



Project Overview



**HP-SEE - High-Performance Computing
Infrastructure for South East Europe**

<http://www.hp-see.eu/>

***HP-SEE receives EC support through FP7 under
the "Research Infrastructures" action.***

Introduction to VRCs



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

➤ **Comp. Physics**

6 countries,
8 apps.

➤ **Comp. Chemistry**

6 countries,
7 apps.

➤ **Life Sciences**

5 countries,
7 apps.

Country	Physics	Chemistry	Life Sciences	Total
Albania	2			1
Armenia			1	1
Bos-Herzeg		1		1
Bulgaria	2	2		4
Georgia			1	1
Greece		1	2	3
Hungary			2	2
Moldova	1			1
Montenegr			1	1
FYR of Mace	1	1		2
Romania	2	1		3
Serbia	1	1		2

Computational Physics VRC



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High-Performance Computing Infrastructure
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➤ Overview

- * Numerically modeling complex systems
- * Fast processing of huge amounts of data
- * Enhancement of the participation in regional, european and international research projects

➤ VCR structure

- * Around 12 target applications
- * Supported by developer groups belonging to 5 project beneficiaries, from 7 Balkan countries

Computational Physics VRC



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➤ Applications Areas

- * High Energy and Particle Physics
- * Plasma Physics
- * Physics of Condensed Matter
- * Atomic Physics
- * Computational Fluid Dynamics

➤ Indicative Applications range

- * Nano-electronics
- * Micro-devices optimization&modeling of robotic devices for biomedicine
- * Feature detection in satellite images
- * Modeling of electron transport
- * Complex gas dynamics&convection

Computational Physics VRC



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➤ Research fields

- **Astrophysics (FAMAD, HAG)**
- **Continuum/Fluid Mechanics (AMR_PAR, SIMPLE-2S 2D)**
- **Geophysics (GIM)**
- **High Energy Physics (HMLQCD)**
- **Physics of semiconductor nano-devices (SET)**
- **Plasma Physics (GENETATOMIC)**
- **Polymer Physics (SFHG)**
- **Quantum Optics (NUQG)**

Computational Physics VRC



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➤ APPLICATION

- **Astrophysics (FAMAD, HAG)**
- **Continuum/Fluid Mechanics (AMR_PAR, SIMPLE-2S 2D)**
- **Geophysics (GIM)**
- **High Energy Physics (HMLQCD)**
- **Physics of semiconductor nano-devices (SET)**
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- 1. SIMPLE-TS 2D - Semi-Implicit Method for Pressure – Linked Equations – Time Step Department of Complex and Multiphase Flow**
- 2. AMR_PAR - Parallel algorithm and program for the solving of continuum mechanics equations using Adaptive Mesh Refinement**
- 3. EagleEye - Feature Extraction from Satellite Images Using a Hybrid Computing Architecture**
- 4. FAMAD - Fractal Algorithms for MAss Distribution High Energy Astrophysics and Advanced Tehnologies**



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- 5. FuzzyCmeans - Parallel Fuzzy C Means for classification/Feature detection Category**
- 6. GENETATOMICS - Genetic algorithms in atomic collisions**
- 7. GIM - Design of fullerene and metal-diothiolene-based materials for photonic applications**
- 8. HAG - High energy physics Algorithms on GPU High Energy Astrophysics and Advanced Tehnologie**
- 9. HMLQCD - Hadron Masses from Lattice QCD**

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10. NUQG - Numerical study of ultra-cold quantum gases Scientific Computing Laboratory

11. SET - Simulation of Electron Transport Department of Grid Technologies and Applications

12. SFHG - Self Avoiding Hamiltonian Walk on Gaskets

Computational *Chemistry* VRC



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➤ Overview

- * Quantum molecular dynamics domain
- * Molecular modelling
- * nano-technology
- * design of new materials

➤ VCR structure

- * Supports 7 applications with main developers in 6 SEE countries
- * collaborating with 5 advanced research centers in Europe and USA
- * 12 regional and national institutions

Computational Chemistry VRC



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➤ Applications Areas

- * Molecular dynamics & simulations
- * Material science

➤ Indicative Applications range

- * Study of physicochemical properties of compound
- * Molecular design of platinum complexes
- * Material design for photonic applications
- * Molecular-orbital simulations
- * Design of chemical reactors, burners, boilers
- * Quantum mechanical simulation of Condensed Phases

Computational Chemistry VR



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- 1. FMD-PA Design of fullerene and metal-diothiolene-based materials for photonic applications
Computational Chemistry**
- 2. CFDOF – CFDOF**
- 3. CompChem - Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation**
- 4. HC-MD-QM-CS - Hybrid Classical/Quantum Molecular Dynamics – Quantum Mechanical Computer Simulation of Condensed Phases**

Computational Chemistry VF



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- 5. ISyMAB - Integrated System for Modeling and data Analysis of complex Biomolecules**
- 6. MDCisplatin - Molecular Design of Platinum Group Metal Complexes as Potential Non-classical Cisplatin Analogues**
- 7. PCACIC - Principal Component Analysis of the Conformational Interconversions in Large-Ring Cyclodextrins Lab. Physical Organic and Computational Chemistry**

Life Sciences VRC



➤ Overview

- * Utilize HPC resources with regional needs
- * Fostering the research process
- * Facilitate the cooperation between RC

➤ VCR structure

- * Supports 7 applications with main developers in 5 SEE countries
- * involve collaborations in Europe and the U.S
- * will foster the development of new collaborations in SEE countries

Life Sciences VRC



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High-Performance Computing Infrastructure
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➤ Applications Areas

- * Neuroscience
- * Proteomics
- * Genomics & DNA sequence analysis

➤ Indicative Applications range

- * Network models of short & long term memory
- * Identification of novel miRNA genes
- * Genomics / sequence analysis
- * Molecular Dynamics
- * Synthesis of nucleotide bases

Life Sciences VRC



- 1. MDSCS - Molecular Dynamics Study of Complex Systems**
- 2. CMSLTM - Computational Models of Short and Long Term Memory Computational Biology Lab**
- 3. DeepAligner - Deep sequencing for short fragment alignment Biotech Group**
- 4. DiseaseGene - In-silico Disease Gene Mapper Biotech Group**

Life Sciences VRC



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- 5. DNAMA - DNA Multicore Analysis**
- 6. miRs - Searching for novel miRNA genes and their targets Computational Biology group**
- 7. MSBP - Modeling of some biochemical processes with the purpose of realization of their thin and purposeful synthesis**

References



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- [1] Project HP-SEE – 261499 – Annex I – “Description of Work”
- [2] HP-SEE Application Questionnaire,
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- [3] HP-SEE survey tool, <http://survey.hp-see.eu/>
- [4] LimeSurvey, <http://www.limesurvey.org/>
- [5] Distributed European Infrastructure for Supercomputing Applications (DEISA), <http://www.deisa.eu/>
- [6] DEISA Extreme Computing Initiative (DECI),
<http://www.deisa.eu/science/decI>
- [7] Partnership for Advanced Computing in Europe (PRACE),
<http://www.praceproject.eu/>

THANK YOU!



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QUESTIONS ?