Supercomputing Support of the Researches and Education

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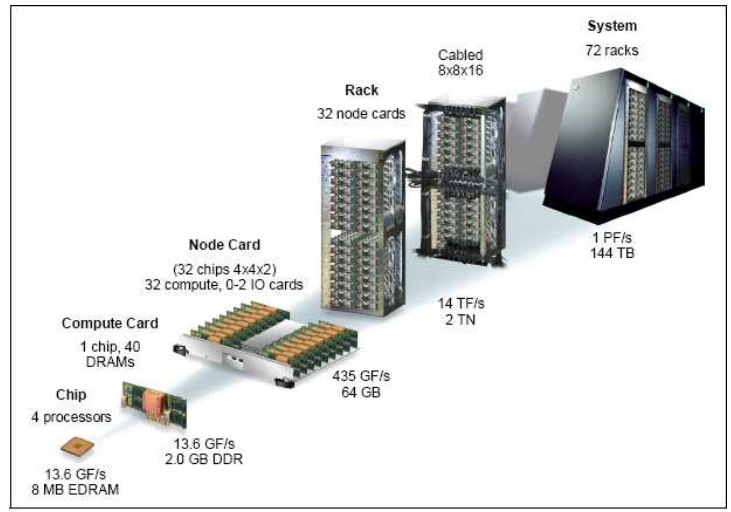
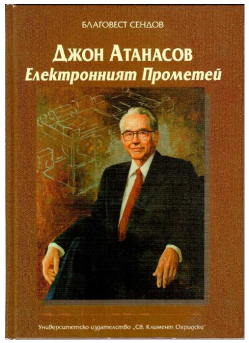
CONTENTS

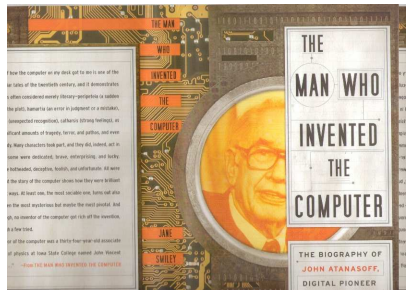
1. Introduction

- 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



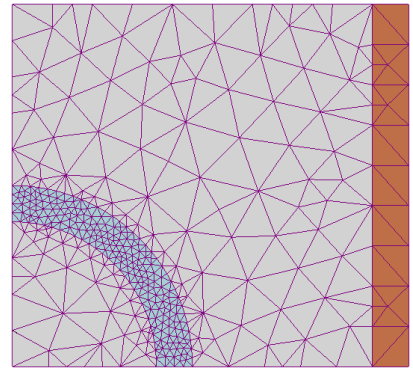


- Atanasoff has been familiar with the numerical **method of Ritz** leading for his problem to a system of **29 linear algebraic equations**.
- Such computations have required many weeks efforts using the Monroe manual rotary Calculator.
- Atanasoff has tried to run several Monroe machines in parallel 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

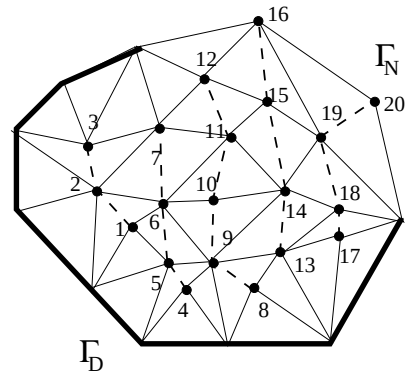
- The Ritz method (1909) is a direct method to find an approximate solution of boundary value problems.
- The Ritz method is described in terms of minimizing the ”energy functional” or Hamiltonian of the system.
- In the language of mathematics, it is exactly the finite element method.
- Not so well 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

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

and the related FEM problem

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



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

$$A\mathbf{u} = \mathbf{f}.$$

PCG scalability

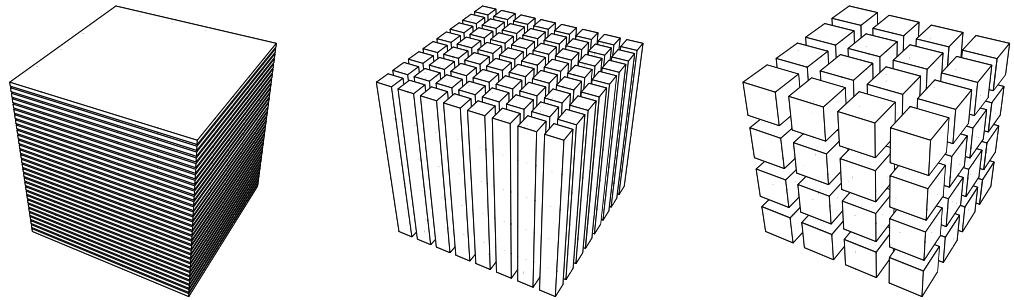
- For large-scale problems, the iterative methods have advantages due to their better/optimal computational complexity and storage requirements.
- The Conjugate Gradient (CG) method is the best iterative solution framework for large scale FEM systems.
- The development of robust Preconditioned Conjugate 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 x 127 x 127	*8 = 8 x 1 x 1*	*2 097 152*	*161*	*1 255.00*	
255 x 255 x 255	*64 = 64 x 1 x 1*	*16 777 216*	*128*	*5 951.08*	*21 %*
511 x 511 x 511	*512 = 512 x 1 x 1*	*134 217 728*	*-*	*> 24* h	*< 2 %*
127 x 127 x 127	*8 = 4 x 2 x 1*	*2 097 152*	*167*	*1 137.83*	
255 x 255 x 255	*64 = 8 x 8 x 1*	*16 777 216*	*129*	*1 203.29*	*95 %*
511 x 511 x 511	*512 = 32 x 16 x 1*	*134 217 728*	*114*	*1 581.13*	*72 %*
127 x 127 x 127	*8 = 4 x 2 x 1*	*2 097 152*	*167*	*1 137.91*	
255 x 255 x 255	*64 = 4 x 4 x 4*	*16 777 216*	*128*	*1 062.30*	*107 %*
511 x 511 x 511	*512 = 8 x 8 x 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

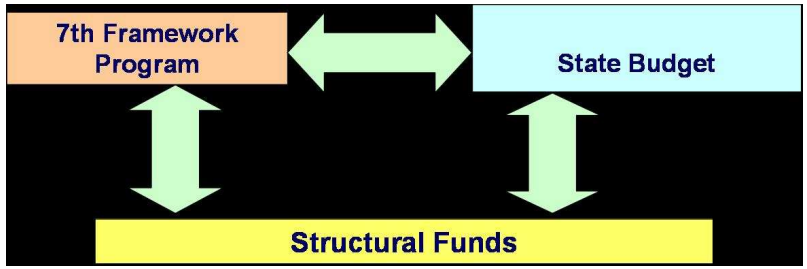
   Scientific and technical coordinator: CoE on Supercomputing applications

   (IICT - BAS is a coordinator of SuperCA++)
6. BG-CLARIN: integration and development of Bulgarian language electronic resources as a part of European CLARIN

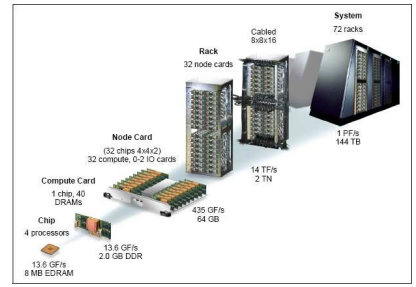
   Scientific and technical coordinator: IICT - BAS
7. Astronomical center for research and education

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.



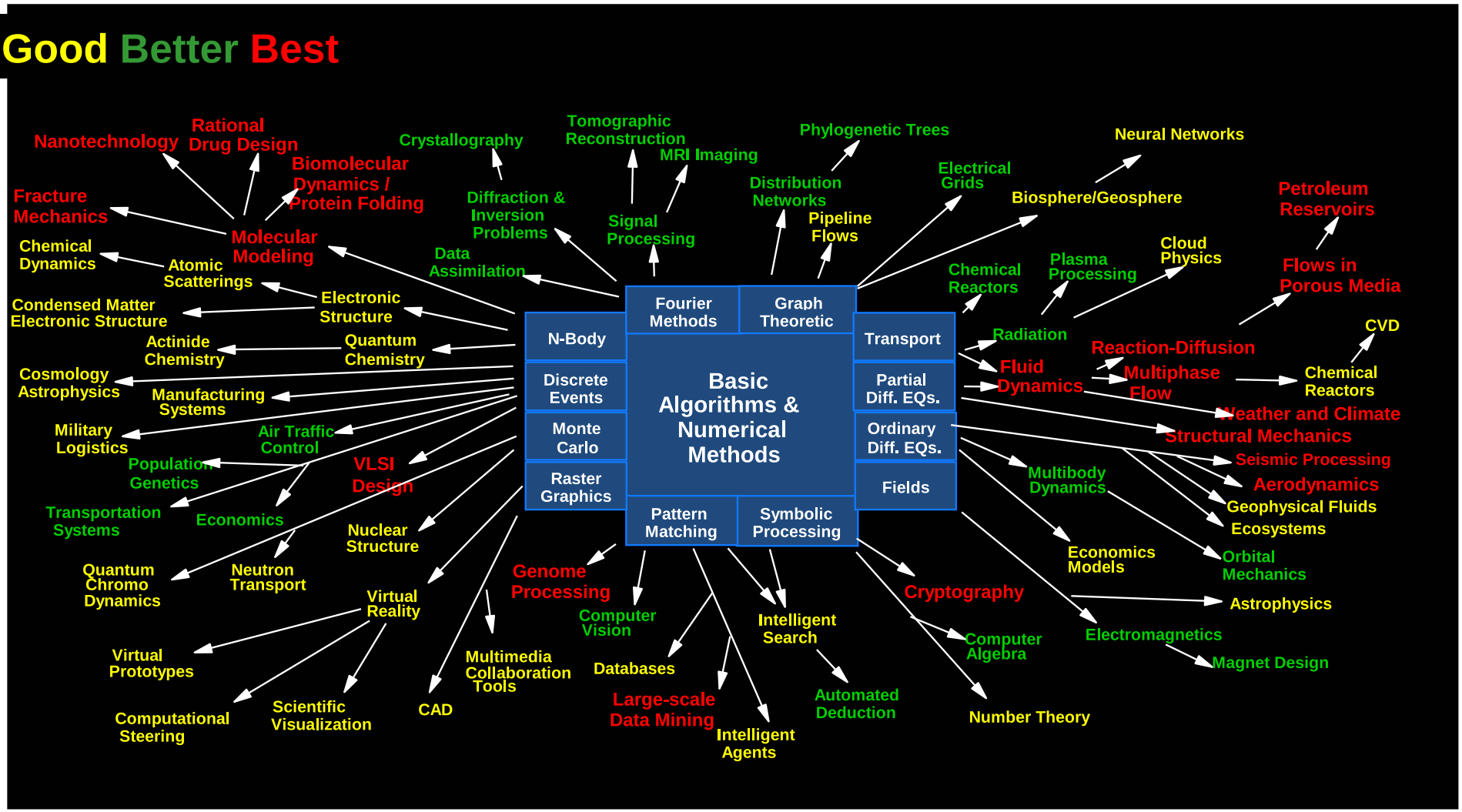
Financial Instruments



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

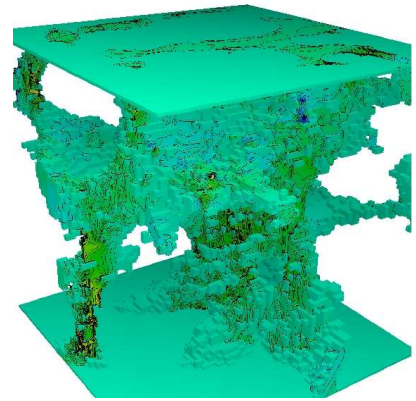


Argonne National Labs GBB

3.A1. Bone microstructure

- μFEM 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.

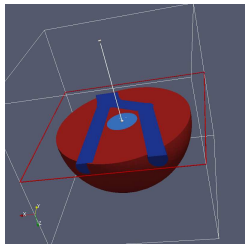
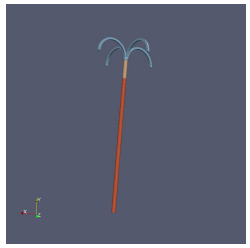
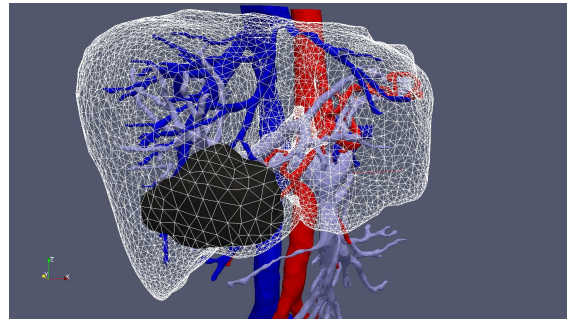
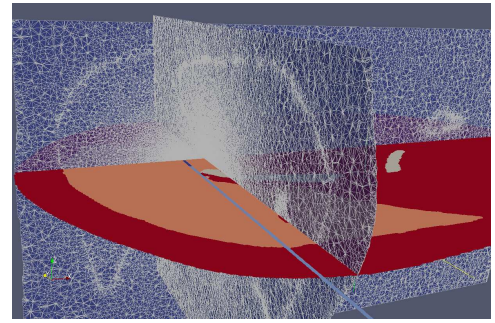
		$\zeta = 0.1$			
		MIC(0)		AMG	
n	p	$T[s]$	It	$T[s]$	It
64	1	1 184	270	1 071	28
128	8	1 831	395	1 147	25
256	64	4 870	888	1 318	25



		$\zeta = 0.01$			
		MIC(0)		AMG	
n	p	$T[s]$	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

		$\zeta = 0.001$			
		MIC(0)		AMG	
n	p	$T[s]$	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

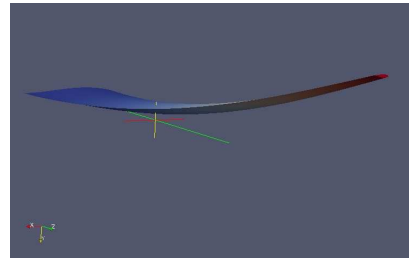





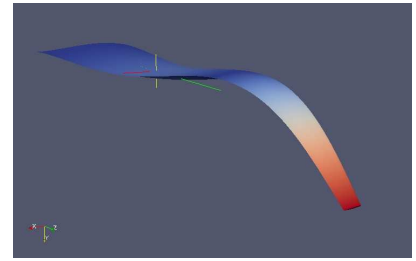
- **The RF ablation destroys the unwanted tissue by heating, arising when the energy dissipated by the electric current flowing through the RF probe is converted to heat.**

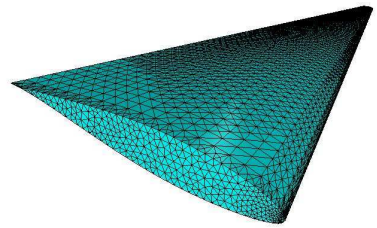
	Degrees of freedom (DOF)		
n_p	2 097 152	16 777 216	134 217 728
32	1 788		
64	884		
128	457		
256	250	1 880	
512	165	1 107	
1 024	155	667	
2 048	387	708	3 340

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

3.A3. Large wind turbine







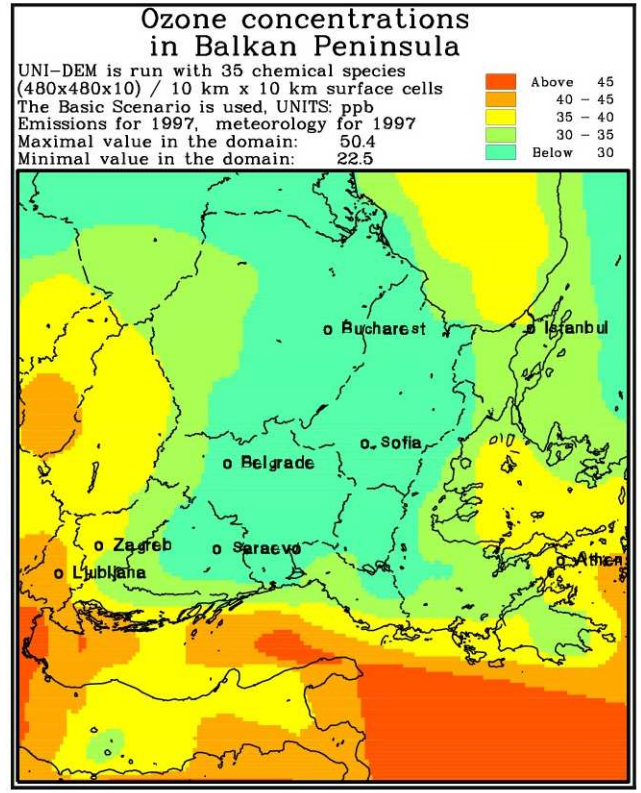
	Linear static problem			Nonlinear static problem			Eigenvalue problem problem		
n_p	T[s]	Sp	E [%]	T[s]	Sp	E [%]	T[s]	Sp	E [%]
16	1 311.92			4 375.24			766.53		
32	666.85	1.97	98. 37	2 213.03	1.98	98.85	395.10	1.94	97.00
64	301.08	4.36	108.93	1 038.75	4.21	105.30	270.92	2.83	70.73
128	180.90	7.25	90.65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

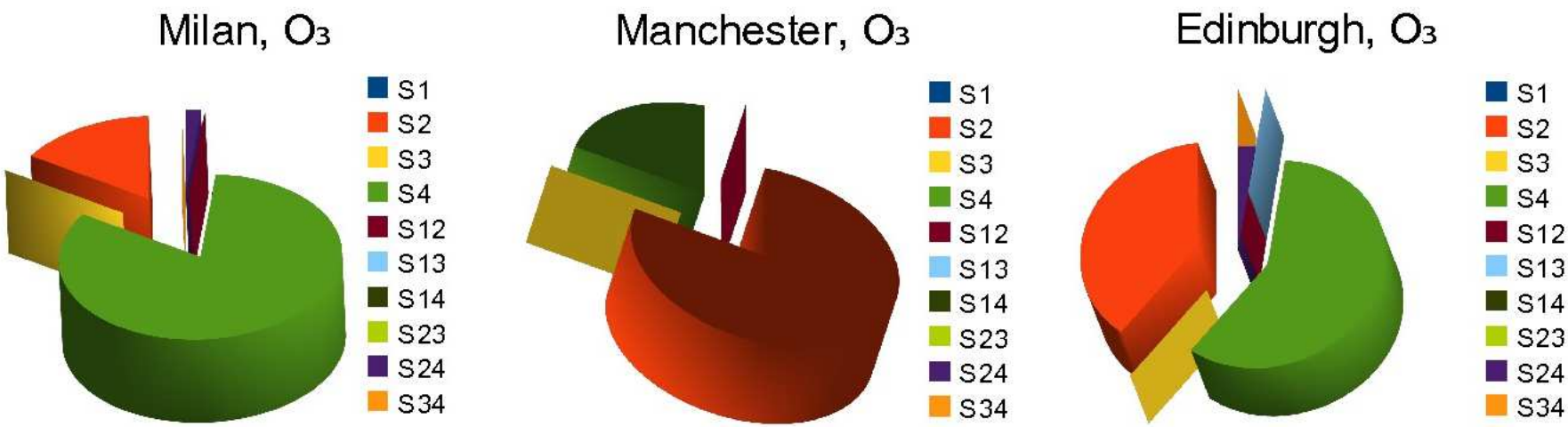
3.B1. Air pollution simulation

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.**



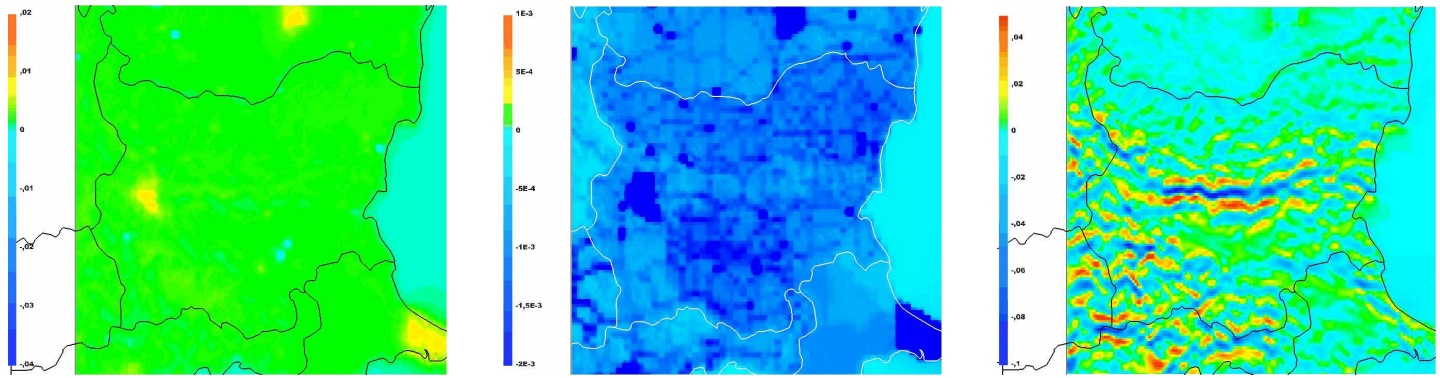
3.B2. Sensitivity analysis



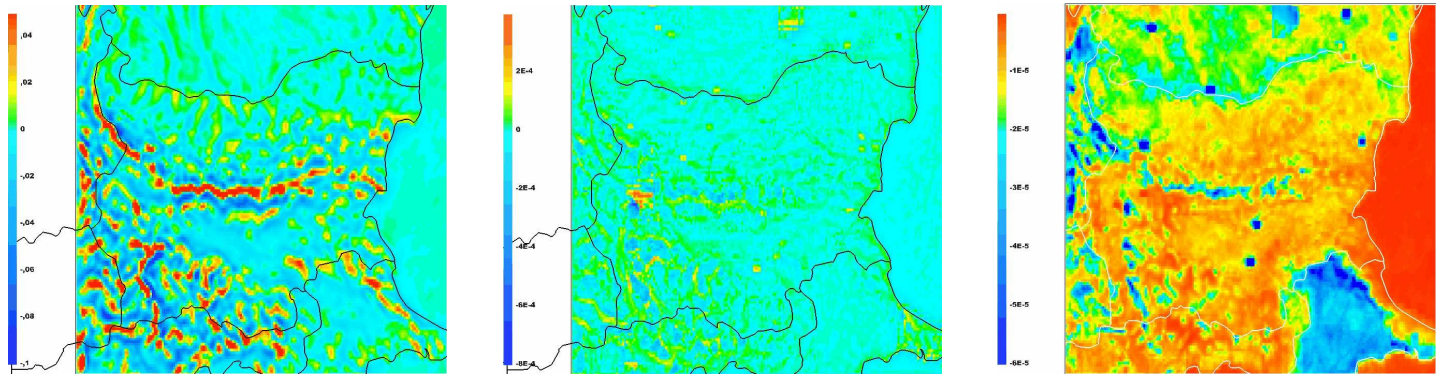
- **Pie charts representation of first- and second-order sensitivity indices of the ozone in Milan, Manchester, and Edinburgh.**

3.B3. Annual contributions

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



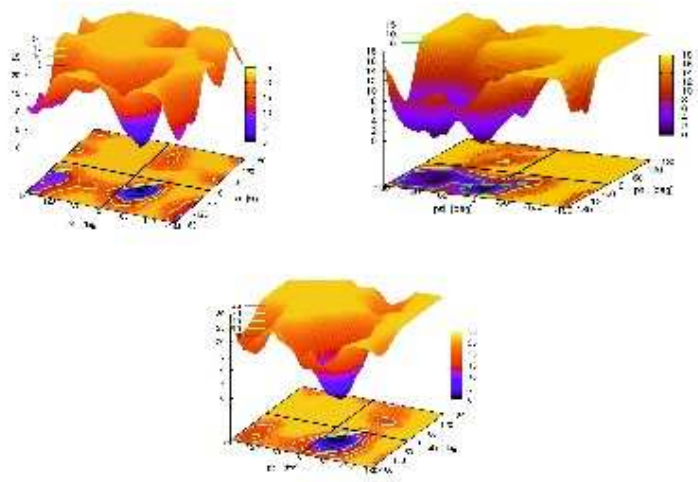
(l) Vertical diffusion; (c) Chemical transformations (r) Horizontal advection;



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

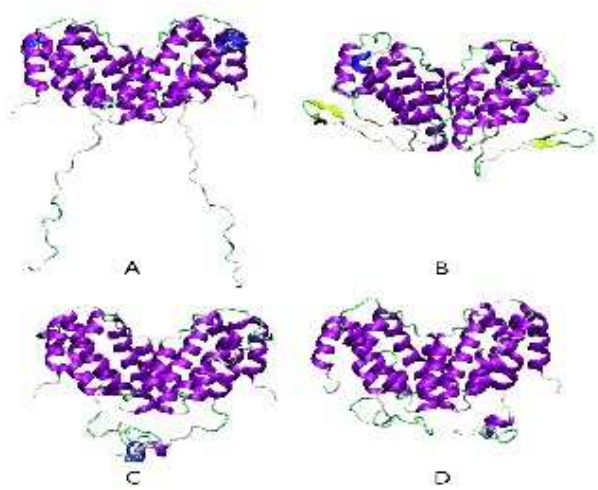
3.C1. Human interferon gamma

- The structural stability of 100 hIFNg 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

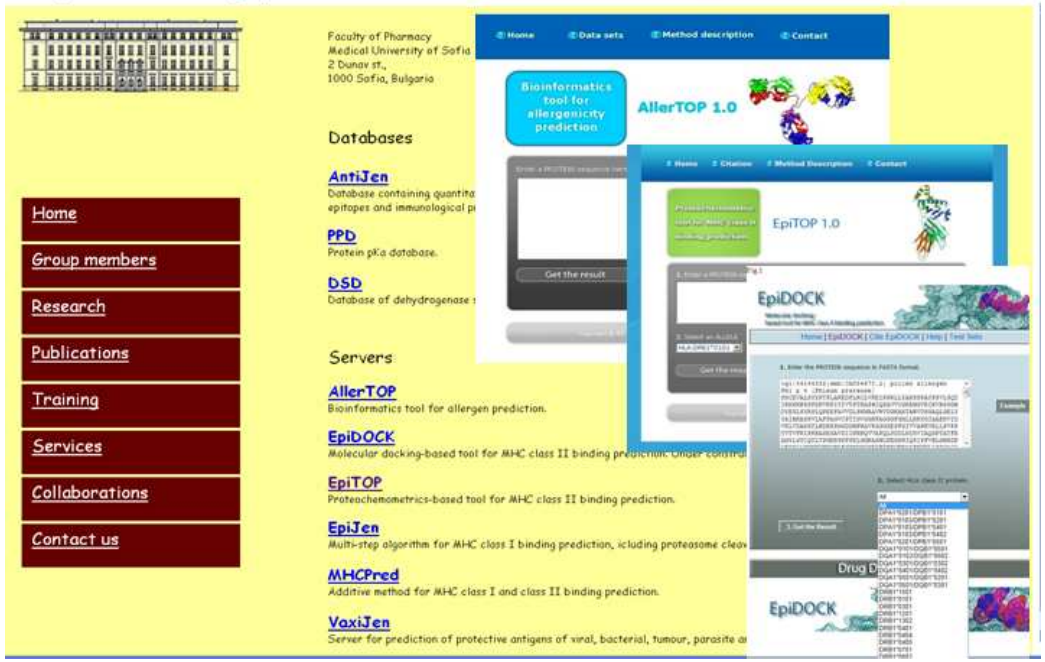
- The length of the tail modifies the affinity to the receptor.
- Two 200 ns MD folding simulations are performed using GROMOS 53a6 + GROMACS 4.5.4 and CHARMM 22 + NAMD 2.9 to cluster the trajectories.
- It was found that in both cases the C-Termini get closer to the globule and the whole protein adopts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



3.C3. In silico drug design

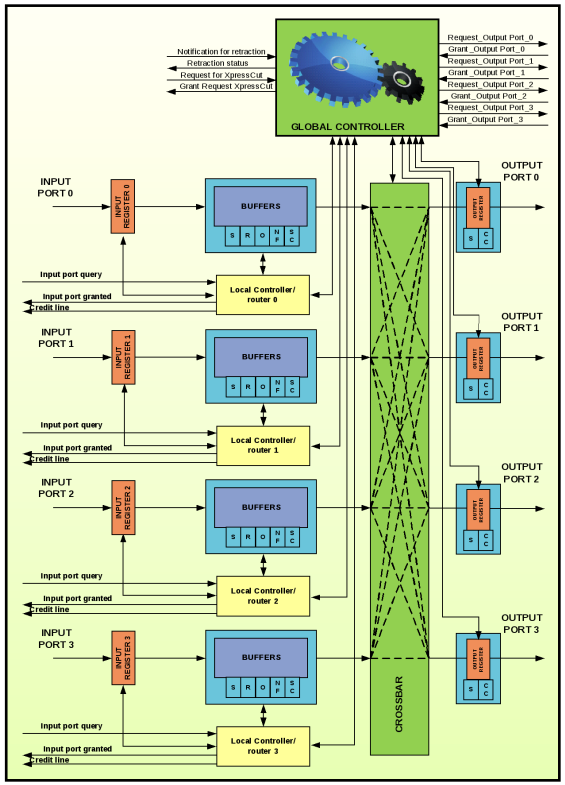
- **Structure-based methods for drug design are used to develop models for allergenicity and immunogenicity predictions of novel proteins.**
- **Molecular dynamics simulations and molecular docking studies are applied on BlueGene-P to derive the models.**
- **Once the models are derived, they are freely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

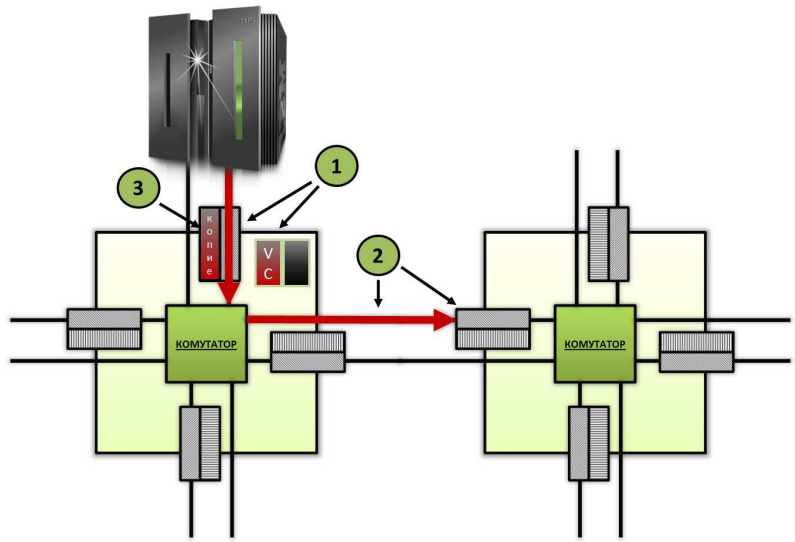
http://www.ddg-pharmfac.net



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.

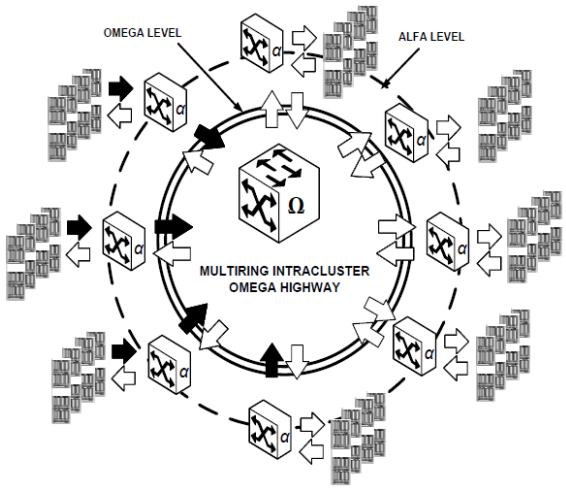


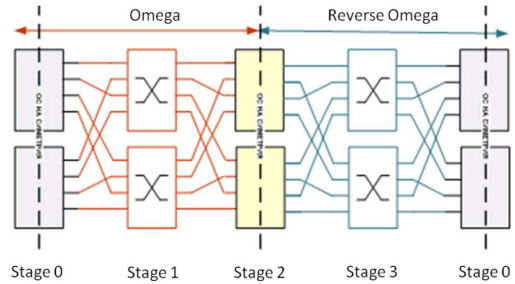


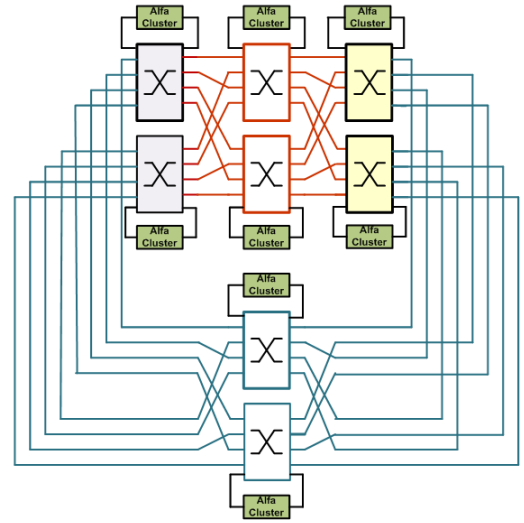
SBB: (l) router with radix 4x4; (r) transfer of the main communication agents

3.D2. αΩ HIGHWAY SAN

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







αΩ **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**

Resent related conferences

- **1st 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.

- **2nd 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 !