European Territorial Cooperation Progamme
Greece - Bulgaria 2007 - 2013

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Project ICoSCIS:
Interregional Cooperation at Scientific Computing in Interdisciplinary Science

European Territorial Cooperation Programme
Greece-Bulgaria 2007-2013
INVESTING IN OUR FUTURE

HPC and GRID at South-West University "Neofit Rilski" - challenges and perspectives for the future

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Presentation of the research interests of SWU Blagoevgrad, BULGARIA

SWU Grid cluster - ICOSCIS project

- Compute Node - Blade (4 number)

  - IBM Flex System x440 Compute Node,

  Intel Xeon 8C Processor Model E5-4620 95W **2.2GHz/1333MHz/16MB**

  8GB (1x8GB, 2Rx4, 1.35V) PC3L-10600 CL9 ECC DDR3 1333MHz LP RDIMM

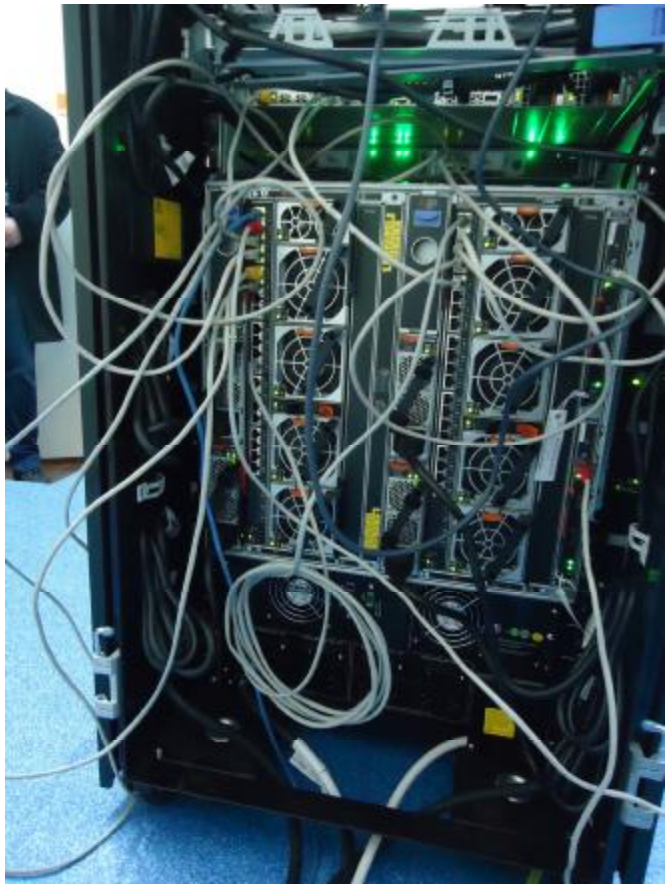
  IBM 300GB 2.5in SFF 10K 6Gbps HS SAS HDD

- Storage

  IBM Storwize V3700 LFF Dual Control Enclosure

  3TB 3.5In 7200 rpm 6Gb SAS NL HDD

SWU Grid cluster



HPC

- **HPC:** any computational technique that solves a large problem faster than possible using single, commodity systems
  - Custom-designed, high-performance processors
  - Parallel computing
  - Distributed computing
  - Grid computing
- **Parallel computing:** single systems with many processors working on the same problem
- **Data parallelism:** each processor performs the same task on different sets or sub-regions of data
- **Task parallelism:** each processor performs a different task

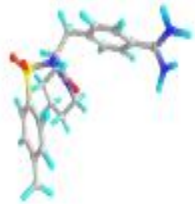
Parallel Programming Models

- The primary programming models in current use are
  - **Data parallelism -** operations are performed in parallel on collections of data structures. A generalization of array operations.
  - **Message passing -** processes possess local memory and communicate with other processes by sending and receiving messages.
  - **Shared memory -** each processor has access to a single shared pool of memory

- Most parallelization efforts fall under the following categories.
  - Codes can be parallelized using message-passing libraries such as **MPI**.
  - Codes can be parallelized using compiler directives such as **OpenMP**.

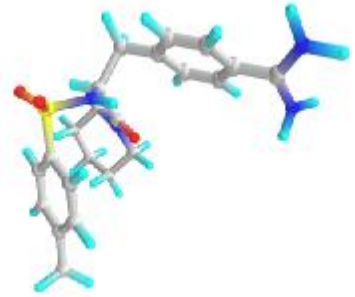
Bioinformatics - docking of protein-ligand complexes

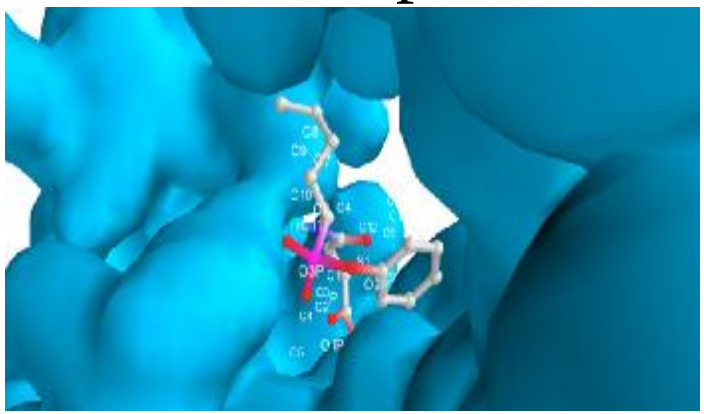
- The binding of **small molecule ligands** to **large protein targets** is central to numerous biological processes.
- The accurate prediction of the binding modes between the ligand and protein (the docking problem) is of fundamental importance in modern structure-based **drug design**.



What is Docking?

- Docking is a **computer simulation procedure to predict the conformation of a receptor-ligand complex**, where the receptor is usually a protein or a nucleic acid molecule (DNA or RNA) and the ligand is either a small molecule or another protein.
- Docking also be defined as a simulation process where a ligand position is estimated in a predicted or pre-defined binding site.





Drug design

- The interactions between the receptor and ligand are **quantum mechanical in nature**, but due to the complexity of biological systems, quantum theory cannot be applied directly.
- Consequently, most methods used in docking and computational drug discovery are more empirical in nature and usually lack generality.
- Quantum mechanical phenomena, such as the formation of a covalent bond between the protein and the ligand upon binding during the transition state of the reaction, cannot be predicted and/or evaluated using these empirical methods.

High-Performance and Parallel Computing with R

R is an integrated suite of software facilities for data manipulation, calculation and graphical display. Among other things it has

- an effective data handling and storage facility,
- a suite of operators for calculations on arrays, in particular matrices,
- a large, coherent, integrated collection of intermediate tools for data analysis, graphical facilities for data analysis and display either directly at the computer or on hardcopy, and
- a well developed, simple and effective programming language (called ‘R’) which includes conditionals, loops, user defined recursive functions and input and output facilities.

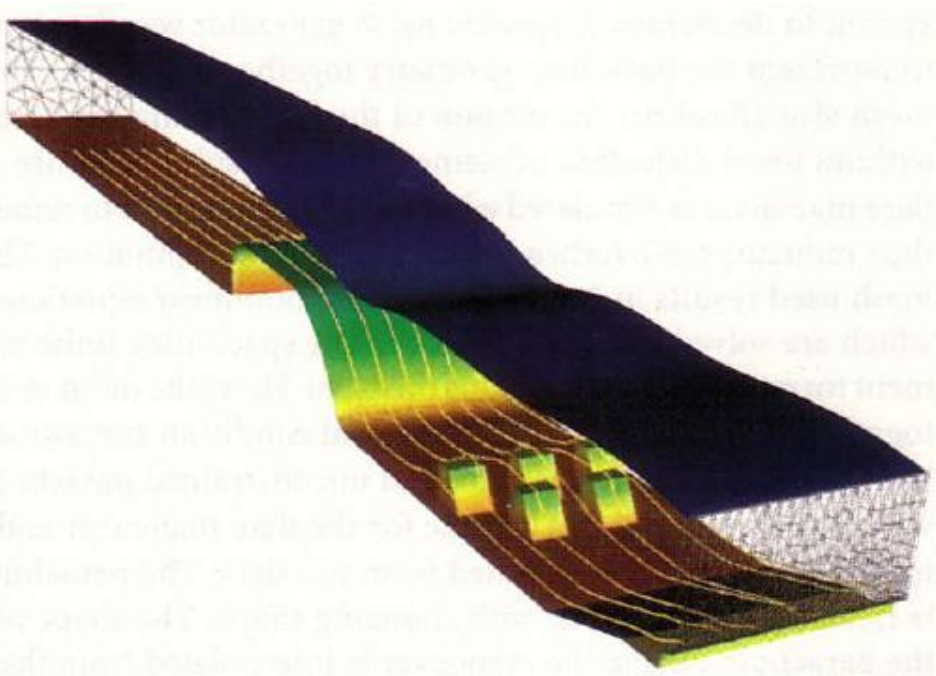
Flow simulation and High Performance Computing

- Flow simulation is a computational tool for exploring science and technology involving flow applications.
- It can provide cost-effective alternatives or complements to laboratory experiments, field tests and prototyping

Flow simulation and High Performance Computing

- Turbulence model - Most computational grids which are in practical use today are not able to resolve the flow features well enough to fully capture turbulence effects. Acknowledging this restriction, significant effort is spent in the computational community to devise and improve turbulence modeling
- Stabilized finite element formulations
- 3D mesh generation for complex geometries
- Iterative solution strategies for large, coupled, nonlinear equation system

Flow simulation and High Performance Computing

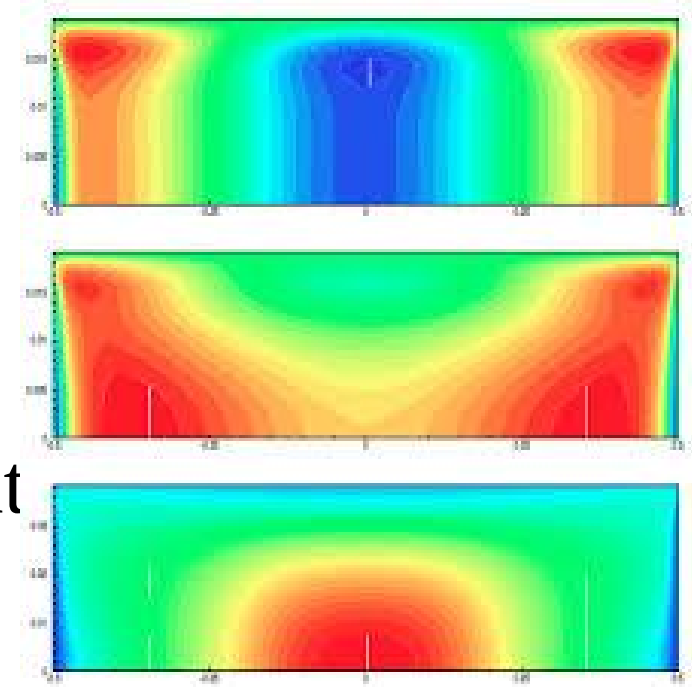


Network Traffic Analysis

- Traffic analysis should be conducted not only up to Layer 2 (SNMP – the number of bytes transferred, or the number of packets transferred at the level of the device interface), but also on Layer 3 (Network layer) and Layer 4 (Transport layer) of OSI model.
- There are a number of tools that can be used for traffic analysis. They are divided into those that require specialised hardware and those that are based on software solutions that are not dependent on the hardware.
- The solutions that rely on hardware are rather expensive, but also significantly faster because they have hardware support. Most often, they are placed in the network so that they are transparent to the rest of the network.

Heat processes

- Multiscale simulations
- Convective heat transfer
- Single phase/multiphase flows and heat transfer
- Micro-/nano flows and heat transfer



High Performance Computing for Weather Prediction

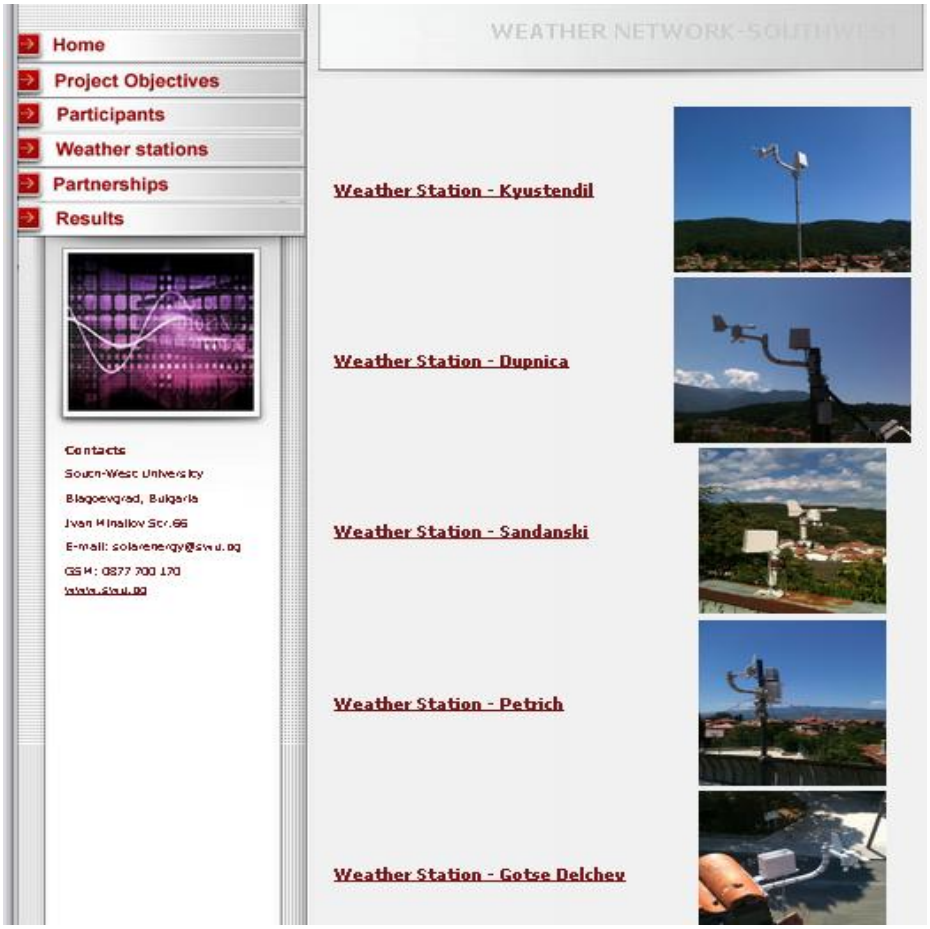
- Medium Range Weather Prediction has great impact on agriculture, disaster management and mitigation purposes
- The partial differential equations governing the dynamics of the atmospheric flow are non-linear in nature. Hence, they need to be solved numerically with very good accuracy.
- For a global weather forecast model of reasonable resolution, huge computation power is needed to provide the forecast well in time.

High Performance Computing for Weather Prediction

Meteorological information obtained in real-time (on-line) by the weather network in six cities in Southwestern Bulgaria:

- Kyustendil
- Dupnitsa
- Sandanski
- Petrich,
- Razlog
- Gotse Delchev

http://solarenergy.swu.bg



High Performance Computing in Finance

- In SWU has a laboratory for econometric study. It was created jointly between faculty of Mathematics and natural Science and Faculty of Economics. Professors from both faculties work on real-world problems of the finance.
- Some of them are:

  - Analysis of the capital adequacy of banks - using the theory of games, “game with nature” and Monte Carlo simulations;

  - Predict the movement of stock indexes - chaos theory and queuing theory;

  - Analysis of financial risk in commercial banks - stochastic models, large optimization mathematical models.

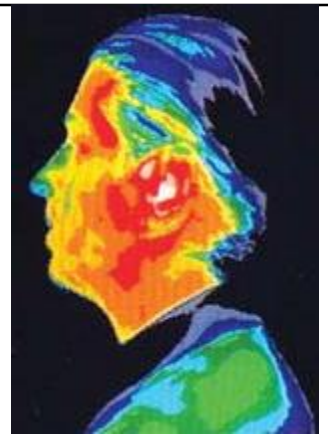
Image Processing

- Why HPC for Image Processing?
  - Image processing algorithms are increasingly sophisticated;
  - Increase in computational complexity, which makes response times inappropriate and algorithms unusable in real applications;
  - The inherent parallelism in image processing and computer vision suggests that high performance computing (HPC) should be readily applicable, and historically image processing and computer vision have been the most common areas proposed for the use of HPC.

- High Performance Computing in 3D Image Processing
  3D Segmentation of the Brain
  3D Tumor Segmentation
  3D Mammography Reconstruction

Impact of electromagnetic waves on humans

- The technologies we use today, from our everyday appliances, cell phones, even our cars, emit electromagnetic radiation & EM radiation that can penetrate and affect us, seriously compromising our health and disturbing our environments.



- For years, scientists have conducted research linking EM radiation to serious diseases like cancer, Alzheimer's, Parkinson's and others.

ICOSCIS team of SWU

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- Prof. Ivan Mirchev
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- Asoc. Prof. Ivan Trenchev
- Assist. Prof. Anton Stoilov
- Assist. Prof. Radoslav Mavrevski
- Assist. Prof. Ivan Todorin