# HP-SEE

## HP-SEE infrastructure and access

www.hp-see.eu

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HP-SEE

High-Performance Computing Infrastructure
for South East Europe's Research Communities

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# OUTLINE

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- Overview
- Types of HPC Infrastructure resources available
- Obtaining access to the HP-SEE resources
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- DEMO

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- **WP5 – Regional HPC operations and interoperation** – will ensure that integrated services will be provided to end users, by deploying the regional HPC infrastructure on top of the existing networking infrastructure, complementary to the existing Grid infrastructure, and fused with end user services.
- Specifically, user community needs in terms of size and availability of HPC resources will be catered for. Current HPC installations in Bulgaria, Romania and Hungary will be integrated at the first stage, followed by the upcoming purchases in Greece and Serbia.
- These will form the backbone of the state-of-the-art regional infrastructure, which will be operated jointly by the project, using a set of operations and management tools that will be supported by WP5. The infrastructure will be open for use of the wider user community from the region, not only infrastructure provision countries

# Types of HPC resources

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- Supercomputers
- HPC clusters with special low-latency MPI interconnection
- HPC clusters with ethernet
- GPU cluster resources
- Storage

# Blue Gene/P supercomputer in Sofia

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- System software:
- Front End Node (bgfen) operating system: SUSE Linux Enterprise Server 10 (SLES 10), Service Pack 1
- Compilers:
  - IBM XL C/C++ Advanced Edition for Blue Gene/P V9.0;
  - IBM XL Fortran Advanced Edition for Blue Gene/P V11.1;
  - GNU Toolchain (gcc, glibc, binutlils, gdb, python);
- Libraries:
  - Engineering and Scientific Subroutine Library (ESSL) for Linux on Power V4.3.1;
  - MPI (MPICH2)
- IBM Tivoli Workload Scheduler LoadLeveler Version 3 Release 4.2 PTF 1;
- Application software:
  - GotoBLAS –currently the fastest implementation of the **Basic Linear Algebra Subroutines (BLAS);**
  - GAMMES-US –a general *ab initio quantum chemistry package;*
  - **NAMD** –a parallel molecular dynamics code for large biomolecular systems;
  - CPMD–a parallelized plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for *ab initio molecular dynamics;*
  - LAMMPS: a classical molecular dynamics simulation code designed to run efficiently on parallel computers
  - **GROMACS –classical molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles;**
  - OpenAtom –a highly scalable and portable parallel application for molecular dynamics simulations at the quantum level, which implements the Car-Parrinello *ab initio Molecular Dynamics (CPAIMD) method;*

# HPC Clusters

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- HPCG at IICT-BAS, BG:
  - BG **36** Intel Xeon  X5560 @2.8Ghz
  - 24 GB per node **576 cores**
  - DDR Infiniband 2.5 μs 20 Gbps
  - /home, /gscratch 22TB, 10TB
  - Small cluster with 4 Nvidia GTX 295 cards, total 1920 GPU cores also connected
- InfraGRID at WUT, RO
  - 50 Intel Xeon E5504 @2.00Ghz
  - 10GB per node **400 cores**
  - QDR 4x Infiniband 1.1μs 40Gbps
  - /home 10TB

# HPC Clusters

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- NCIT at UPB
  - 48 28*HS21 Dual Intel Quad-Core Xeon E5504 @2.00Ghz, 4*QS22 Dual IBM PowerXCell 8i @3.2GHz, 20*LS22 Dual AMD Opteron Hex-Core @2.6GHz 16GB/HS21, 8GB/QS22, 12GB/LS22
  - **544 cores,** 4 * Gigabit Ethernet, QDR 4x Infiniband 1.1μs 40Gbps
  - Lustre FS 20TB 400MB/s
- SUN E15K supercomputer cluster at NIIFI, HU
  - 2 US-III+ @1.2GHz, US-IV+ @1.8Ghz 158Gbyte, 286GByte 144 cores
  - 2 x Gigabit Ethernet cca 300 μs 1 Gbps
  - 6.4 Tbyte

# HPC Clusters

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- PARADOX at IPB
  - 84 Intel Xeon E5345@2.33GHz 8GB per node
  - **672 cores**
  - Gigabit Ethernet 50μs 1 Gbps
  - /home, /scratch, /storage 3 TB , 100GB per node, up to 50 TB

# Software

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- Operating systems – mostly Scientific Linux 5
- Batch systems – torque/maui or Sun Grid Engine
- Software – compilers, mpi, lapack, fftw, etc.
- Gaussian03 in RO and HU

# Obtaining access

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- Most HPC centers in the worlds have their own policy for requesting resources. Usually there is an application form, describing the goals of the application, requested amount and type of resources, and other such details.

# Example Application form

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- The request forms for obtaining access to HPCG and BG-FEN are available as part of the training materials.
- It is important to fill out the requested CPU usage quota, because a default amount of 10 000 CPU hours will be applied.

# Application's phases

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- Each application should choose their "home" cluster to do development there
- Once the application is usable, they can request access to other clusters, and strive to improve scalability
- When good scalability is achieved, some application related bencharking results should be produced and the most suitable resources should be used for production utilization and achieving scientific results.

# Conclusions

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- First steps after the training: filling access forms, obtaining access
- Start compiling application for the target architecture.

# DEMO

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- Demonstration of access