Supercomputer and grid infrastructure in Poland

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Outline of the talk:

• presentation of the Polish High Performance Computer centres, and the Grid they are forming.

• presentation of the Warsaw HPC centre: ICM University of Warsaw

• overview of the services, competences and projects led by, and provided at ICM UW

• summary of the neuroinformatics activities facilitated by the resources of HPC centres
Five HPC centres in Poland

- were founded 22 years ago,
- they are independent, although closely collaborating entities,
- theirs mission is to provide free access to the HPC resources for entire academic community in Poland
- since a couple of years part of the resources are accessible via web based grid services: PLGrid
- research and education is also carried out in the HPC units.
Polish Grid Infrastructure PLGrid

- computational resources: 576 TFLOPs; 41 248 cores
- memory: 113,26 TB RAM
- storage: 5,58 PB
- cores: Intel Xeon, AMD Opteron, GPU Nvidia TESLA

Advanced Service Platforms

Grid infrastructure (Grid services) PL-Grid
- Clusters
- High Performance Computers
- Data repositories

National Computer Network PIONIER
Applications

- quantum chemistry
  Gaussian, Dalton, Turbomole, ...
- life sciences
  Amber, Namd, Charmm, AutoDock, Neuron
- material sciences
  VASP, Medea, ...
- physics and engineering
  Abaqus, OpenFOAM, Mede, ...
- general purpose
  R, Matlab, Mathematica, Nmag, Python ...
- user owns codes
Access, grants, webService

- PLGrid resources are granted for free, disclosing the acknowledgement in scientific papers.
- There is no direct access to the computers. Job submission, monitoring and output retrieving process is carried out by the WebPortal www.plgrid.pl
Interdisciplinary Centre for Mathematical and Computational Modelling
University of Warsaw

- One of the HPC centres in Poland

- computational and storage infrastructure
- research projects based at ICM:
  - Meteo - numerical weather forecast
  - VisNow - general purpose visualisation package;
  - CeON - Centre for Open Science
  - many others

- computational and algorithmic support for external projects: Cosmology, Nuclear Physics, Fluid Dynamics …

- OCEAN - large infrastructural and research project on Big Data science.
An example: *Nostromo* – IBM Blue Gene/Q

Architecture: IBM Blue Gene/Q
Number of cores: 16384
Memory: 16 TB
CPU: PowerPC A2 @ 1.6GHz
Interconnect: 5D Torus
Binary format: big-endian
Cores per node: 16 cores (64 threads)
Memory per node: 16 GB
Storage: GPFS
OS: BG/Q Linux
Batch system: Slurm

Installation of the **Neuron** software. Large simulations are carried out.
Selected project based at ICM UW

Numerical weather forecast.
• Based on the Unified Model – 60h forecast
• Computations are carried out 4 time a day
• Computational engine: BlueGene/Q (IBM Power7)
Selected project based at ICM UW

Visualisation software

- **VisNow**, is a comprehensive visualisation software developed entirely at ICM UW
- It is a general purpose, workflow based, modular environment for both:
  - data visualisation
  - visual data analysis
- It is an OpenSource project
- Written in Java, with intuitive GUI
VisNow

- Sample Applications
  - Solid State Physics
  - Fluid dynamics
  - Molecular Mechanics ekularna
  - Cosmology
  - Medical Science
  - Neuroscience

- Functionality
  - Direct Access to selected DBasis.
  - **Data transformations** (e.g., denoising, reduction, segmentation, sections, ...)
  - Data mapping
  - Presentation
Computational and algorithmic support for external projects:

**Cosmology**
- Evolution of the Universe

**Epidemiology**
- Agent Based Modelling of the Influenza Disease spread across Poland
Computational and algorithmic support for external projects:

Biomolecular modelling

- Modelling of spatial RNA structures
- Design of new therapeutic targets aimed at the RNA
OCEAN: the forth paradigm of science.

- OCEAN is a infrastructural and research project totally devoted to big data issue
- The new Big Data centre (building and machines) is currently under construction.
- OCEAN will be also a centre of Big Data research and expertise:
  - data collection and storage
  - data curation
  - advanced data analysis

Science development stages (by Jim Gray):
Paradigms:
1st. Empirical facts
2nd. Theoretical approaches
3rd. Computer simulations
4th. Data Science
Computational neuroscience projects:

- C. Elegans locomotion: command neuron circuit simulations

\[
\frac{dAVB}{dt} = -AVB + \varepsilon_{ASH} \omega_{AVB,ASH} H(ASH) + \varepsilon_{PVC} \omega_{AVB,PVC} H(PVC) + \\
\varepsilon_{AVB}^2 \varepsilon_{DVA}^2 g_{AVB,DVA} (DVA - AVB) + \varepsilon_{AVB}^2 \varepsilon_{DVA}^2 g_{AVB,F} (E_f - AVB) + X_{AVB}
\]

- EEG based Alzheimer disease biomarkers

- Cognitive system simulations - emergence of linguistic categories
Thank You!