High-Performance Computing and Groundbreaking Applications

Svetozar Margenov
Institute of Information and Communication Technologies
(IICT-BAS)
margenov@parallel.bas.bg

Academic HPC Resources

AVITOHOL at IICT-BAS

150x HP ProLiant SL250s Gen8 each with
2x Intel Xeon E5-2650 v2 (8C/16T),
64 GB DDR3-1866 RAM and
2x Intel Xeopn Phi 7120P
6x HP ProLiant DL380p Gen8 nodes with
2x Intel Xeon E5-2650v2 (8C/16T),
64 GB DDR3-1866 RAM
Infiniband 56 Gb/s FDR
Storage system with 96 TB

AVITOHOL

Total Performance:
RPeak:412.3 TFlop/s
RMax: 264.2 TFlop/s
Top 500 position: 389

HPCG cluster at IICT-BAS

36 blades BL 280c(2x Intel X5560(4C/8T); 24GB DDR3);
8 management nodes HP DL 380 G6(2x Intel X5560(4C/8T); 32GB DDR3);
2 HP ProLiant SL390s G7(2x Intel E5649(6C/12T);96GB DDR3)
8x nVidia TESLA M2090 per server;
2 HP SL270s Gen8 (2x Intel Xeon E5-2650 v2(8C/16T); 128GB DDR3)
Total number of Xeon Phi 5110P coprocessors: 9
Total 132TBs of system storage

TOTAL PERFORMANCE:
RPEAK:22.94 TFlop/s

NCSA IBM Blue Gene/P

8192 PowerPC 450 processors
4TBs of system memory
12TBs of system stotage
IBM proprietary interconnect with
2.5 μs latency and 10GBps bandwidth

TOTAL PERFORMANCE:
RPEAK:27.85 TFlop/s
RMAX:23.45 TFlop/s

PHYSON at Sofia University

53 Intel Xeon x86_64 processors
524Gibs of system memory
6.5TBs of system storage
2x nVidia Tesla M2090 graphics processors

TOTAL PERFORMANCE:
RPEAK:3.57 TFlop/s
RMAX: 3.22 TFlop/s

MADARA at IIOCCP-BAS

54 Primergy RX200 S5 servers with
2 Intel Xeon E5520(4C/8T) each
and a total of 800GB DDR3 1066MHz
20Gb/s DDR Infiniband
108TB System Storage by Fujitsu FibreCat SX100

CoE on Supercomputing Applications

Consortium of the Project DCVP 02/1, SuperCA++:

Institute of Information and Communication Technologies – BAS (coordinator)

Sofia University “St. Climent Ohridski”

Technical University – Sofia

Medical University – Sofia

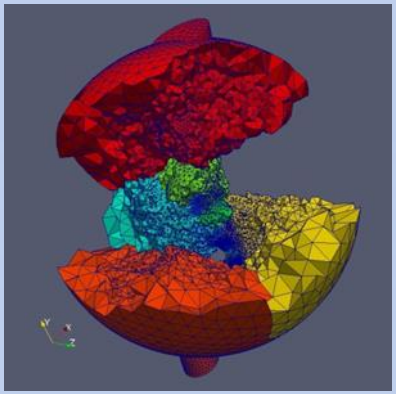
Institute of Mechanics - BAS

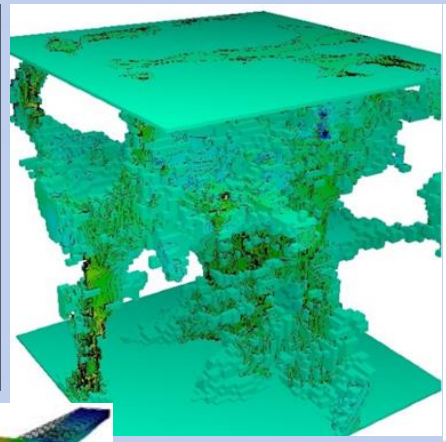
National Institute of Geophysics, Geodesy and Geography – BAS

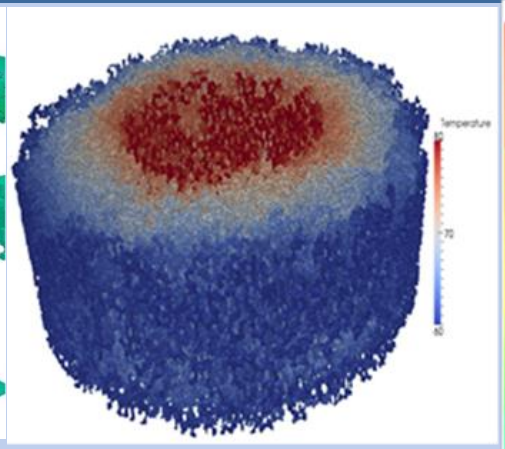
Basic Infrastructure:

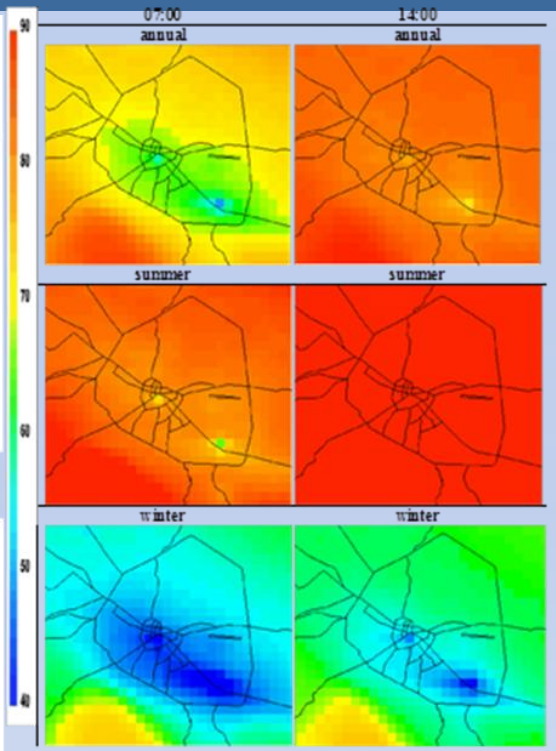
- Supercomputer IBM Blue Gene/P
- HPC Cluster at IICT

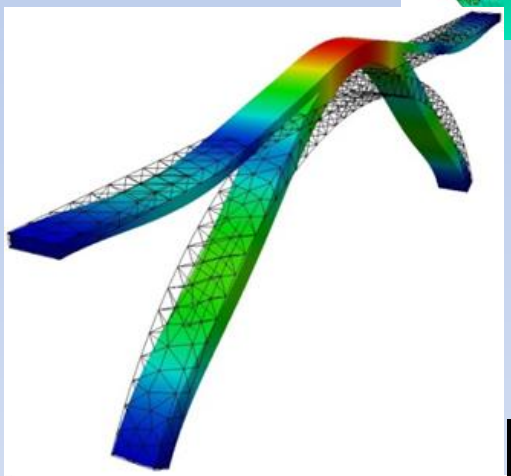
SuperCA++

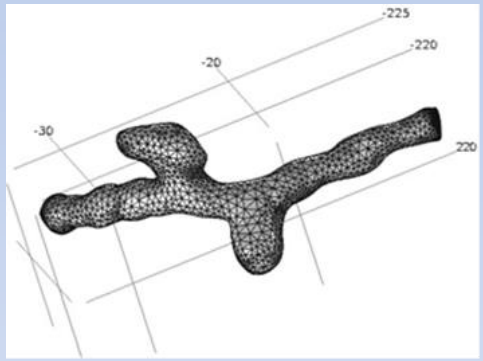


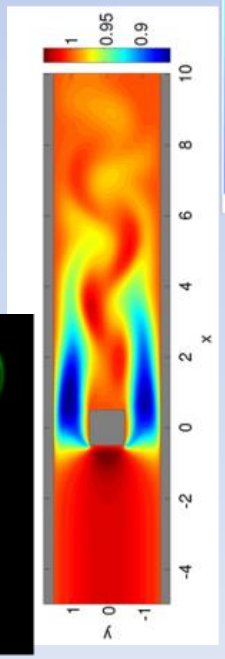


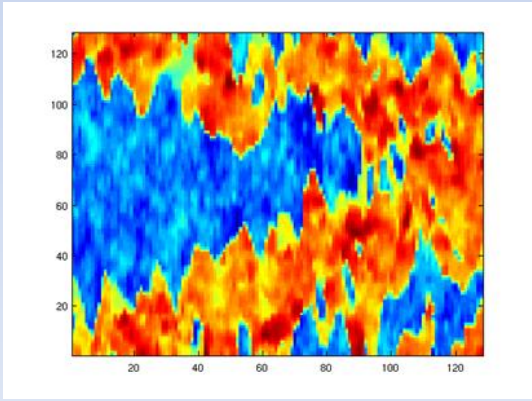

Temperature

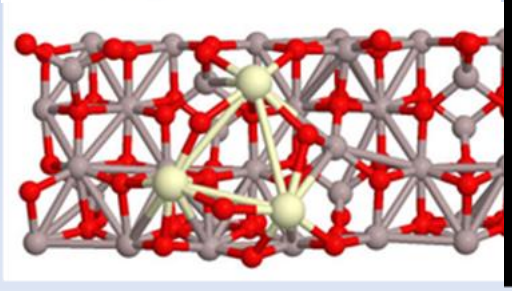

07:00
14:00
annual
annual
summer
summer
winter
winter

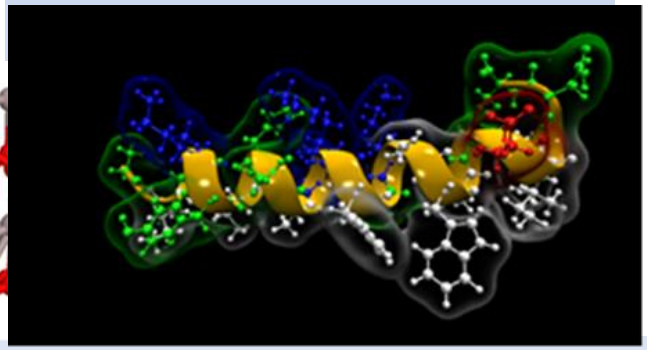



-225
-220
-20
-30
220

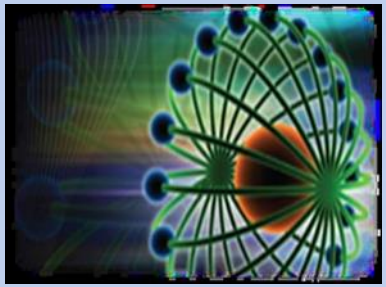

1
0.95
0.9
10
8
6
4
2
0
-2
-4
x
y


120
100
80
60
40
20
20
40
60
80
100
120





National Roadmap for Research Infrastructures 2017-2023



National Center for High Performance and Distributed Computing (HP&DC)

- **Coordinator**

  Institute of Information and Communication Technologies

- **Location**

  Institute of Information and Communication Technologies

- **Financial coordinator**

  Ministry of Education and Science

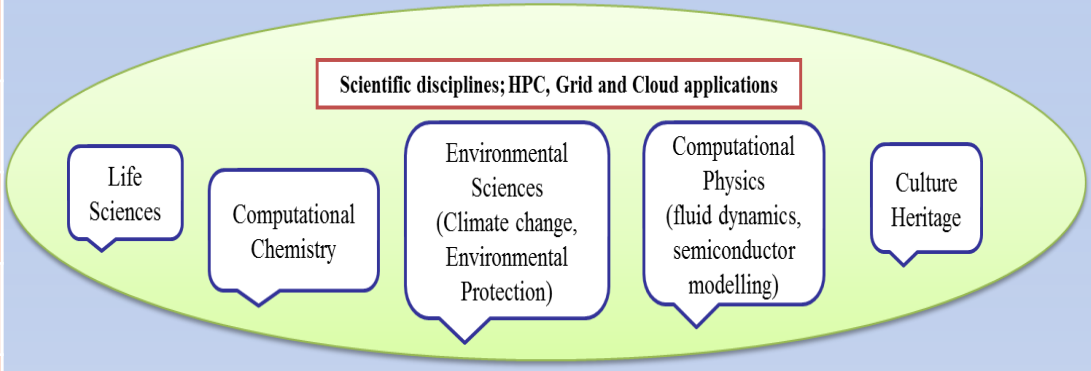
- **Participation in European Infrastructures**

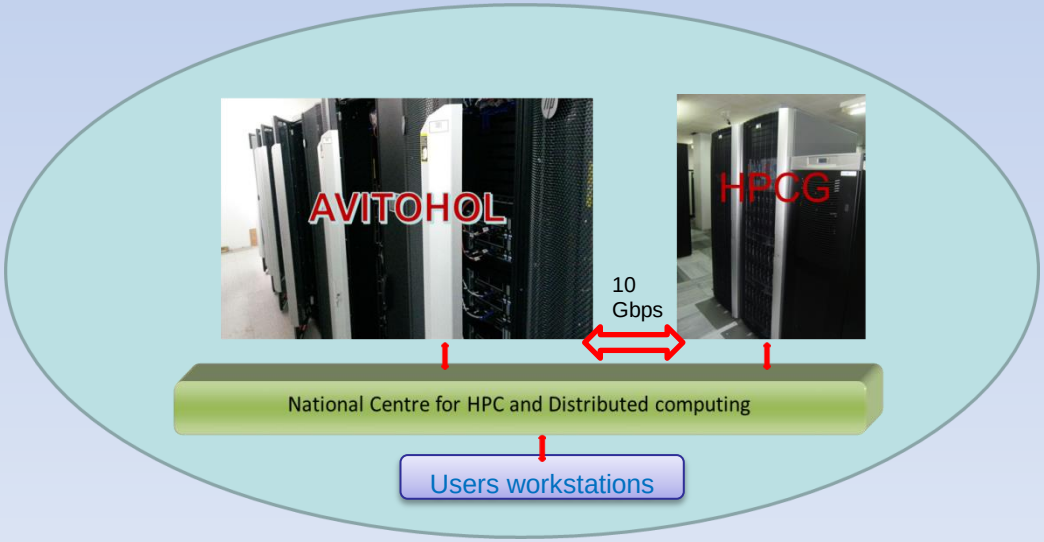
  EGI and PRACE through cooperation with NCSA

National Center for HP&DC at IICT

150 HP Cluster Platform SL250S GEN8 servers with 2 Intel Xeon E 2650 v2 CPUs and 2 Intel Xeon Phi 7120P coprocessors	
Site	IICT-BAS/Avitohol
Manufacturer	Hewlett-Packard
Cores	20700
Interconnection	FDR InfiniBand
Theoretical Peak Performance	412.3 Tflop/s
RMAX Performance	264.0 Tflop/s
Memory	9600 GB
Operation System	Red Hat Enterprise Linux for HPC
Storage capacity	96 TB SAN

Top500 List on 389 place (Nov 2015)
http://www.top500.org/system/178609



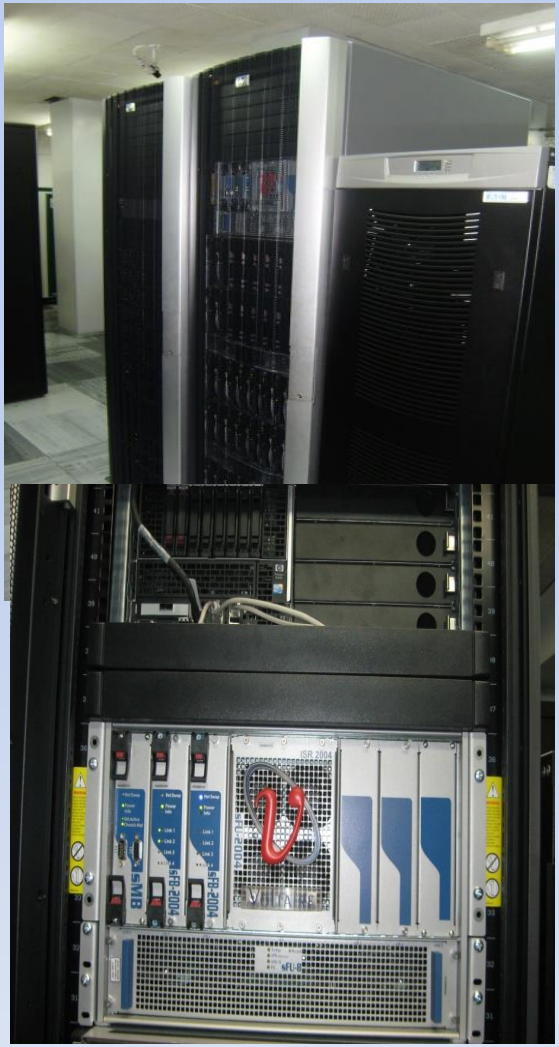


Supercomputer Avitohol at IICT

- The system consists of 8 racks of type HP MCS 200, paired in couples.
- Each pair provides power and cooling for up to 50 kW of equipment, cooled by water cooling.
- About 90% of the computational power comes from the accelerators – one 7120P coprocessor achieves 1.25 TFlop/s in double precision.
- RedHat Enterprise for HPC
- Intel Cluster Studio (compilers, MPI,MKL)
- GNU Compiler Collection
- Torque/moab for resource management with web and command line interface
- Monitoring and accounting tools
- Services running on virtual machines

HPCG Cluster at IICT

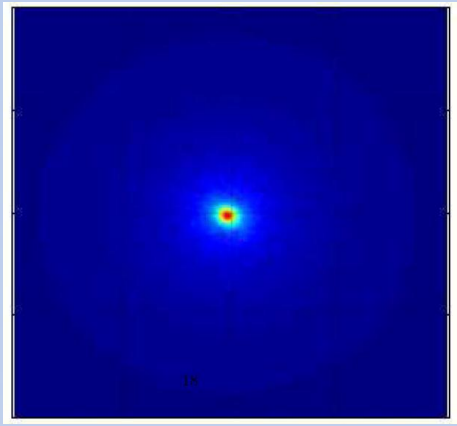
- 36 blade servers HP BL 280c, deployed in 3 HP Cluster Platform Express 7000 enclosures, each with 2 Xeon X5560 @ 2.80GHz, 24 GB RAM – 576 cores total with more than 3 Tflops peak performance; 8 dual-socket HP DL 380 G6 with dual Intel X5560 @ 2.8 Ghz, 32 GB RAM. Non-blocking Infiniband interconnection @ 20 Gbps, 92% efficiency on LINPACK
- Total disk storage more than 132 TB from three disk systems, interconnected with Fiber Channel.
- 2 HP ProLiant SL390s G7 4U servers with 16 NVIDIA Tesla M2090 graphic cards (total 8192 GPU cores with 10.64 TFlops in double precision); HP SL270s Gen8 4U server with 8 Intel Xeon Phi 5110P Coprocessors (total 480 cores, 1920 threads, 8.088 TFlops of double-precision peak performance per server).
- Total peak theoretical peak performance 22.93 TFlops

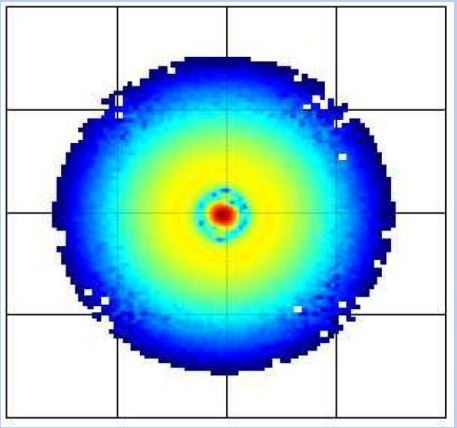


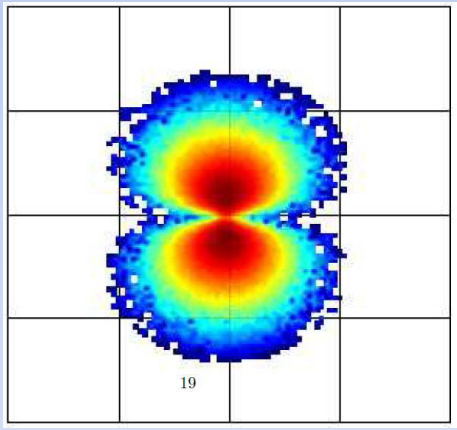
Quantum Computing

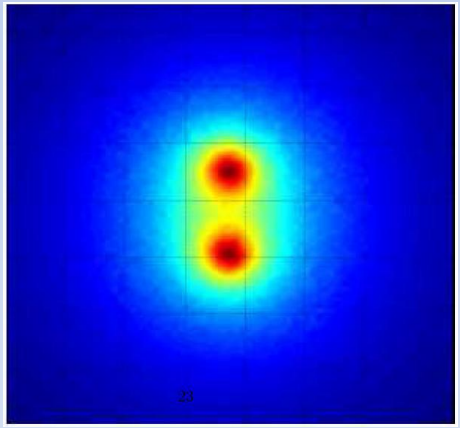
Quantum Computing in the Wigner Formulation of Quantum Mechanics:

- The signed particle formulation of quantum mechanics is a generalization of the Wigner Monte Carlo method which can deal with time-dependent, full quantum and multi-dimensional many-body problems .
- The quantum chemistry is possible in the Wigner formalism, offers an intuitive physical picture and allowing time-dependent quantum chemistry, thus opening access to the excited states of atoms, molecules, crystals, etc.









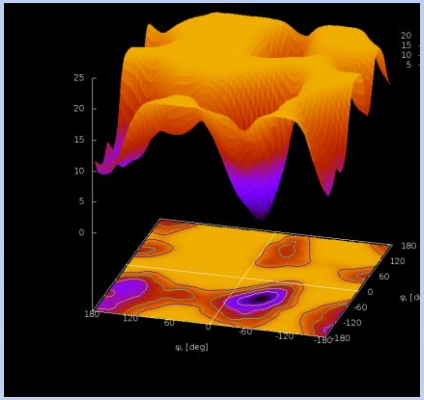
Collaboration: IICT-BAS and TU Wien

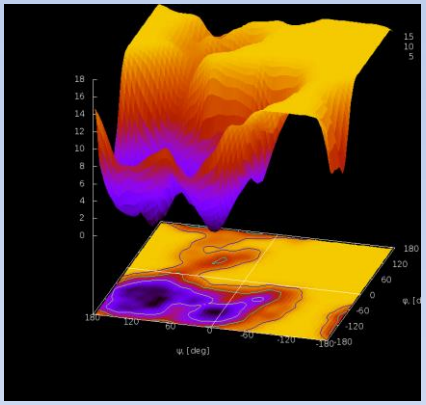
In-Silico Drug Design

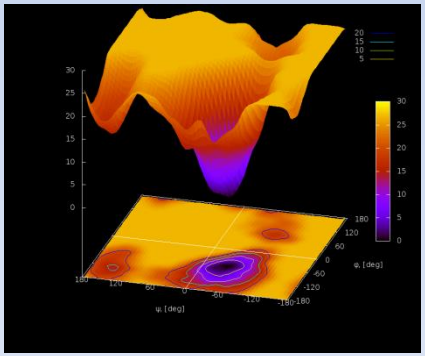
Supercomputer Simulation in Molecular Dynamics

Example:

- The root cause of autoimmune diseases (including multiple sclerosis) is the elevated expression of cytokininase-interferon, hIFNg.
- Ability to control these currently incurable diseases provides artificially mutated hIFNg forms.
- The assembled *In-Silico* protocol has selected 12 potential drug candidates with a stable local structure in the mutation region, preserved affinity for the receptor and low activity, from a library of 100 mutant forms, which reduces the required *In-Vitro* experiments tenfold.





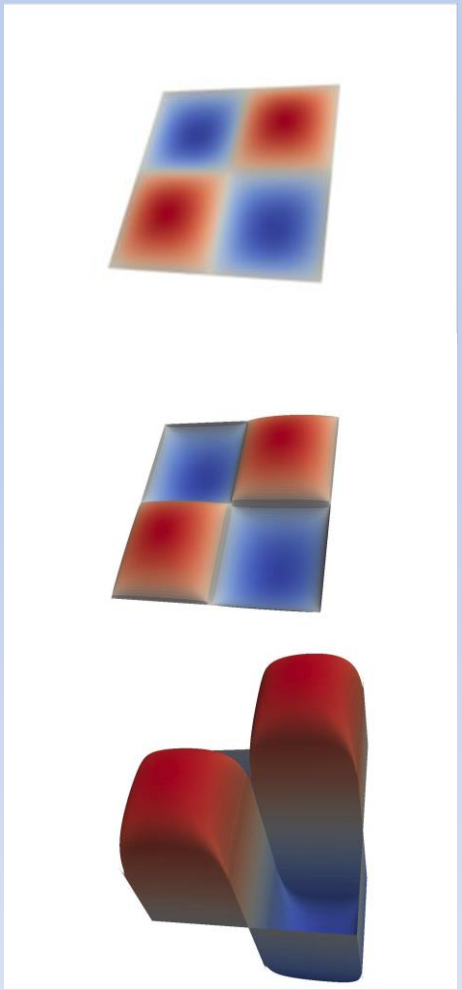


Collaboration: IMB-BAS, SU "St. Climent Ohridski". IICT-BAS

Super-Diffusion

Fractional Diffusion:

- Anomalously fast diffusion (also known as super-diffusion) is described by fraction elliptic operator in space.
- For instance, such a phenomena appears when the **Brownian motion hypothesis is violated**.
- The applications include underground flow, diffusion in fractal domains, dynamics of protein molecules, heat conduction with memory.



Supercomputer Avitohol				
DOFs	128^3		256^3	
Nodes	Time [s]	Efficiency	Time [s]	Efficiency
1	235		1 623	
2	103	115 %	729	111 %
4	52	113 %	360	113 %

Collaboration: IICT-BAS, TU Vilnius and Texas A&M University

Digital Composite

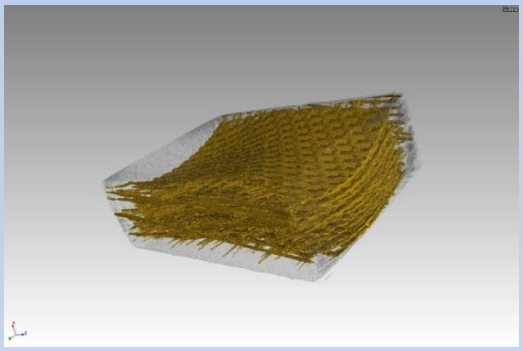
Digital Composite is an advanced approach for estimation of material properties based on:

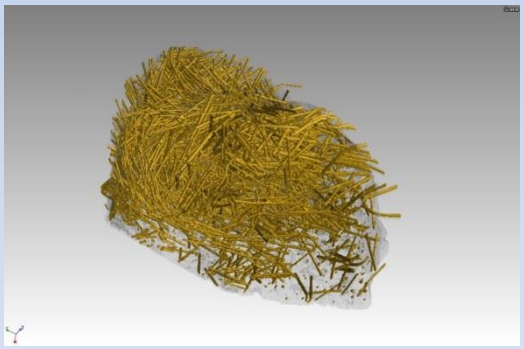
- High resolution industrial Computed Tomography (CT) images (SmartLab at IICT-BAS);
- Micro finite element (μ-FEM) analysis;
- Numerical upscaling;
- Supercomputing simulations.

Fiber Reinforced Concrete:

- Numerical upscaling of elastic properties;
- Representative Volume Element (RVE) of 1000 x 1000 x 1000 voxels;

		Avitohol			Salomon		
#P	#It	T[s]	T_1[s]	S_1	T[s]	T_1[s]	S_1
1	219	10975	50,11		5636	25,71	
8	439	2788	6,35	7,89	1763	4,02	6,40
64	535	517	0,97	51,76	292	0,55	47,11

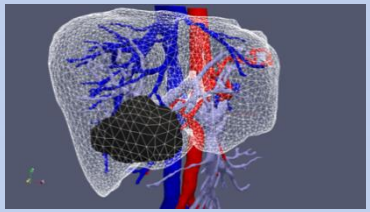
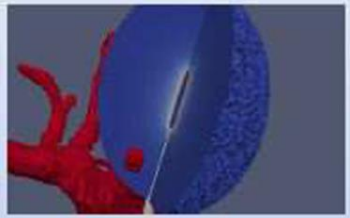
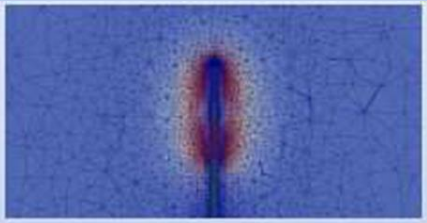




Collaboration: IICT-BAS, IG CAS – Ostrava and Czech National Supercomputing Center

Radio Frequency Hepatic 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.


Test Problem	V_1[cm^3]	Impact	$V_{4.6}$[cm^3]	Impact
Without blood circulation	20.7		14.0	
Portal vane is included	10.8	1.91	6.7	2.09
Portal vane and capillary network are included	7.8	2.65	5.3	2.64

Pralution Library, NVIDIA K20 GPU: N = 89 169 (left) and N = 2 693 437 (right)

Preconditioner	N_{it}	T [s]
Jacoby	444	0.2
FSAI	202	0.15
ILU(0,1)	166	0.4
AMG	21	12.9

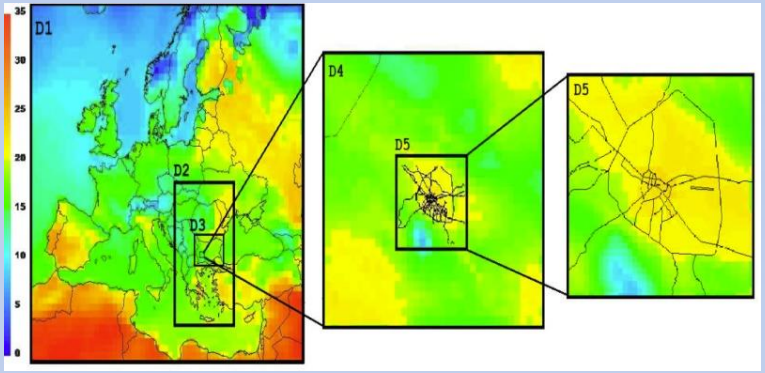
Preconditioner	N_{it}	T [s]
Jacoby	2 741	16
FSAI	1 453	15.6
ILU(0,1)	1 373	26
AMG	26	3

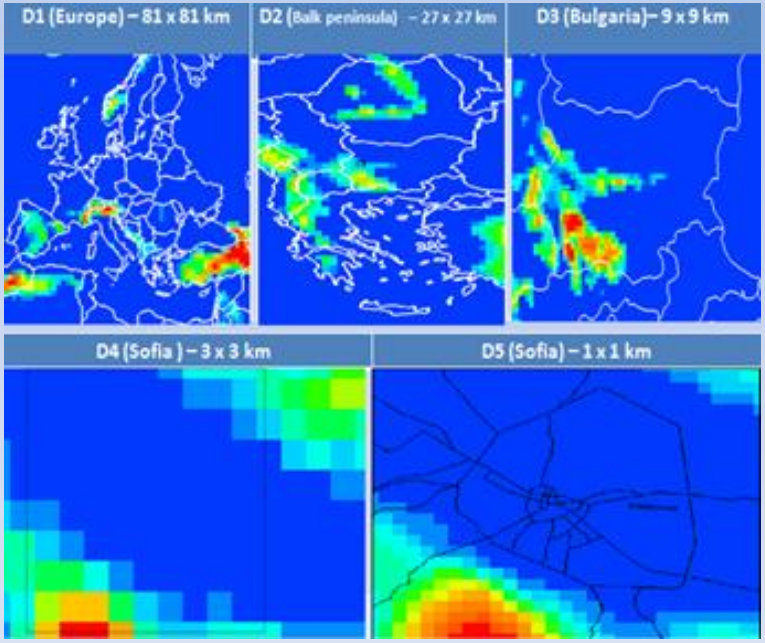
Collaboration: IICT-BAS, AMET Ltd. and German partner

Global Climate Changes and Quality of Life

Atmospheric composition - impact on the quality of life and human health in Sofia:

- WRF and CMAQ nesting capabilities are applied for downscaling the simulations to a 1 km x 1 km resolution in space for the innermost domain.
- The simulations is performed day by day for a period of 7 years (2008-2014).
- The surface concentrations are calculated for the four seasons and annually by averaging the typical fields.



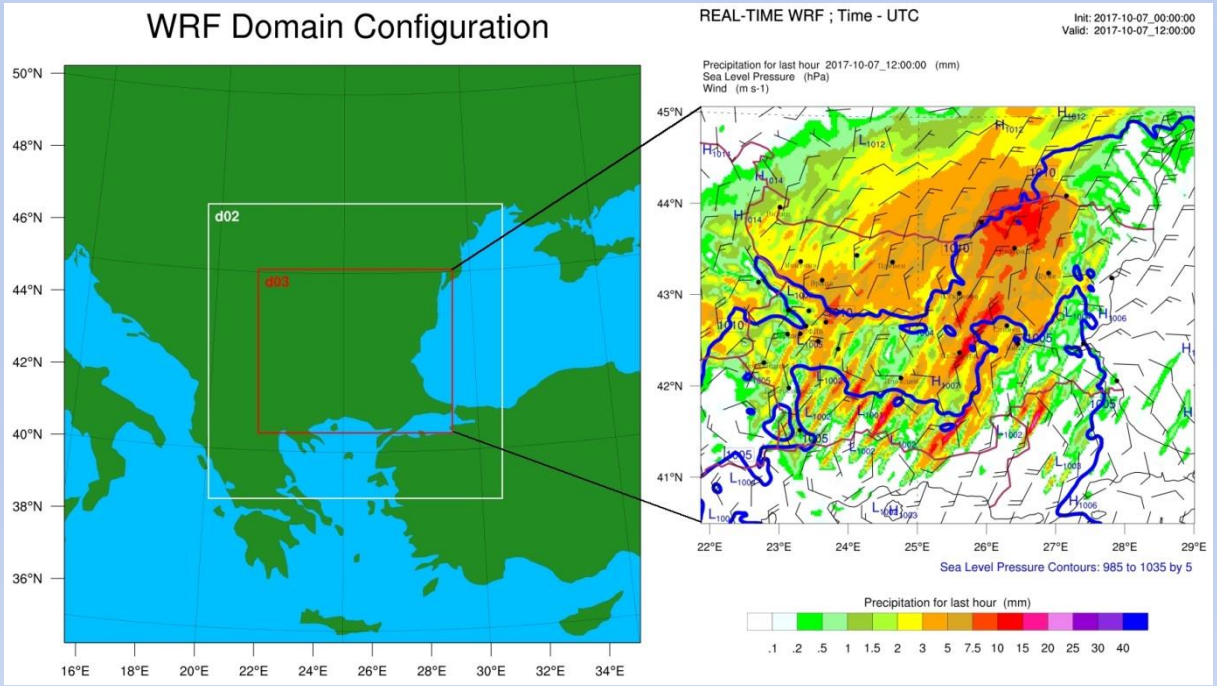


Collaboration: NIGGG-BAS and IICT-BAS

Supercomputing in Weather Forecast Research

Locally Refined Weather Forecast and Environmental Applications:

- The WRF recursive parched refinement is applied for downscaling the simulations targeted at 400 m x 400 m resolution in space.



- "Every day NIMH will make predictions about the expected dusting of the capital.
- **Without Avitohol the calculations will take 2 years.** "
  Prof.Branzov, director of the National Institute of Meteorology and Hydrology (NIMH),

"Trud", 16.02.2017

Collaboration: NIMH-BAS and IICT-BAS

Digital Transformations of the Society

The challenges faced by scientists in today's digital society and their role and responsibilities for building, developing and widest implementation into the practice of innovative digital technologies and skills include:

- Building up and development of **open access e-science infrastructures**, including critical research capacity for digital transition in all areas of the economy and society.
- Developing a scientific methodology and innovative capacity in order to efficiently realize the cycle **modeling, simulation, optimization in the conditions of the contemporary digital society.**
- Developing **a platform for open science and open access to research results** created with public funding.
- Developing a platform for **open educational resources** to ensure that publicly funded materials are available to all and that training can be done at any time and in any place.
- Work on **attracting private investment to support digital transformations** and for research and innovation in priority areas of ICT.

Thank you for your Attention!

- **„There is nothing more useful for the practice than the good theory.“**

  Kurt Lewin

  (1890-1947)

- **„In theory, the theory and practice are one and the same. However, in practice they are not.“**

  Albert Einstein

  (1879-1955)