High Performance Scientific Computing Requirements and Resources

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OVERVIEW

- PURPOSES
- OVERVIEW ON SUPERCOMPUTING
- EUROPEAN/REGIONAL HPC INFRASTRUCTURE
- ROMANIAN RESEARCH VISIBILITY AT INTERNATIONAL LEVEL
- NATIONAL HPC INFRASTRUCTURE
- HPC NEEDS FOR RESEARCH
- LONG-TERM PROSPECTS
- CONCLUSIONS: DISCUSSIONS

PURPOSES OF THE MEETING

- ❑ Initiate a dialogue between the participants to the various HPC activities (users & developers from different disciplines, IT professionals, funding agencies, etc.)
- ❑ Initiate a survey on the existing HPC resources and the needs of HPC for the scientific research
- ❑ First steps towards an estimation of the HPC resources which will be necessary for research on a longer term

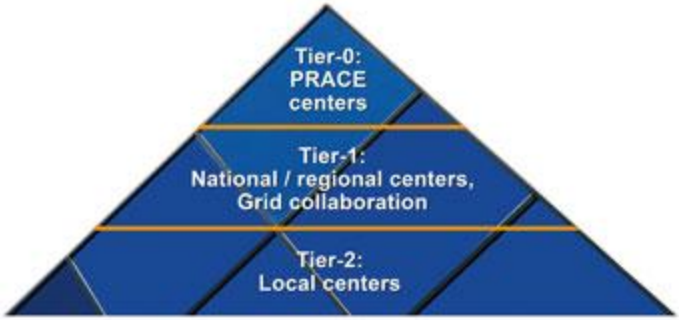
OVERVIEW ON SUPERCOMPUTING

Tianhe-1A-NUDT, NVIDIA GPU
Jaguar-Cray, Opteron 6 core
Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla
TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C, Nvidia
Hopper - Cray XE6 12-core
Tera-100 - Bull
Roadrunner-BladeCenter, PowerXCell 8i / Opteron
Kraken XT5 - Cray, Opteron 6-c
JUGENE - Blue Gene/P
Cielo - Cray XE6 8-core

(Top500, November 2010)

EUROPEAN HPC INFRASTRUCTURE

PRACE = Partnership for Advanced Computing in Europe
pan-European Research Infrastructure for HPC
Up to 6 Tier-0 centers (PetaFlops)



JUGENE (1 PFlops) ->
Juelich, DE

CURIE (1,6 PFlops) ->
CEA, FR

20 members: Austria, Bulgaria, Cyprus, Czech Rep, Finland, France, Germany, Greece, Ireland, Italy, The Netherlands, Norway, Poland, Portugal, Serbia, Spain, Sweden, Switzerland, Turkey, UK.

All partners contribute in cash or in-kind to the management of the resource infrastructure and the delivery of services.

REGIONAL HPC INFRASTRUCTURE AND HP-SEE

Bulgaria: - IBM Blue Gene/P (Min. Trans. ITC), 8192 cores, 23.42 TFlops

Upgrade hard 2011-2018: > 1 MEur/year. Software, operation.

- HPC Grid Cluster (IICT-BAS), 576 procs, 3 TFlops.

Serbia: - PARADOX (Inst. Phys. Belgrade-IPB), 672 procs, 5.25 TFlops

IPB in PRACE since 2008, will host Blue Danube National Supercomputing Facility. 10 MEur in 7 years.

Similar developments in Greece (10 MEur) and Hungary.

FP7 **HP-SEE project** (*High-Performance Computing Infrastructure for South East Europe's Research Communities*), 2010-2012

Coordinated by GRNET - Greece; 13 partners in SEE and Caucasus region.

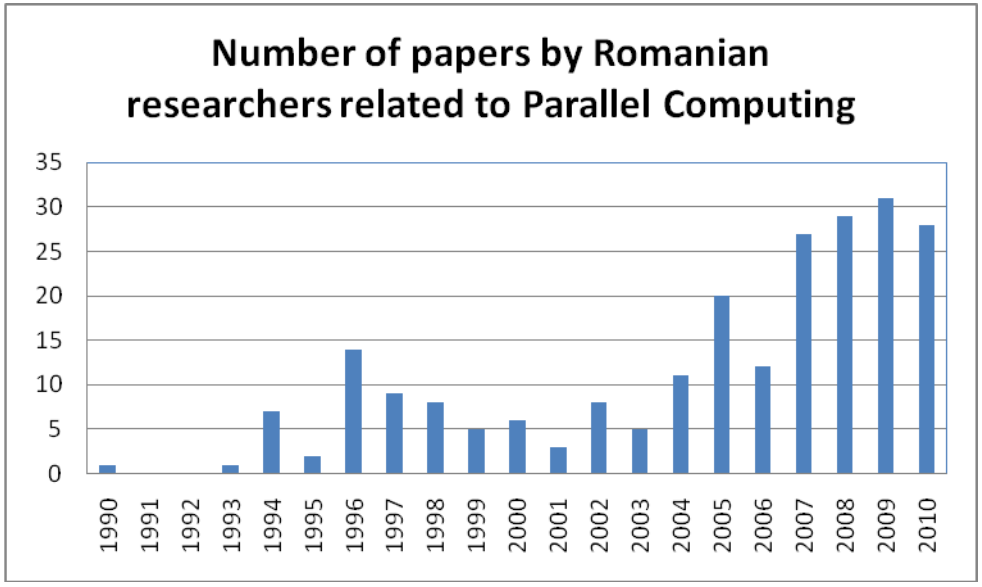
Objectives:

- link existing and upcoming HPC facilities in the region in a common infrastructure, and provide operational solutions for it
- open the HPC infrastructure to new user communities in comp. Chemistry, Physics, Life Sci.
- act as a SEE bridge for PRACE

ROMANIAN RESEARCH VISIBILITY - 1

Source: SCOPUS database, http://www.scopus.com/ (courtesy of D. Zaharie, UVT)

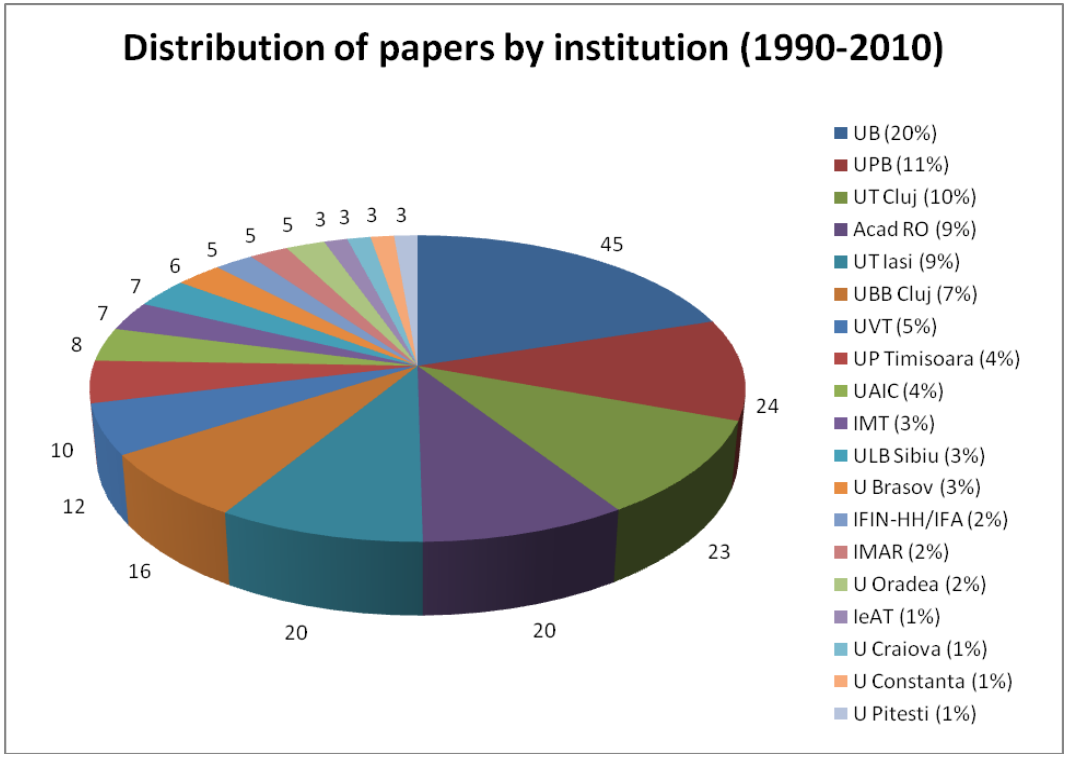
TITLE-ABS-KEY("parallel computing" OR "parallel algorithm" OR "parallel implementation" OR "parallel program" OR "parallel architecture")AND AFFILCOUNTRY(Romania)



Total: 228 records, 860 citations.

ROMANIAN RESEARCH VISIBILITY - 2

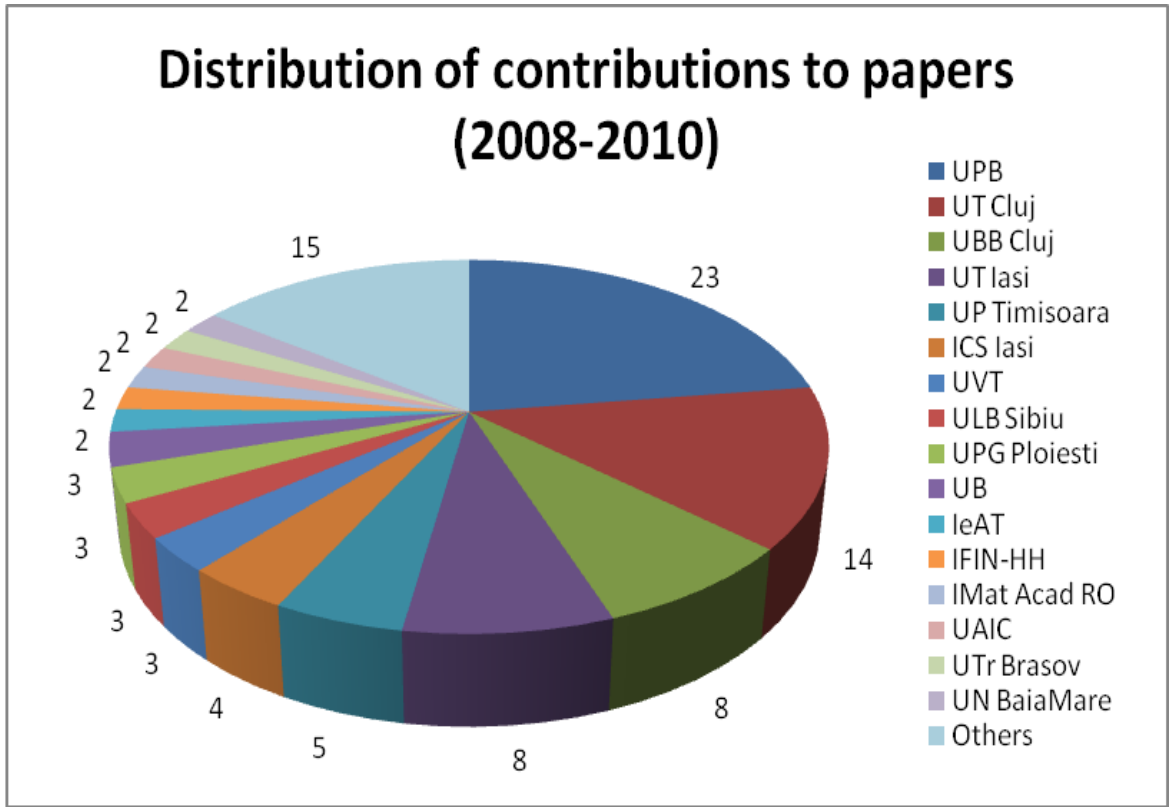
Distribution of papers according to the institution to which the authors are affiliated



Only the contributions >1% are represented above (225 papers).

ROMANIAN RESEARCH VISIBILITY - 3

101 institutional contributions to papers published between **2008-2010**



NATIONAL SUPERCOMPUTING CENTRE

August 2009: "*MCSI pregateste, impreuna cu IBM, un proiect de mare importanta strategica pentru mediul universitar, de cercetare si privat din Romania, tinta principala fiind punerea la dispozitia tuturor potentialilor beneficiari a unui instrument extrem de puternic de calcul (Supercomputing).*"

November 2009: HG - National Center for Supercomputing (established in spring 2010)

December 2009: First bid for purchasing HPC equipment (1,6 MEur)

January 2011: MCSI is looking for (new) ways of using the purchased equipment (112 blades = 896 cores)

February 2011: ANCS initiates a survey about the need for HPC resources in the scientific community

Further upgrades are possible

NATIONAL HPC INFRASTRUCTURE - 1

CONSORTIUM FOR HPC AND SUPERCOMPUTING

Open collaborative entity (JRU), established in October 2009 by the signing of a MoU* by: IFIN-HH, ISS, UPB, UVT, recognized by the authorities (**MoU privind Dezvoltarea Infrastructurii Nationale de Calcul de Inalta Performanta si Supercomputing*).

Participation to the FP7 HP-SEE project, since 2010

MAJOR HPC RESOURCES

Name	Institution	Cores	CPU type	Interconnect	TFlops(teo)
NCIT-Cluster	UPB	562	PowerXCell+Intel+AMD	Infiniband+GbEth.	3,4
RO-09-UTCN	UTCN	512	Intel	-	-
InfraGRID	UVT	499	Intel	Infiniband	2,5
IFIN_BC	IFIN-HH	368	PowerXCell8i+AMD	Infiniband	3,9
IFIN_Bio	IFIN-HH	256	Intel	Myrinet2000	2,72
Rospace	ISS	212	-	-	-
MDEO-Cluster	FF-UB	192			-

HPC NEEDS FOR RESEARCH - MAGURELE PLATFORM

IFIN-HH

- NUCLEAR PHYSICS
  - Transport phenomena in quark-gluon plasma, based on a Boltzmann or hydrodynamic approach [Descrierea in modele de transport relativiste a dinamicii plasmei de cuarci si gluoni la energii corespunzind experimentelor de la RHIC si potential de la LHC in ciocnirile cu ioni grei (Au si Pb) - colab. FF-UB, Univ Catania]
  - Multifragmentation of nuclei [Dinamica nucleara la energii intermediare (generarea unui numar mare de evenimente) - colab. FF-UB, CHIMERA - Catania si GSI]
- HIGH ENERGY PHYSICS
  Reconstructia evenimentelor obtinute folosind aranjamentele experimentale de la LHC, CERN si CBM - FAIR, Darmstadt
- NONLINEAR OPTICS
  Physics of Bose-Einstein condensates (collab. with IPB in HP-SEE)
- PHYSICS OF CONDENSED MATTER
  1) Modeling and simulation of granular flow (colab. Oslo, Strasbourg Universities)
  2) Phonon dynamics in complex media (slab, wire, bridge structures), with disorder, with application to the modeling of nano-detectors for electromagnetic radiation. Interaction with defects, charges and particles.
- MOLECULAR DYNAMICS SIMULATIONS
  Biophysics: protein-membrane interaction (colab. cu Fac. Biol. - UB)

HPC NEEDS FOR RESEARCH - MAGURELE PLATFORM

INFLPR

- Colectiv Modelarea matematica a plasmelor de fuziune

  - Modelarea numerica a plasmelor tokamak descriptibile prin modele MHD, in cadrul **Integrated Tokamak Modelling Task Force** (EFDA ITM-TF) – EURATOM Fuziune ; Modelele elaborate de grup si calculele se refera la instalatii tokamak reale: ASDEX_Upgrade si JET. Calcule pe BlueGene/P+clusteri de la Max Planck, GATEWAY - Italia. Trecerea 2D->3D va necesita resurse suplimentare de calcul par.
  - dezvoltate aplicatii ale caror date sunt stocate intr-o baza de date de mari dimensiuni, gazduita in sistemul paralel de fisiere al cluster-ului ITM GATEWAY.
  - prj. ITM AMNS (Atomic, Molecular, Nuclear and Surface Data): realizarea unei structuri de baze de date, ce urmeaza sa fie utilizata in coduri masiv paralele ce vor fi rulate intr-o prima faza pe ITM Gateway

- Programare CUDA pt. algoritmi de reconstructie tomografica (Tesla NVIDIA)

HPC NEEDS FOR RESEARCH - MAGURELE PLATFORM

ISS

1. Space missions: ISS HPC clusters process, analyse, interpret data gathered by:

Planck mission: image the anisotropies of the Cosmic Background Radiation Field

Cluster mission: Solar wind interaction with a magnetized Planet (Earth, Jupiter). Cluster is currently investigating the Earth's magnetic environment and its interaction with the solar wind in three dimensions

Venus Express: is a satellite optimised for studying the atmosphere of Venus, from the surface right up to the ionosphere.

2. Other collaborations

ANTARES Collaboration: data collected by a large area water Cherenkov detector in the deep Mediterranean Sea, optimised for the detection of muons from high-energy astrophysical neutrinos.

High Energy Physics

UrQMD Viewer with CUDA (GPU development, deploying and dissemination in the framework of the FP7 HP-SEE project

ALICE/LHC-CERN: jet detection in Pb-Pb interactions; grid data are locally processed on HPC cluster (see also GSI). Currently implementing the algorithms.

HPC NEEDS FOR RESEARCH - MAGURELE PLATFORM

INFP

The main direction related to HPC that has been developed in NIEP involved data acquisition, archiving and real-time processing. Recently, new interest has been shown for numerical simulation of earthquake generation process.
Many of the major research activities in geophysics and seismology require to considerably expand of the present computing capacity. Particularly promising areas for future research include simulations of earthquake processes, advanced modeling techniques for seismic wave propagation, and new methodologies for high-resolution images of the Earth's interior.
Examples of research challenging issues are:

- Earthquake rupture processes
- Computation of seismic wave propagation in complex media
- Strong motion response of sedimentary basins
- Geophysical inversion applications
- Data acquisition and archiving
- Seismic tomography
- Discrimination between earthquakes and nuclear explosions

HPC NEEDS FOR RESEARCH - MAGURELE PLATFORM

PHYSICS FACULTY - UB

Grupul de Fizica Nucleara Relativista (Prof. Al. Jipa**)**

- Investigarea formarii plasmei de cuarci si gluoni si a hadronizarii in ciocniri nucleu-nucleu si proton-proton la energii relativiste si ultrarelativiste
- Studiul parametrilor termodinamici pentru tranzitiile de faza care apar in ciocniri nucleare la energii ultrarelativiste. -> evolutia Universului
- mii de particule produse intr-o ciocnire nucleara la energii relativiste -> folosire coduri de simulare complexe (UrQMD, HIJING, AMPT) pentru descrierea mecanismelor de producere de particule si a comportarii acestora -> putere mare de calcul ~1Tflops

Dotari: cluster 1,7 Tflops, uzura fizica si morala

Materials and Devices for Electronics and Optoelectronics Research Center (Nemnes)

1) Stochastic simulations for interacting fermionic and bosonic systems, in the framework of fractional exclusion statistics (cu IFIN-HH); 2) mezoscopic systems, nanodevices modeling

HPC NEEDS FOR RESEARCH - 2

UTCN

Areas of expertise:

- •parallel algorithms and applications,
- •visualization, imaging, virtual reality,
- •multicore applications,
- •real-time systems.

Research examples:

- •image processing for automotive systems,
- •spatial data modeling and visualization,
- •Earth Science and environment-oriented applications development,
- •simulation of biological neural microcircuits,
- •simulations of fluid-structure interactions,
- •autonomous driving, cryptography,
- •structural mechanics and material sciences,
- •complex optimization for real-time applications

Expertise in parallel application area:

Development of parallel simulation software for CFD, MD, Neuroscience for classical and multicore HPC systems

Development of parallel applicative software for real time applications on NVIDIA multicore GPU: stereo reconstruction engine, optical flow engine, ego motion estimation, medical imaging

Computing on DEISA infrastructure (DEISA DECI 5, DEISA DECI 6 Projects)

HPC NEEDS FOR RESEARCH - 2

UPB

National Center for Information Technology (NCIT) (Prof. N. Tapus)

The Centre is dedicated to research, education and training in computer science and other areas.
Ensures a collaborative virtual environment using HPC resources and computer-supported cooperative work tools. Includes project development, training, consultancy, technology transfer, etc.
The mission of the Center is to promote advanced and inter-disciplinary research, to develop a new paradigm for intimate collaboration among computer scientists, computational scientists and researchers from a diversity of domains, to develop human resources by postgraduate educational programs (MSc, Ph.D., long-life learning) and a local "culture" in advanced Information Technology, and to offer local and remote access to a shared powerful computer infrastructure for the Romanian academic and industry communities.
Multiple international cooperation with similar centers, partnerships with IT companies and development of many national and international projects.
HPC resources: multiple development stages -> NCIT Cluster.
Contribution to HP-SEE: "EagleEye" application.

HPC NEEDS FOR RESEARCH - 2

Biology Faculty - UB (Prof. Dan Mihailescu)

Studiul computational al biomoleculelor: **modelarea** structurii si **simularea** functionarii

Simularea functionarii proteinelor: a) dinamica moleculara; b) analiza modurilor normale de vibratie

Aplicatii:

- Lipopolizaharidele bacteriene,
- Canalul epitelial de sodiu (ENaC),
- Structura proteinei GP120,
- Triptofan-hidroxilaza Ii umana: analiza modurilor normale de vibratie;
- Simularea spectrului THz al albuminei serice bovine (BSA): modificari conformationale.

Cluster de modelare:

1X (Switch 24Port Infiniband); 16X (cablu Infiniband 3M); 2X (UPS APC SURT8000RMXLI); 1X (1U 17 inch next generation LCD key drawer); 2X (cabinet 42HU800X1000); 16X Server Thruster (2X CPU Intel Quad Core Xeon X5450, 3GHz, 12 Mb Cache; DDRAM 64Gb KVR667D2D4F5; 3X HDD 146 Gb/15K SAS SEAGATE; 1X HCA MELLANOX INFINIHOST III Lx; 4X DDR HCA PCI-E X8; 1X DVDRW SLIM PIONEER); Sistem de operare: 16 X (RED HAT ENTERPRISE LINUX);

HPC NEEDS FOR RESEARCH - 2

UVT-1

Computing Science Centre (Prof. Dana Petcu) Excerpts:

The Centre intends to considerable expand in the near future its capacity, in order to become a HPC centre of Romania. It intends to install until Spring 2011 to its site a super-computer. This acquisition is scheduled in the frame of the EC Structural Funds project started in September 2010 by UVT to build an Institute for Environmental Research, project to which the Centre takes active part. The acquisition will lead to an improvement of the contributions to the FP7 HP-SEE project dealing with HPC in South Eastern Europe.
Multiple international cooperation with similar centers, and development of many national and international projects in HPC and Grid.
Participated in an IBM funded project together with UPB concerning satellite image processing on IBM Blue Gene; UVT and UPB team trained to work with the supercomputer and the activities have concern code development and tests on supercomputer
Contribution to HP-SEE: FuzzyCmeans application
One key person is acting as national expert in the FP7-ICT Committee and European e-Infrastructure Reflection Group (e-IRG). Moreover, two key persons are involved in the management board of COST Actions: I0805 - Open Network for High-Performance Computing on Complex Environments (www.complexhpc.org) and respectively, IC0801 related to Agreement Technologies.

HPC NEEDS FOR RESEARCH - 2

UVT-2

Facultatea de Fizica.

Grupul pentru modelarea proceselor fizice din instalatiile de crestere a cristalelor.
Prof.dr. Daniel Vizman
Teme de cercetare care necesita HPC:
-Modelarea convectiei topiturii in instalatiile industriale de crestere a cristalelor
-Modelarea influentei campurilor magnetice asupra curgerii topiturii in instalatiile industriale de crestere a cristalelor
-Modelarea proceselor de difuzie a dopantilor in procesele industriale de crestere a cristalelor
-Studiul influentei diferitilor parametrii de crestere(viteza de crestere, rotatia creuzetului, campuri magnetice) asupra formei interfetei de cristalizare

Modelarea numerica a acestor fenomene necesita HPC datorita marimii retelelor 3D folosite (peste 1.000.000 de volume finite). Folosirea HPC ar duce la imbunatatirea considerabila a timpului de calcul. In prezent modelarea a 500s timp real poate dura si 2 saptamani pe un cluster obisnuit (pina in 10 cores).

HPC NEEDS FOR RESEARCH - 2

Universitatea Tehnica Gh. Asachi - Iasi

Department of Computer Science and Engineering.

HPC Research TeamC

Infrastructures

The main node (frontend) of the GRAI Grid
Located at the Faculty of Automatic Control and Computer Science, Department of Computer Science and Engineering, HPC Laboratory;
Composed by an IBM x3800 (4 Intel Xeon processors, 8 GB RAM, 4 x x146 GB SAS HDD), twelve Dell Optiplex 755 (each with Intel Core 2 Duo E6550, 2 GB RAM) as working nodes, a NVIDIA Quadro Plex 1000 graphic system dedicated to graphic processing applications.

Research areas

Grid and cluster computing, Quantum computing, Combinatorial optimization, Data analysis, Computer graphics, GPU systems, Visualization, Multi-agent systems.

HPC NEEDS FOR RESEARCH - 2

Centrul de Cercetari Tehnice Fundamentale si Avansate -AR-Timisoara

Victor Sofonea:
Modelarea/simularea pe calculator a comportarii fluidelor complexe (tranzitii de faza, structuri si auto-organizare, microfluidica, aplicatii) utilizand tehnici de calcul paralel.

Sistem de calcul modest ->
Se asigura portabilitatea programelor si rularea versiunii finale pe sisteme mai puternice cand este posibil

Granturi acordate pt. folosire resurse
CASPUR (Roma)
CINECA (Bologna)

Implementarea algoritmilor de tip "lattice Boltzmann" folositi in fizica fluidelor pe GPU

HPC NEEDS FOR RESEARCH - 2

Physics Faculty - Univ. Craiova

Elaborarea unor algoritmi numerici eficienti, cu aplicatii la algoritmi de tip Monte-Carlo si prelucrarea semnalelor.

In cadrul studiului algoritmilor de tip “quantum diffusion Monte-Carlo” s-a elaborat un algoritm conceptual nou de inversare numerica a transformatei Laplace, cu aplicabilitate in prelucrarea semnalelor RMN.

S-au studiat algoritmii numerici pentru localizarea rezonantelor in plasma din tokamak, in colaborare cu CEA-Cadarache .

Algoritmii numerici pentru generarea de procese stochastice utilizate in simularea Monte-Carlo a transportului anomal in plasma au fost elaborati pe baza rezultatelor din lucrarile

Metode numerice speciale pentru calculul inverselor unor distributii de probabilitate standard au fost elaborate in. Un rezultat este postat pe situl prestigioasei firme Wolfram, producator al softului MATHEMATICA.

Una din preocuparile prezente este legata de metode noi Monte-Carlo de rezolvare a ecuatiei Fokker-Planck asociate procesului de incalzire, in cadrul proiectului Integrated Tokamak Modelling, proiectul IMP5.

HPC NEEDS FOR RESEARCH - 2

INCAS

Interesul pentru HPC la INCAS este legat in primul rand de

1. Aerodinamica industriala (studiul configuratilor de aeronave - RANS, LES).
Partea academica: LES sau DNS la numere Reynolds mici pe geometrii simple, consacrate.

2. Computational Structure Dynamics: folosind un solver comercial - Dytran, parte a pachetului Nastran/Patran.

Cluster (configuratia la care va fi upgradat in curand):

Number of nodes 20; CPU Intel E5640; RAM 16GB per node; Max number of parallel processes:160
Clusterul este la 1/10 din capacitatea declarata in tabel, dar in 2011planificata si finantata echiparea completa, ajungand la 160CPU, intr-o carcasa foarte mica, la un consum maxim de 10KW (320GB RAM, 20TB HDD).

LONG-TERM PROSPECTS

HPC support for large scale scientific collaborations:

- **ELI-NP** (IFIN-HH, IFTAR)

Modelling of high-intensity laser interaction with matter: new phenomena (condensed matter physics + nuclear physics)

Unified Nuclear Energy Density Functional (UNEDF) collaboration: find an optimum 'nuclear' functional based on by the nucleonic Hamiltonian and existing experimental data (UNEDF SciDAC collaboration, Central Michigan University, M. Horoi; University of Washington, I. Stetcu). ELI best tool for the evaluation of the theory. Compare experimental results with HPC simulations.

- **KM3NeT** (ISS)

KM3NeT, an European deep-sea research infrastructure, will host a neutrino telescope with a volume of at least one cubic kilometre at the bottom of the Mediterranean Sea. Search for neutrinos from distant astrophysical sources like gamma ray bursters, supernovae or colliding stars and will be a powerful tool in the search for dark matter in the Universe.

- **CERN** EXPERIMENTS (IFIN-HH, ISS, ITIM-CJ, UPB, etc.) (20 years)
- **EURATOM-MEdC** (INFLPR, IFIN-HH, INCDFM, UTCN, UAIC, ...) EU Fusion Programme
- **FAIR** (IFIN-HH, FF-UB, ...) CBM, PANDA, etc.

THANK YOU FOR YOUR ATTENTION !

DISCUSSIONS