | PCG-MILU     | PCG-AMLI-V    | PCG-AMLI-W  |
|--------------------|----------|--------------|--------------|---------------|-------------|
| 1 024              | 0.02     | 0.05 (84)    | 0.04 (21)    | < 0.01 (16)   | < 0.01 (16) |
| 4 096              | 0.17     | 0.12 (163)   | 0.09 (30)    | 0.02 (18)     | 0.02 (17)   |
| 16 384             | 2.21     | 0.91 (320)   | 0.52 (46)    | 0.09 (22)     | 0.09 (17)   |
| 65 536             | 30.08    | 9.2 (630)    | 3.8 (68)     | 0.49 (25)     | 0.45 (17)   |
| 262 144            | *        | 81.6 (1 256) | 27.8 (102)   | 2.7 (28)      | 2.3 (17)    |
| 1 048 576          | *        | 805 (2 439)  | 214 (152)    | 13.3 (31)     | 10.5 (17)   |
| complexity         | $O(N^2)$ | $O(N^{3/2})$ | $O(N^{5/4})$ | $O(N \log N)$ | $O(N)$      |

Solution time in seconds (and  $n_{it}$ ) for Poisson equation on a unit square



# BoomerAMG parallel scalability

Figure: 1D, 2D and 3D partitioning: voxel triangulation of a cubic domain



Parallel numerical tests based on BoomerAMG solver for a parabolic problem in a cubic space domain, voxel FEM mesh, and 96 implicit backward Euler time steps, are given bellow.

| Parallel scalability        |                                   |             |          |            |        |
|-----------------------------|-----------------------------------|-------------|----------|------------|--------|
| Mesh                        | $N_p = P_x \times P_y \times P_z$ | $N$         | $N_{it}$ | $T(p)$ [s] | $E(p)$ |
| $127 \times 127 \times 127$ | $8 = 8 \times 1 \times 1$         | 2 097 152   | 161      | 1 255.00   |        |
| $255 \times 255 \times 255$ | $64 = 64 \times 1 \times 1$       | 16 777 216  | 128      | 5 951.08   | 21 %   |
| $511 \times 511 \times 511$ | $512 = 512 \times 1 \times 1$     | 134 217 728 | -        | > 24 h     | < 2 %  |
| $127 \times 127 \times 127$ | $8 = 4 \times 2 \times 1$         | 2 097 152   | 167      | 1 137.83   |        |
| $255 \times 255 \times 255$ | $64 = 8 \times 8 \times 1$        | 16 777 216  | 129      | 1 203.29   | 95 %   |
| $511 \times 511 \times 511$ | $512 = 32 \times 16 \times 1$     | 134 217 728 | 114      | 1 581.13   | 72 %   |
| $127 \times 127 \times 127$ | $8 = 4 \times 2 \times 1$         | 2 097 152   | 167      | 1 137.91   |        |
| $255 \times 255 \times 255$ | $64 = 4 \times 4 \times 4$        | 16 777 216  | 128      | 1 062.30   | 107 %  |
| $511 \times 511 \times 511$ | $512 = 8 \times 8 \times 8$       | 134 217 728 | 114      | 1 155.08   | 99 %   |



# 2. Strategic documents

- **Draft National Reform Programme (2011-2015)**
- **National Roadmap for Research Infrastructure (2011-2020)**
- **National Broadband Strategy (2009-2013)**
- **National Program on Accelerated IS development (2008-2010)**
- **Operational Programmes (2007-2013)**
- **National Strategic Reference Framework (2007-2013)**
- **State Policy on Accelerated IS development (2007-2010)**



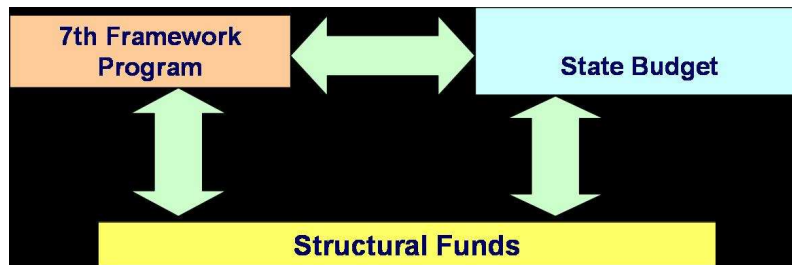
# Roadmap for RI (2011-2020)

1. Infrastructure for sustainable development in the area of sea research
2. Infrastructure for the production and research of new materials
3. **Infrastructure for genome, proteome and metabolome researches**  
**IICT - BAS is a member of the consortium**
4. Infrastructure in the area of renewable energy sources and energy efficiency
5. **Bulgarian supercomputing center**  
**Scientific and technical coordinator: CoE on Supercomputing applications**  
**(IICT - BAS is a coordinator of SuperCA++)**
6. **BG-CLARIN: integration and development of Bulgarian language electronic resources as a part of European CLARIN**  
**Scientific and technical coordinator: IICT - BAS**
7. Astronomical center for research and education

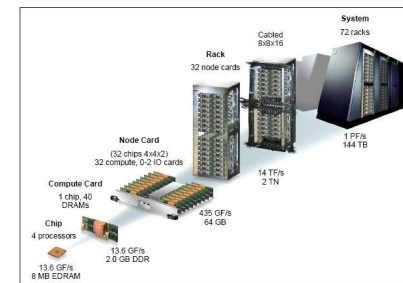


# Approach towards SuperCA

- Concentrate on better management and exploitation of existing supercomputing resources.
- Definition of new directions in areas important to ensure the catching up process.
- Stepping up collaboration with other countries and international organisations.



Financial Instruments



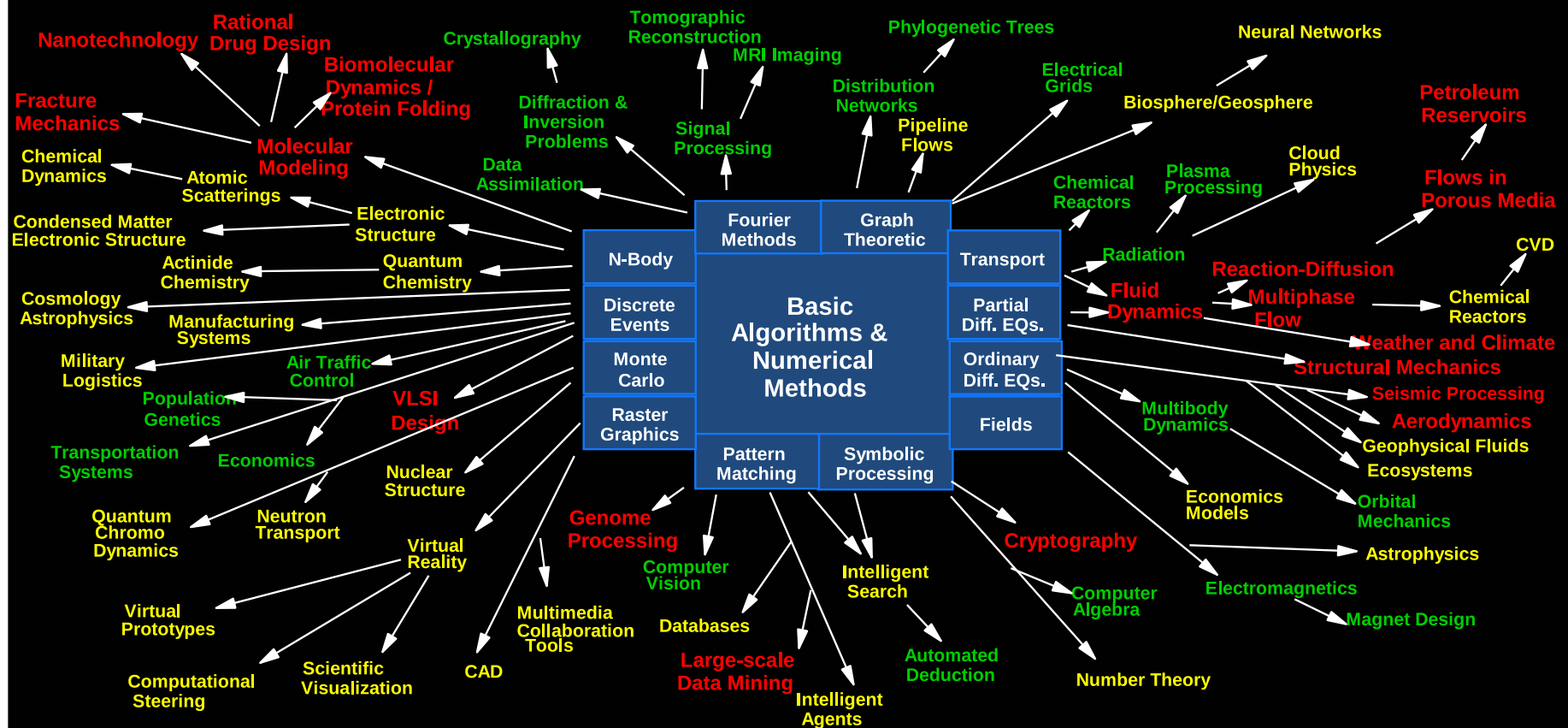
IBM Blue Gene/P

- It is attractive speaking about supercomputing, but keep in mind exponential growing overall expectations.
- Supercomputing is an enabler of scientific and innovative results, but not a ready solution or result.



# 3. Supercomputing applications

Good Better Best



Argonne National Labs GBB



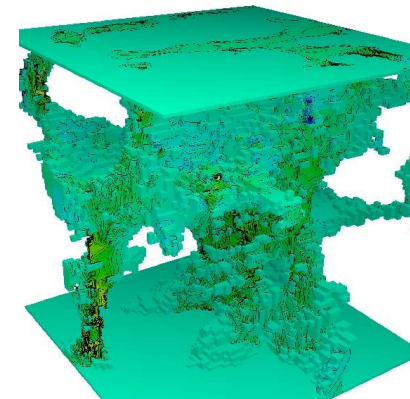


# 3.A1. Bone microstructure

- $\mu$ FEM analysis with NC Rannacher-Turek FEs is applied in a voxel setting.
- solid skeleton at micro level  $\Rightarrow$  anisotropic tensor at macro level.
- MIC(0) and BoomerAMG in combination with Displacement Decomposition.

|     |     | $\zeta = 0.1$ |      |        |      |
|-----|-----|---------------|------|--------|------|
| $n$ | $p$ | MIC(0)        |      | AMG    |      |
|     |     | $T[s]$        | $It$ | $T[s]$ | $It$ |
| 64  | 1   | 1 184         | 270  | 1 071  | 28   |
| 128 | 8   | 1 831         | 395  | 1 147  | 25   |
| 256 | 64  | 4 870         | 888  | 1 318  | 25   |

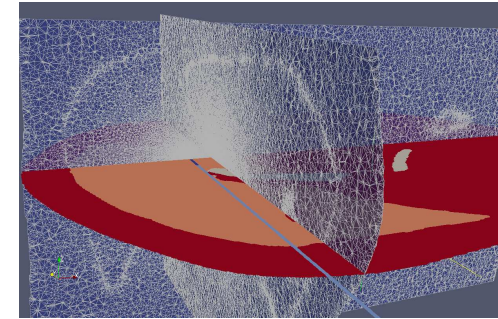
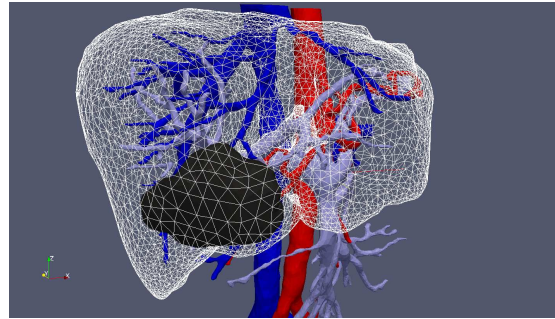
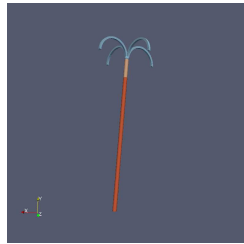
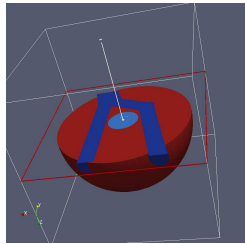
|     |     | $\zeta = 0.01$ |       |        |      |
|-----|-----|----------------|-------|--------|------|
| $n$ | $p$ | MIC(0)         |       | AMG    |      |
|     |     | $T[s]$         | $It$  | $T[s]$ | $It$ |
| 64  | 1   | 2 634          | 601   | 2 384  | 63   |
| 128 | 8   | 4 905          | 1 060 | 2 860  | 63   |
| 256 | 64  | 10 177         | 1 863 | 2 715  | 52   |



|     |     | $\zeta = 0.001$ |       |        |      |
|-----|-----|-----------------|-------|--------|------|
| $n$ | $p$ | MIC(0)          |       | AMG    |      |
|     |     | $T[s]$          | $It$  | $T[s]$ | $It$ |
| 64  | 1   | 4 477           | 1 022 | 4 412  | 117  |
| 128 | 8   | 9 626           | 2 081 | 5 928  | 131  |
| 256 | 64  | 16 182          | 2 965 | 6 939  | 102  |



# 3.A2. RF tumor ablation



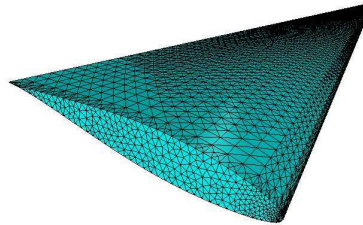
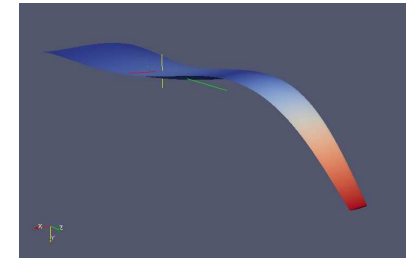
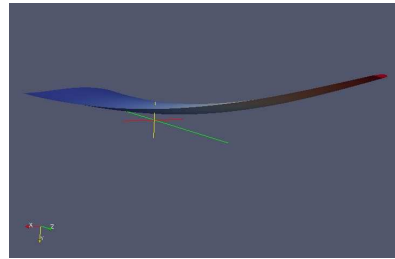
- The RF ablation destroys the unwanted tissue by heating, arising when the energy dissipated by the electric current flowing through the RF probe is converted to heat.

|       | Degrees of freedom (DOF) |            |             |
|-------|--------------------------|------------|-------------|
| $n_p$ | 2 097 152                | 16 777 216 | 134 217 728 |
| 32    | 1 788                    |            |             |
| 64    | 884                      |            |             |
| 128   | 457                      |            |             |
| 256   | 250                      | 1 880      |             |
| 512   | 165                      | 1 107      |             |
| 1 024 | 155                      | 667        |             |
| 2 048 | 387                      | 708        | 3 340       |

Parallel times T[s] for simulation of 8' of HTA with time step of 1''



# 3.A3. Large wind turbine



| $n_p$ | Linear static problem |      |        | Nonlinear static problem |      |        | Eigenvalue problem problem |      |       |
|-------|-----------------------|------|--------|--------------------------|------|--------|----------------------------|------|-------|
|       | T[s]                  | Sp   | E [%]  | T[s]                     | Sp   | E [%]  | T[s]                       | Sp   | E [%] |
| 16    | 1 311.92              |      |        | 4 375.24                 |      |        | 766.53                     |      |       |
| 32    | 666.85                | 1.97 | 98. 37 | 2 213.03                 | 1.98 | 98.85  | 395.10                     | 1.94 | 97.00 |
| 64    | 301.08                | 4.36 | 108.93 | 1 038.75                 | 4.21 | 105.30 | 270.92                     | 2.83 | 70.73 |
| 128   | 180.90                | 7.25 | 90.65  | 612.24                   | 7.15 | 89.33  | 243.96                     | 3.14 | 39.27 |

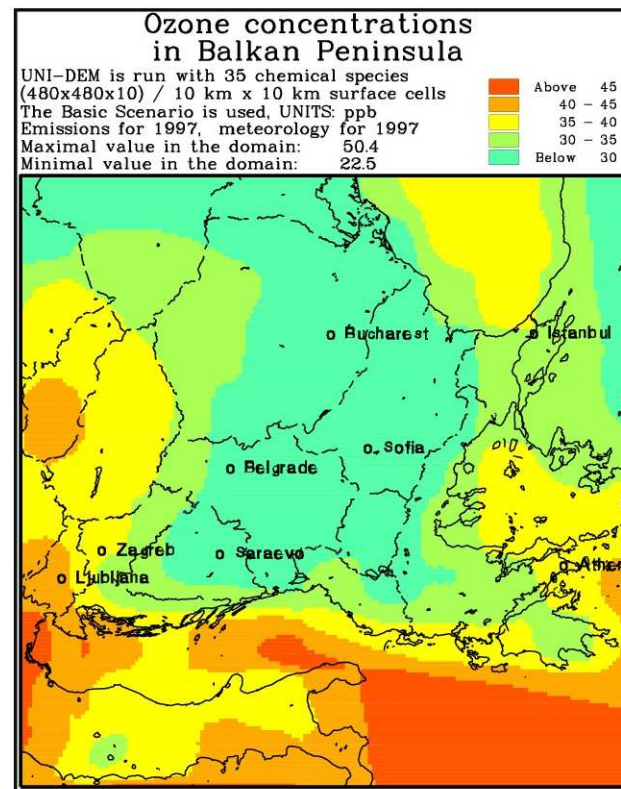
Elmer Multifrontal Massively Parallel Solver (MUMPS) for 3D elasticity problems: N = 1 774 074



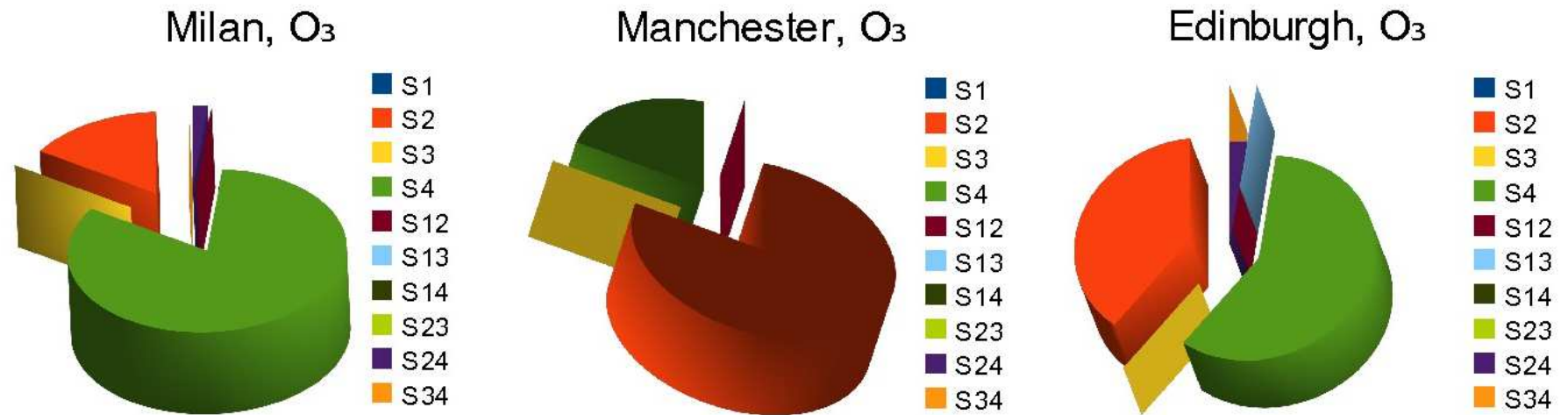
# 3.B1. Air pollution simulation

The results of supercomputer modeling of effects of global climate change scenarios and some emissions amendment over the air pollution level in South-East Europe and particularly over the Bulgarian territory are studied.

- Several hundred runs are performed on IBM Blue Gene/P computer in Sofia including fourteen scenarios over a period of sixteen years.
- The major conclusion is that the increase of the temperature, alone or in combination with some other factors, leads to rather considerable increases of some pollution levels, which might become dangerous for the environment.



# 3.B2. Sensitivity analysis



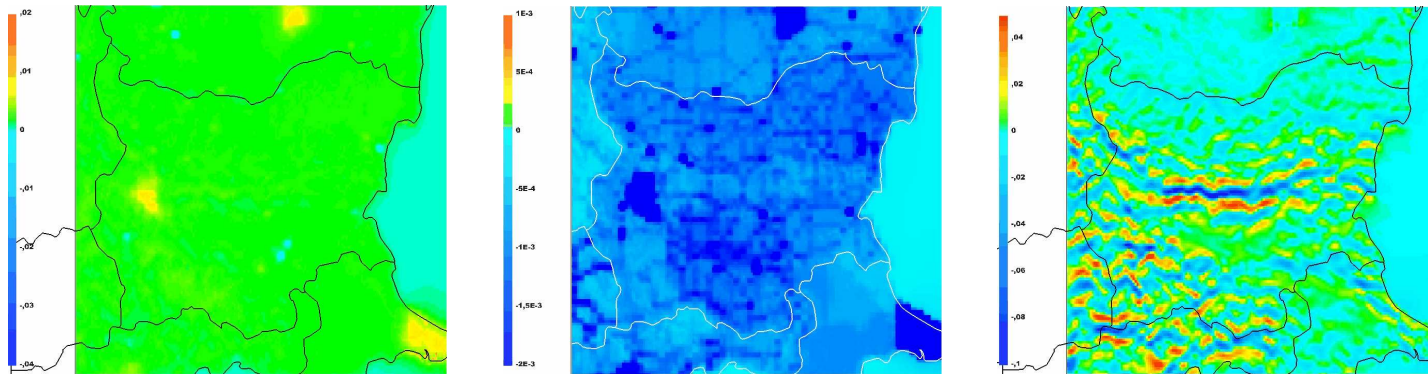
- Pie charts representation of first- and second-order sensitivity indices of the ozone in Milan, Manchester, and Edinburgh.



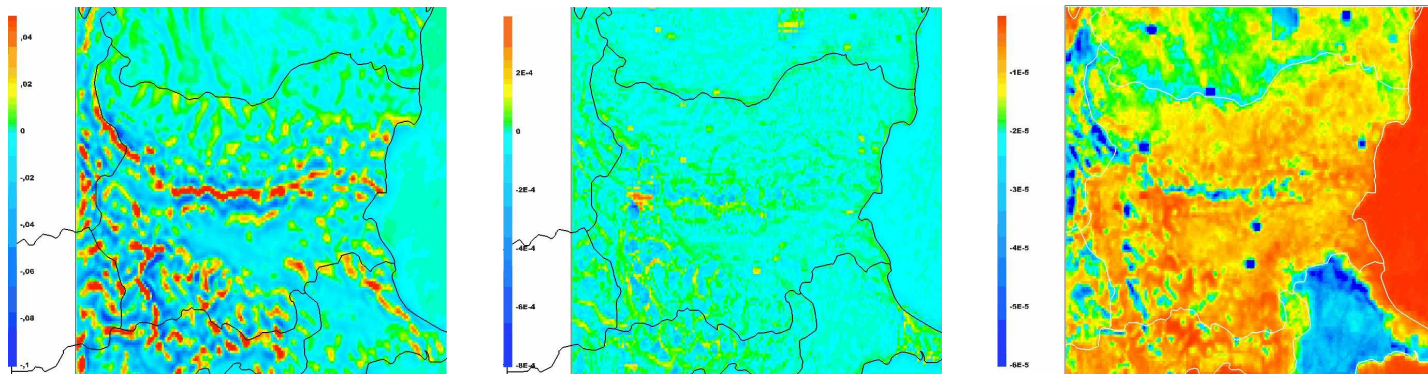


# 3.B3. Annual contributions

Typical annual contributions of different processes to the surface ozone concentrations hourly changes in Bulgaria.



(l) Vertical diffusion; (c) Chemical transformations (r) Horizontal advection;

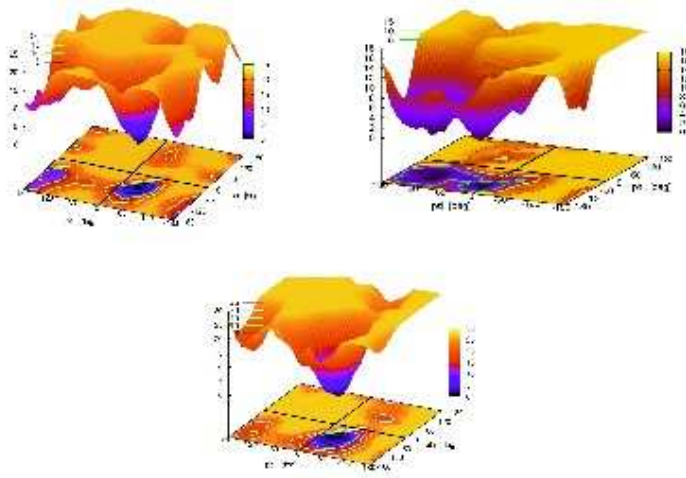


(l) Vertical advection; (c) Horizontal diffusion; (r) Cloud processes



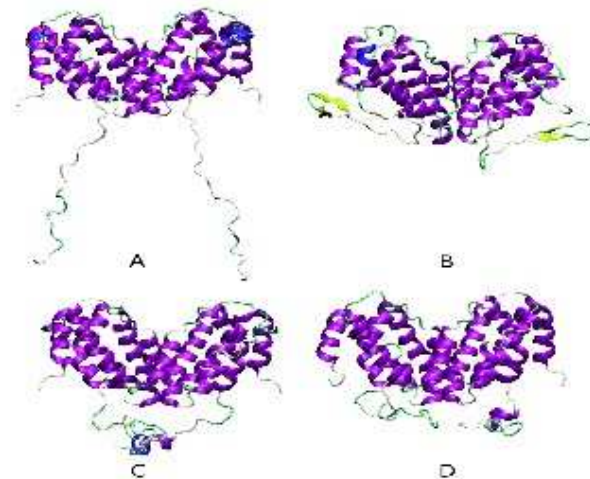
# 3.C1. Human interferon gamma

- The structural stability of 100 hIFN $\gamma$  mutants with 3 random mutations in the upstream NLS (aa 86-89) are studied using metadynamics based on collective variables the backbone dihedral angles of the 86-th amino acid.
- The free energy profile of the native and mutated forms of the protein are reconducted by comparing the profiles to the native form.



# 3.C2. Conformation of C-terminus

- The length of the tail modifies the affinity to the receptor.
- Two 200 ns MD folding simulations are performed using GROMOS 53a6 + GROMACS 4.5.4 and CHARMM 22 + NAMD 2.9 to cluster the trajectories.
- It was found that in both cases the C-Termini get closer to the globule and the whole protein adopts more compact conformation.





# 3.C3. In silico drug design

- Structure-based methods for drug design are used to develop models for allergenicity and immunogenicity predictions of novel proteins.
- Molecular dynamics simulations and molecular docking studies are applied on BlueGene-P to derive the models.
- Once the models are derived, they are freely accessible via the web site:

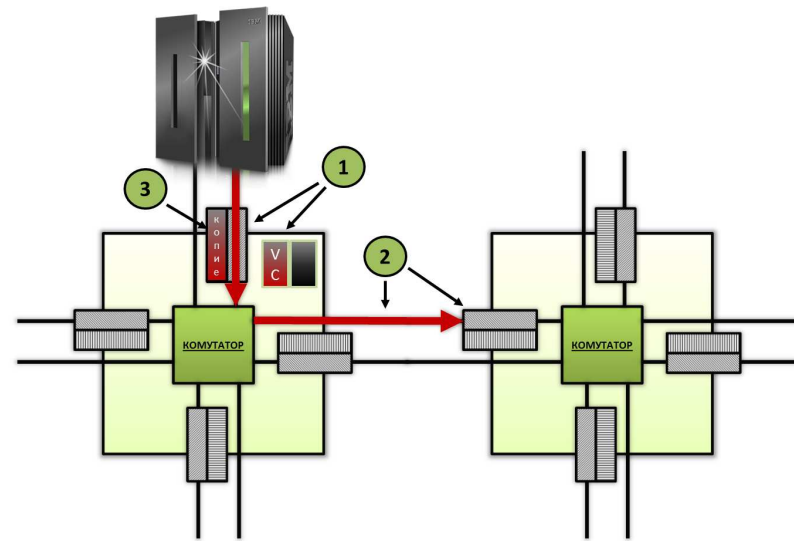
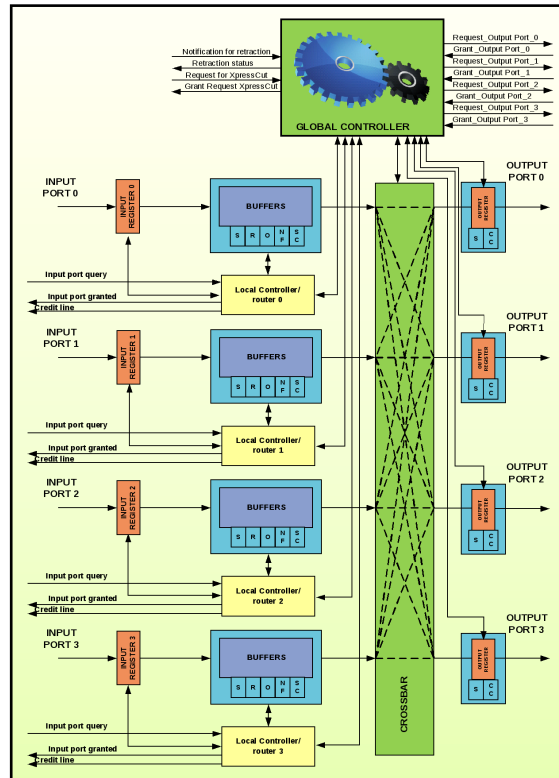
<http://www.ddg-pharmfac.net>

The screenshot displays the homepage of the ddg-pharmfac.net website. On the left, there is a navigation menu with links: Home, Group members, Research, Publications, Training, Services, Collaborations, and Contact us. The main content area is divided into sections: Faculty of Pharmacy, Medical University of Sofia (2 Dunay st., 1000 Sofia, Bulgaria); Databases (AntiJen, PPD, DSD); Servers (AllerTOP, EpiDOCK, EpiTOP, EpiJen, MHCPred, VaxiJen); and a central area featuring tool descriptions and screenshots for AllerTOP 1.0, EpiTOP 1.0, and EpiDOCK. The AllerTOP 1.0 section describes it as a 'Bioinformatics tool for allergenicity prediction'. The EpiTOP 1.0 section describes it as a 'Protein structure-based tool for MHC class II binding prediction'. The EpiDOCK section describes it as a 'Molecular docking tool for MHC class II binding prediction'. The VaxiJen section describes it as a 'Server for prediction of protective antigens of viral, bacterial, tumour, parasite and fungal proteins'.



# 3.D1. SBB flow control in SAN

Step-Back-on-Blocking (SBB) flow control in system area networks (SAN) is applied for utilization of the network resources.

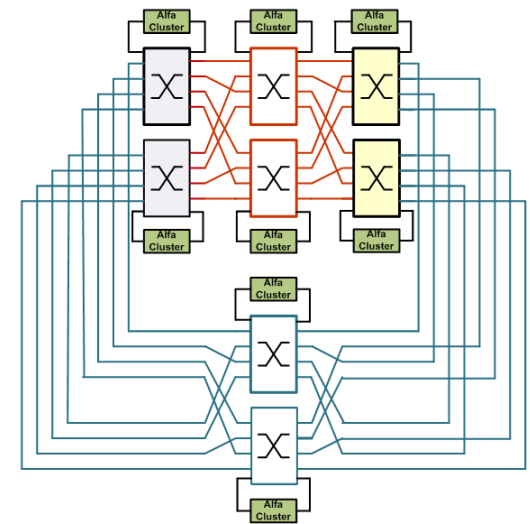
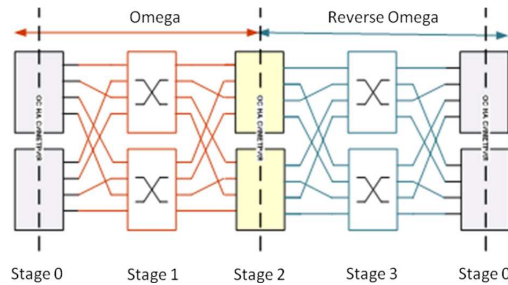
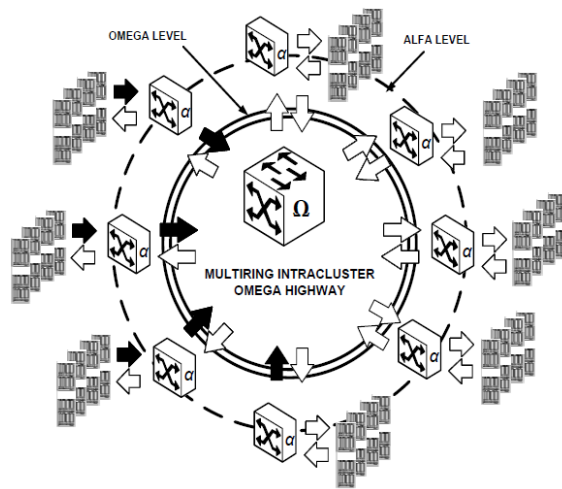


SBB: (l) router with radix 4x4; (r) transfer of the main communication agents



# 3.D2. $\alpha\Omega$ HIGHWAY SAN

The hierarchical structure of the system area network is studied on two levels:  
level Omega and level Alpha.



$\alpha\Omega$  HIGHWAY system area network architecture



# 5. Education and training

The consortium SuperCA++ includes:

- Bulgarian Academy of Sciences
  - **Institute of Information and Communication Technologies (C)**
  - National Institute for Geophysics, Geodesy and Geography
  - Institute of Mechanics
- Sofia University
  - Department of Mathematics and Informatics
  - Department of Physics
- Technical University - Sofia
  - Department of Electronics
- Medical University - Sofia
  - Department of Pharmacology

**60% of SuperCA++ team are students or young researchers.**



# Structure of SuperCA++

- **WG1: High performance architectures of multi-core processors - [V. Lazarov](#)**
- **WG2: Multi processors interconnection networks - [P. Borovska](#)**
- **WG3: High performance framework for Grid applications - [E. Atanasov](#)**
- **WG4: Finite element simulation of strongly heterogeneous media - [S. Margenov](#)**
- **WG5: Monte Carlo sensitivity analysis - [I. Dimov](#)**
- **WG6: Wind energy and atmospheric quality - [K. Ganev](#)**
- **WG7: Computational fluid dynamics - [N. Popivanov](#)**
- **WG8: Processes and phenomena in micro-electro-mechanical systems - [E. Manoach](#)**
- **WG9: Quantum simulations - [I. Christov](#)**
- **WG10: Simulation of biological molecules and systems - [L. Litov](#)**
- **WG11: In silico analysis of immunogenic and allergenic proteins - [I. Doytchinova](#)**



# Graduate sources

## Regular graduate sources in supercomputing and supercomputing applications:

- Parallel architectures and high performance computing
- Parallel numerical methods and algorithms
- Computational physics
- Computational chemistry
- Computational pharmacy

## Academic institutions:

- Bulgarian Academy of Sciences
- Sofia University
- Technical University - Sofia
- Medical University - Sofia
- University of Library Studies and Information Technologies



# Training courses

## ● **Supercomputer applications in natural sciences**

- **Organizers:** Bulgarian Supercomputing Center, Sofia University, Medical University - Sofia, Bulgarian Academy of Sciences
- **Time:** October - December 2011, February - April 2012
- **Topics:** Introduction to parallel calculations, Physics, Chemistry, Biology and Pharmacy

## ● **High-performance computing**

- **Organizer:** Institute of Information and Communication Technologies (IICT-BAS)
- **Time:** March 2011, February 2012
- **Topics:** Introduction to parallel computing, Programing with MPI, Open MP and CUDA, Application software deployed on BG/P and IICT HPC cluster





# SuperCA++ events

- Workshop SuperCA++, Hisarya, 20-22 May 2011
- Workshop SuperCA++, Bansko, 23-24 April 2012
- Workshop SuperCA++, Tryavna, 31 March 2 April 2013



Център за върхови научни постижения „Суперкомпютърни приложения“

**Center of Excellence "Supercomputing Applications" (SuperCA++)**



| Консорциум   | Приложения Applications  | Инфраструктура Infrastructure  |
|--|--|--|
| <p>Институт по информационни и комуникационни технологии – БАН (Координатор)</p> <p>Софийски университет "Св. Климент Охридски"</p> <p>Технически университет – София</p> <p>Медицински университет – София</p> <p>Институт по механика – БАН</p> <p>Национален институт по геофизика, геодезия и география – БАН</p> <p style="color: green; text-align: center;"><b>Consortium</b></p> <p><i>Institute of Information and Communication Technologies, BAS (Coordinator)</i></p> <p><i>Sofia University "St. Kliment Ohridski"</i></p> <p><i>Technical University of Sofia</i></p> <p><i>Medical University of Sofia</i></p> <p><i>Institute of Mechanics, BAS</i></p> <p><i>National Institute of Geophysics, Geodesy and Geography, BAS</i></p> <p style="color: green; text-align: center;"><b>Работни пакети</b></p> <div style="font-size: 0.8em;"> <p><b>P01:</b> Високопроизводителни компютърни архитектури в областта на PetaFLOPS с използване на многоядрени процесори</p> <p><b>P02:</b> Многопроцесорни комуникационни мрежи за PetaFLOPS суперкомпютри</p> <p><b>P03:</b> Високопроизводителна среда за иновативни Грид приложения</p> <p><b>P04:</b> Компютърна симулация с крайни елементи на силно хетерогенни среди</p> <p><b>P05:</b> Монте Карло методи за анализ на чувствителността на големи математически модели</p> <p><b>P06:</b> Изучаване енергията на вятъра и качеството на въздуха в България с използване на интензивни симулации в каскада от машини</p> <p><b>P07:</b> Суперкомпютърни приложения в изчислителната механика на флуидите</p> <p><b>P08:</b> Паралелни алгоритми и Грид приложения за компютърно моделиране на процеси и феномени в Микро-Електро-Механични системи (MEMS)</p> <p><b>P09:</b> Квантови суперкомпютърни симулации</p> <p><b>P10:</b> Суперкомпютърни симулации на биологични молекули и системи</p> <p><b>P11:</b> In Silico анализ на имуногенни и алергени протеини</p> </div> | <div style="text-align: center;">   </div> <p><b>IBM Blue Gene/P Supercomputer</b></p> <p>Симулации на пренос на звук в кристали и вълнуване с използване на IBM Blue Gene/P</p> <p><i>IBM Blue Gene/P simulation of air pollution transport</i></p> <div style="display: flex; justify-content: space-around;">   </div> <p><b>Исследване на мултигредови архитектури</b></p> <p><i>Multi-Thread architecture simulations</i></p> <p><b>Симулация на разпространение на вирус</b></p> <p><i>Developed Grid service with using Advanced Message Queueing Protocol</i></p> <p style="color: green; text-align: center;"><b>Work packages</b></p> <div style="font-size: 0.8em;"> <p><b>WP1:</b> High Performance Architectures towards PetaFLOPS based on Multi-Core Processors</p> <p><b>WP2:</b> Multiprocessors Communication Networks for PetaFLOPS Supercomputers</p> <p><b>WP3:</b> High-Performance Framework for Advanced Grid Applications</p> <p><b>WP4:</b> Finite Element Computer Simulation of Strongly Heterogeneous Media</p> <p><b>WP5:</b> Monte Carlo Methods for Sensitivity Analysis of Large Mathematical Models</p> <p><b>WP6:</b> Wind Energy and Atmospheric Quality Studies in Bulgaria using Extensive Multi-scale Simulations</p> <p><b>WP7:</b> Supercomputer Applications in Computational Fluid Mechanics</p> <p><b>WP8:</b> Computer Simulation of Micro-gas Flows in Elements of Micro-Electro-Mechanical Systems (MEMS)</p> <p><b>WP9:</b> Quantum Supercomputer Simulations</p> <p><b>WP10:</b> Supercomputer Simulations of Biological Molecules and Systems</p> <p><b>WP11:</b> In Silico Prediction of Immunogenic and Allergenic Proteins</p> </div> | <p><b>IBM Blue Gene/P Supercomputer</b></p> <p>Consists of two racks, 2048 Power PC 605 based computer nodes, 1024 process in core and a total of 4TB random access memory. Each processor core has a double precision, dual pipe floating-point core accelerator. System I/O nodes are connected via fibre optics to a 10 Gb/s Ethernet switch. The installed partition size, available currently, is 128 compute nodes (312 processed cores).</p> <p>The theoretical performance of the computer is 27.65 TFlops while the maximum LINPACK performance achieved is 12.85 TFlops/s.</p> <p><b>ICT HPC Cluster</b></p> <p>HP Cluster Platform Express 7000 enclosure with 20 blades 10, 206 with dual Intel Xeon X5550 Q 3.06GHz (total 576 cores, 34 GB RAM per blade).</p> <p>There are 8 storage and management controlling nodes 6 HP DL 380 G5 with dual Intel X5550 Q 3.0 GHz and 12 GB RAM and 50 TB disk storage.</p> <p>All these servers are interconnected via non-blocking QDR Infiniband interconnect of 100Gbps line speed. The theoretical peak performance is 1.23 TFlops.</p> <p>The HPC cluster was upgraded with two HP DL 380 G7 all in half Tray Servers with series NVIDIA Tesla M2090 G20 Modules, included in ProLiant BL460c Scalable System Rack. The GPU cards have 3048 CUDA cores. The peak GPU computing performance exceeds the value of 4.05 TFlops in double precision or 1.23 TFlops in single precision.</p> <p>The GPU computing modules are connected to the InfiniBand cluster with QDR Infiniband cards.</p> <div style="text-align: center;">  </div> <p style="color: green; text-align: center;"><b>Годишен семинар, Банско'2012</b></p> <p style="color: green; text-align: center;"><b>Annual Seminar, Bansko'2012</b></p> |

Проект ДЦВР 02/1 с НФ "Научни изследвания", MOMH (DCVР 02/1 Grant with Bulgarian NSF)





# Recent related conferences



- **1<sup>st</sup> Regional Conference “Supercomputing-New Challenge for Science and Industry” in Bulgaria, December 09-10.2010, Sheraton Hotel, Sofia.**

**More than 200 participants from Germany, Poland, Turkey, Greece, Croatia, Romania, Latvia and Lithuania.**

- **2<sup>nd</sup> Regional Conference “Supercomputing Applications in Science and Industry”, Rodopi Hotel, Sunny Beach, September 20-21, 2011.**

**More than 80 participants from Bulgaria, Germany, Italy, Greece, Croatia, Japan, UK and Russia.**

**Both conferences bridge scientific and industrial perspectives and provide a forum for exchange of different views and opinions.**



# 5. Theory and practice

- "There is nothing so practical as the good theory."  
Kurt Lewin
- "In theory, theory and practice are the same. In practice, they are not."  
Albert Einstein



**THANK YOU !**

