High Performance Computing infrastructure
The POWIEW Project

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POWIEW

HPC Infrastructure for Grand Challenges of Science and Engineering

http://wielkiewyzwania.pl

HPC: new computational architectures
new-scale research

POWIEW Consortium:

- Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw (**ICM**)
- Poznań Supercomputing and Networking Center, Institute of Bioorganic Chemistry PAS (**PSNC**)
- Academic Computer Centre CYFRONET, AGH University of Science and Technology, Krakow (**CYFRONET**)

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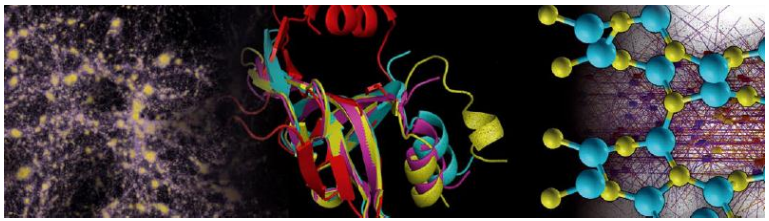
Large scale scientific computing projects:

- Numerical Weather Prediction
- Semiconductor modelling
- Modelling and Visualization of RNA Structures
- Neuroinformatics Simulations
- Modelling of the Structure of the Universe
- Molecular Modelling
- Reservoir Modelling
- Astrophysics and Radio Astronomy
- Visual Analysis



Main computing architectures:

- MPP systems – IBM BlueGene/P
- Fat Node systems – IBM POWER7 IH
- SMP systems – HP Blade Center Versatile SMP (vSMP)
- GPU-based hybrid systems – HP SL390s nVidia Fermi

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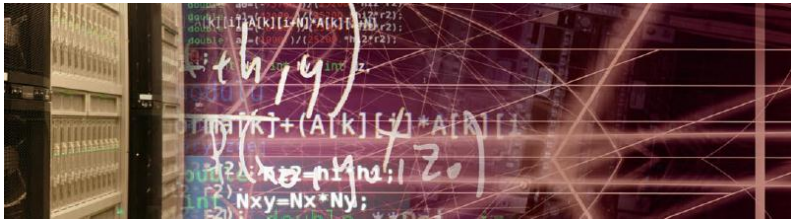
New computational models

new algorithms and computational models for future HPC systems



Competence

synergy of research

& new developments in HPC programming

Training

new programming techniques and tools,

novel HPC paradigms

New HPC strategy for academia in Poland

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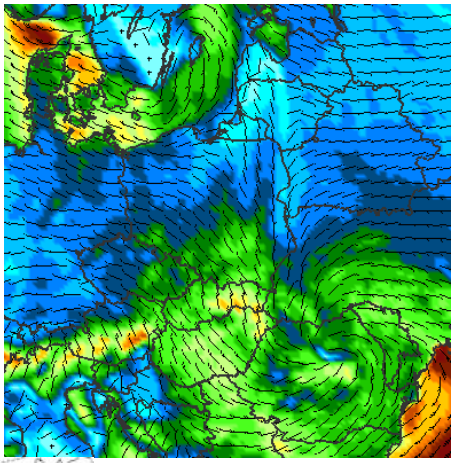
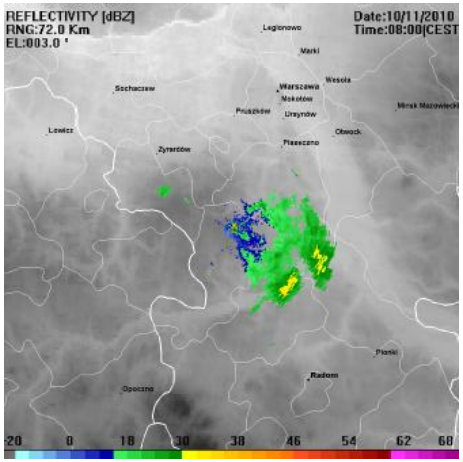
Main research areas: an overview

- New insights
- New scales of resolution
- New temporal ranges

New scales of resolution in numerical weather prediction

- NWP (http://meteo.pl):
  - Down to 1 km horizontal resolution on mesoscale
  - New concepts in ensemble modelling

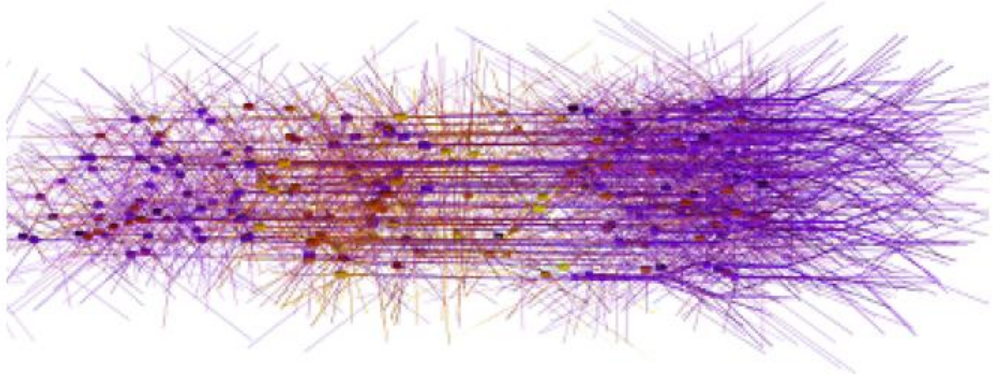




Neurocomputing

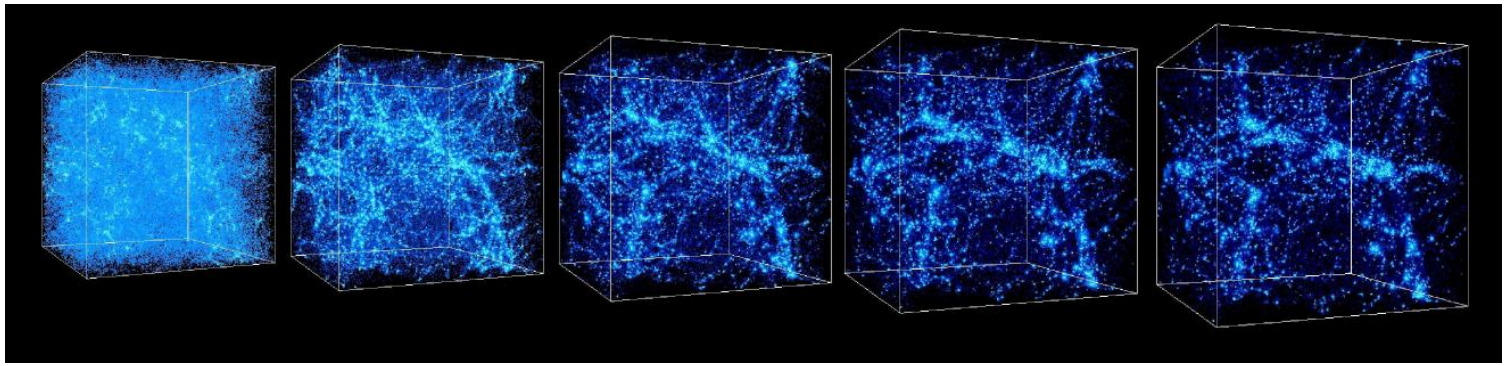
- **Modelling of Local Field Potentials (LFP)**

- **Analysis of dynamics of thalamic activation**
  in stimulation of somato-sensory pathway in anesthetized rat and activity in the barrel cortex in behaving rats



Modelling of the Structure of the Universe

- Large scale simulations with N-body codes (Gadget3, GotPM)
- **Warsaw Universe Simulation**, 2048^3 particles
- MPP-based results analysis:
  - Statistical methods
  - Topological classification
  - Geometrical classification
  - Delaunay Tesselation, Alpha-shapes and Beti numbers



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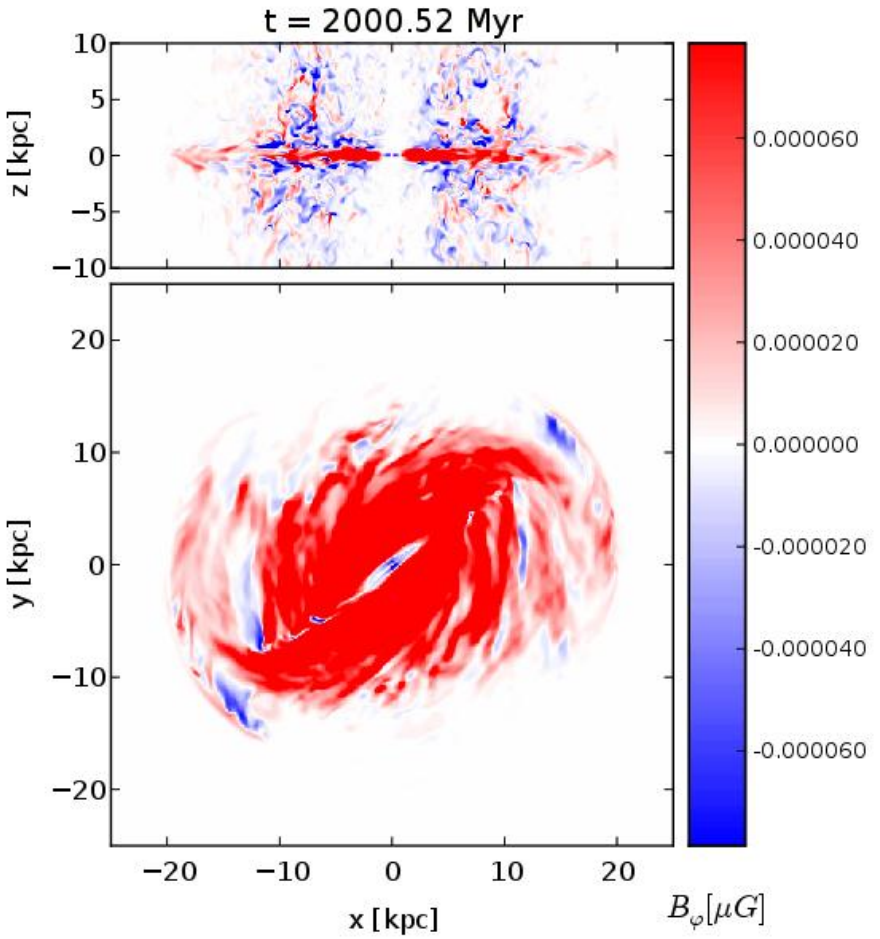
Large-scale numerical simulations of astrophysical structures formation

- Planet formation processes in protoplanetary discs
- Dust coagulation processes assisted by gravitational interactions
- Gravitational instability and formation processes of molecular clouds and stars in magnetized multiphase interstellar media
- Generation of magnetic fields in spiral galaxies evolving from a dynamo process, driven by cosmic rays



Astrophysics

- Development of new parallel, reconfigurable and hybrid (software & hardware) solutions for specific simulations and computational models

- *Simulation of N-body problems* codes

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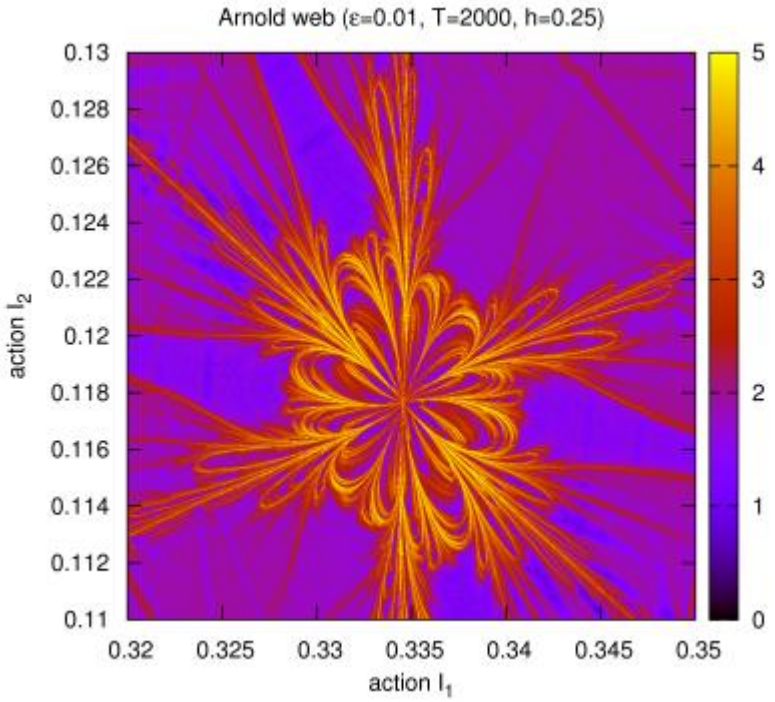
Analysis of the observations and the global dynamics of extrasolar planetary systems

- Analysis of global dynamics and stability of extrasolar planetary systems
- Dynamic analysis of multiple planetary systems observations
- Simulations of terrestrial planets formation and their orbital evolution

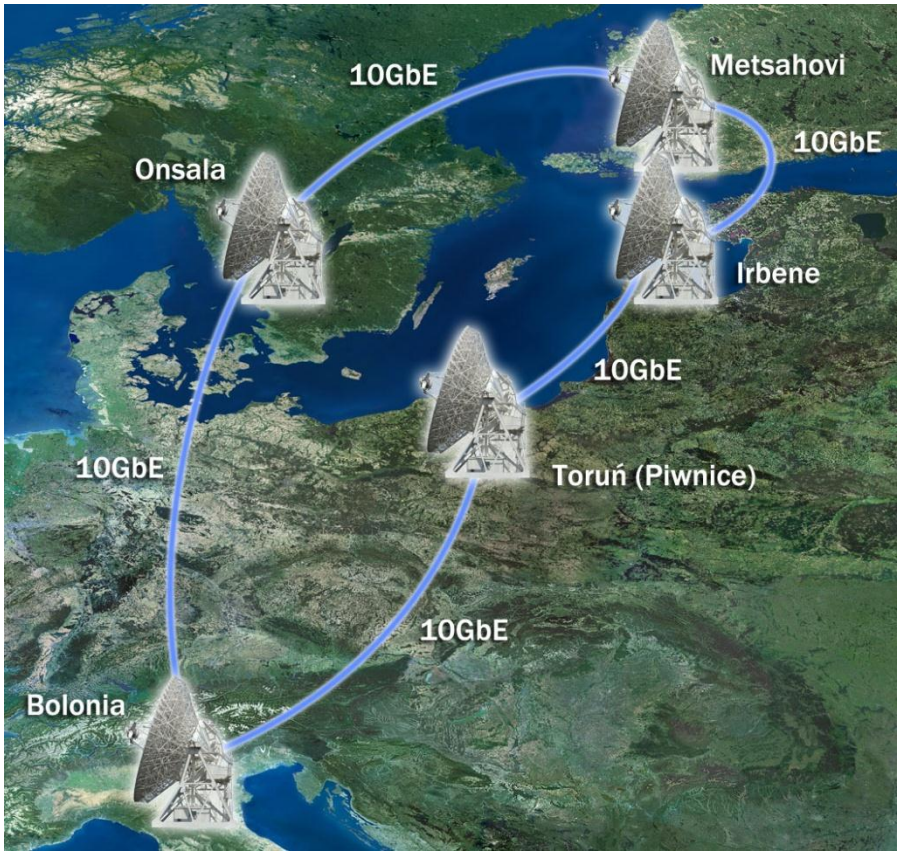


Shape of the Universe

- Analysis of cosmic background maps
- Planning strategy for analyzing sky maps (generated by Planck Surveyor telescope)

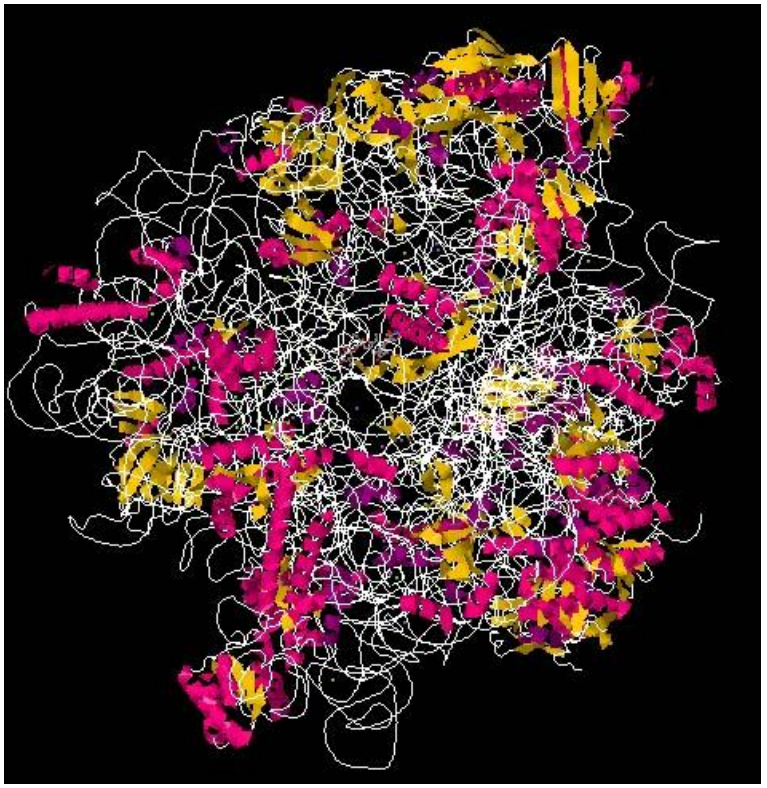
Baltic e-VLBI interferometer

- Environmental initiative of common research in radioastronomy
- Software correlation using PSNC hardware resources
- Cooperation of the astronomy centers: Toruń (Piwnice) - Poland, Onsala - Sweden, Irbene - Latvia, Metsahovi Finland and Bologna – Italy
- Quasi realtime correlation using virtual 10 Gb Eth network



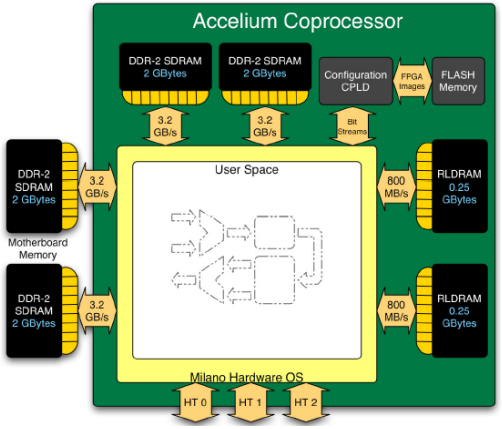
High-throughput modelling of functionally and therapeutically relevant spatial RNA structures

- Modelling of spatial RNA structures
- Design of new therapeutic targets aimed at the RNA
- Validation of RNAComposer software for fully automated spatial RNA models generation from structural fragments



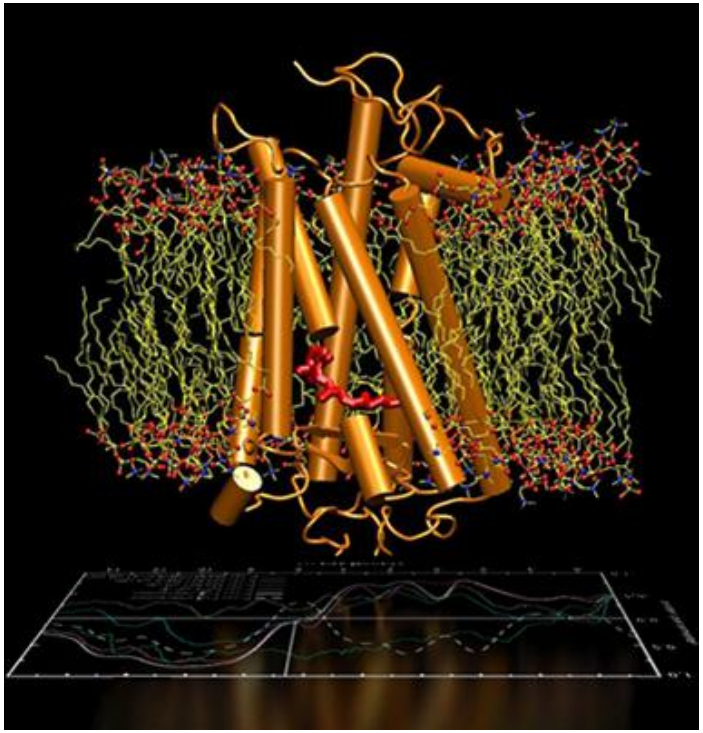
Quantum Chemistry and Molecular Dynamics

- **Applications of FPGA-based systems:**
  - Quantum Chemistry simulations
  - Molecular Dynamics simulations



Molecular Dynamics

- Hardware acceleration of GROMACS and NAMD code
- Design of Fourier coprocessor, based on the FPGA devices
- New programming/designing technique based on the Impulse C language



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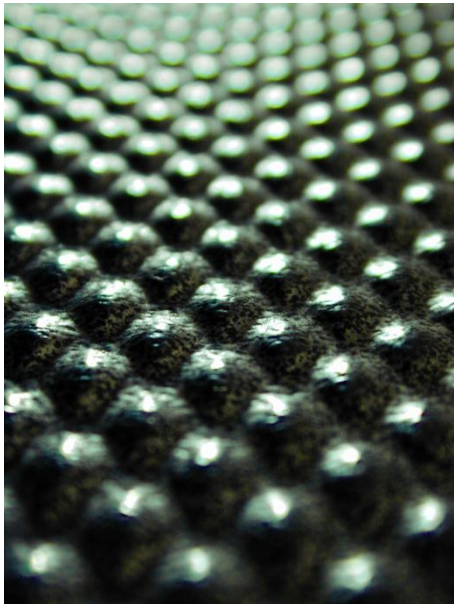
Semiconductor modelling

- Crystal Growth Modelling
- Development of new DFT software for specific computational models (parallel, many-core)
- **RSchr** – C++ & MPI Finite Element B-spline solver of one-electron Schroedinger equation with arbitrary potential



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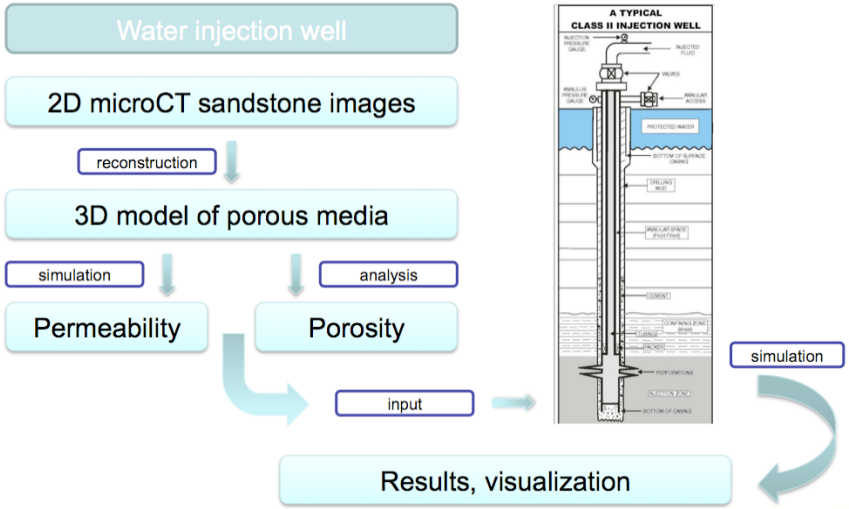
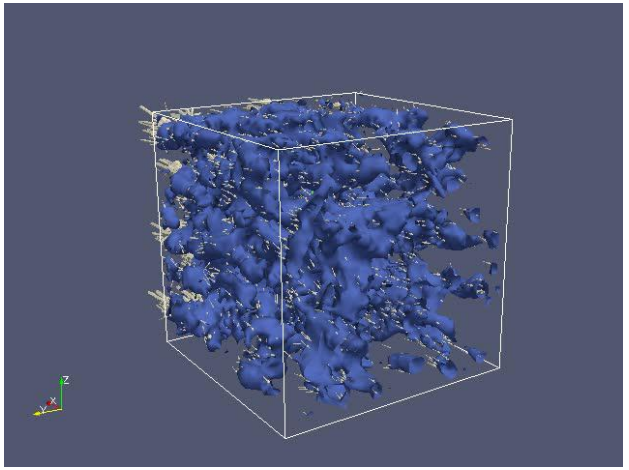
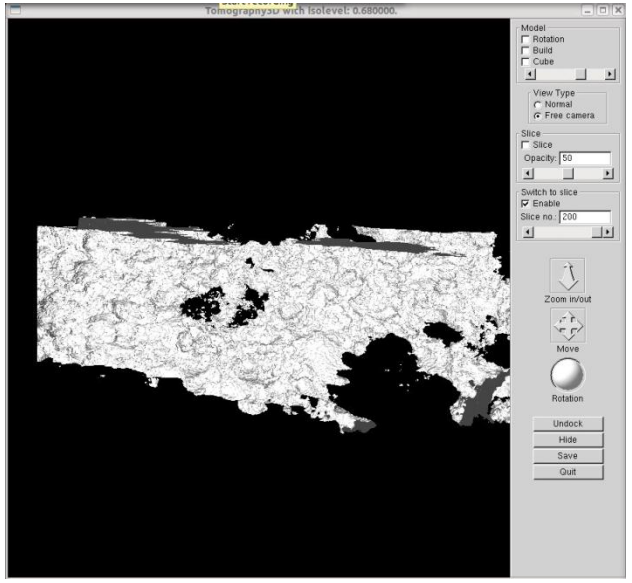
Integrated reservoir simulations on GPU-based systems

USE CASE







3D model	GPU-cluster-ready	Support for MPI-IO
	Real-time visualization	Model ready in just few secons
Porosity	GPU-cluster-ready	Real-time visualization
Permeability	Lattice Boltzmann approach	Scales well up to thousands of cores
	Cluster-ready	Support for MPI-IO

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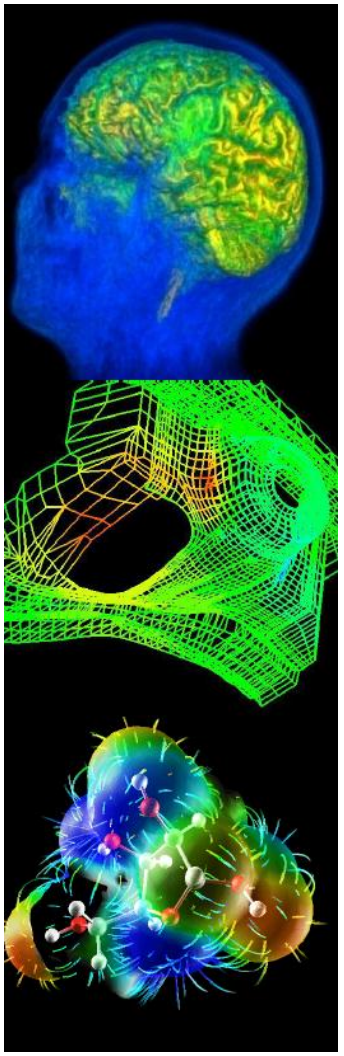
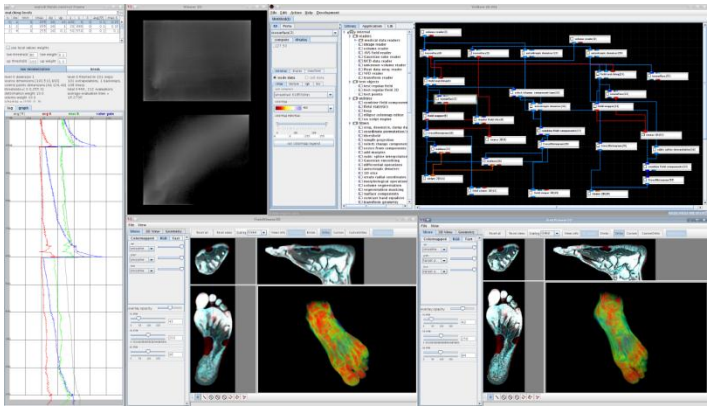
Visual Computing and Data Analysis

- **New solutions: VisNow** Visual Analysis Software – http://visnow.icm.edu.pl
- Distributed Visualization Engine (MPP,SMP, GPGPU)
- In situ Visualization
- **Visualization of simulation results**
  - Cosmology
  - Turbulent flows
  - Neurobiology
  - Biomedicine





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Outlook

- Collaborative plans
- New national allocation concepts
- Synchronised key infrastructure investments
- Open software repository
- Joint training actions
- At the way towards petascale for Polish academic community

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