EU Centre of Excellence for
COMPUTER MODELLING OF COMPLEX SYSTEMS

## Project vision:

The basic strategic objective of the CX-CMCS project is to transform the Scientific Computing Laboratory (http://scl.phy.bg.ac.yu/) into a centre of excellence, i.e. to decisively increase the quality of research conducted at SCL, and make it a preferred West Balkan research partner for EU institutions working in the fields of simulation of complex systems and of GRID technology.

SCL is a unit of the Institute of Physics in Belgrade. The Institute contributes more than 10% of the total scientific output of Serbia and constantly ranks among the best R&D institutions in the region. SCL currently has 18 staff members, and participates in several international and national projects, including FP6 projects CX-CMCS, SEE-GRID, SEE-GRID-2, EGEE-II, and Cost action P10. SCL defines the current state of the art in high performance computing in the West Balkan region with its PARADOX cluster.

CX-CMCS aims to reinforce the research capacity of the SCL by: hiring young researchers; providing training and mobility for the research staff; upgrading the computing infrastructure. The success of this endeavour will be measured through a benchmarking exercise to be performed in the project's last year. Our networking partners (4 from EU and 3 from Serbia) have been carefully selected to provide the skills and expertise necessary to reinforce the research potential of SCL through training and joint research. The proposed equipment upgrade will make it possible to tackle even the most complex GRID applications allowing SCL to become a key regional player in deployment and use of this emerging technology. The CX-CMCS International Advisory Board will help SCL develop a long term strategy and facilitate its integration into ERA.

CX-CMCS aims to be a living example that it is possible to bridge the "digital divide" between countries and regions having high tech ICT technologies and those that do not.
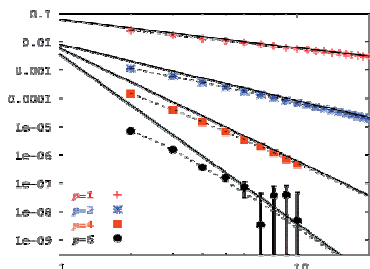
Science at SCL: Systematic speedup of path integrals

The figure on the left shows the many order of magnitude speed-up in the evaluation of path integrals of a generic quantum theory obtained at SCL. This success illustrates SCL's general approach to scientific computing as a heuristic tool:

- *True success in numerical simulations is obtained through the input of key new analytical knowledge into the algorithms.*

- *The ultimate outcome of the simulations of complex systems are not*

Planned impacts:

- **Impact on technology –** Maintain and extend SCL infrastructure representing the current state of the art of computing and communication facilities in the West Balkan region; Implement latest GRID-related technologies.

- **Impact on research** – Improve research environment, human and computing capacities making it possible to study complex systems characterized with very large data sets and requiring extensive computing power. This will allow: comprehensive survey of near-Earth objects and estimation of catastrophic impacts, modelling the formation of Earth-like planets around other stars; study of the large-scale topology of the Internet, study of granular systems, efficient simulations in High Energy Physics.

- **Social impact** – The brain-drain of tens of thousands of young professionals with key skills is a phenomenon of paramount social impact on a region that has until recently endured a decade of wars, social instability and economic hardship. Of those that left, many were educated in the physical sciences and engineering and their continued education in the USA coincided with the emergence of robust new research fields as well as with the birth of several new technologies. Today, West Balkan (and EU) RTD has the potential of tapping into this extremely important human resource. The key precondition for alleviating the consequences of brain-drain is in identifying of high quality research centres to serve as brain-gain focal points.

- **Impact on national RTD policy** – Develop a set of recommendations for policy makers at national and local levels for fostering growth of research excellence in a rapidly changing high-tech environment.

- **Contribution to EU policies –** In particular those addressing the issue of bridging the "digital divide" between countries and regions.

- **Dissemination and exploitation of results –** Improve EU-wide visibility and future participation in ERA; Maintain leading position of SCL in Serbian research; Promote modelling of complex systems using high performance computing resources in fundamental and applied research; Enhance interest of general public in S&T by showing examples of how scientific computing research can benefit every day life; Provide relevant data and recommendations regarding scientific computing to policy makers at national and local levels.

- **Impact on related national and international research activities –** SCL is active in two overlapping research fields: investigation of complex systems and development and deployment of GRID-based technologies. As a result of its expertise in both fields SCL is a prominent participant in several international and national projects. It is the driving force of the Academic and Educational Grid Initiative of Serbia (AEGIS), and the instigator of the ARETE initiative (Advancing Research Excellence and Technological Efficiency).
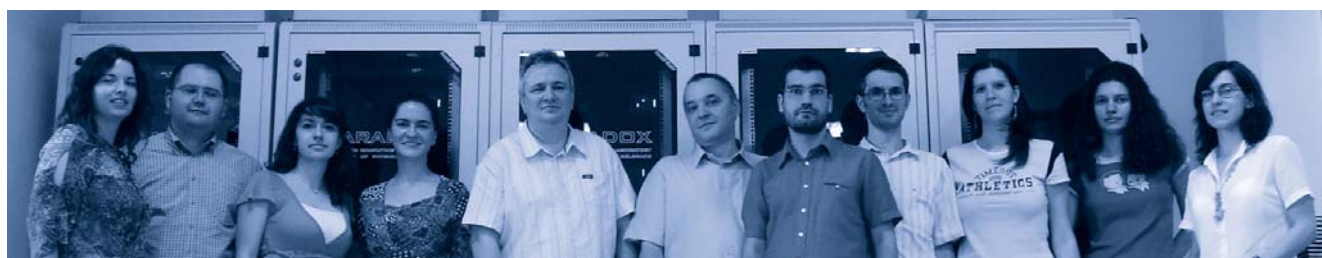
Reinforced human capacity:

From the start of CX-CMCS a total of eight new young researchers have come to SCL. Each of these talented young physicists have been recipients of prestigious Ministry of Science stipends that serve as matching funds that complement their CX-CMCS stipends. As a result of this matching, CX-CMCS has doubled the planned number of young researchers brought to SCL. During the first year of CX-CMCS four of these new researchers have already been hired by the Institute of Physics in Belgrade.
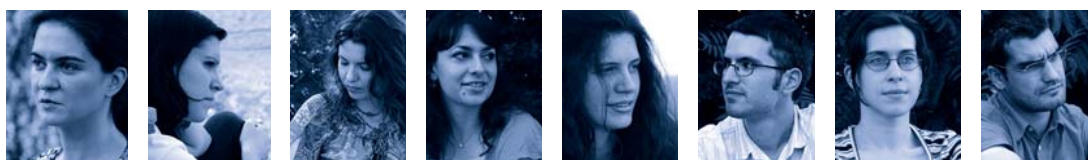

SCL has also attracted four young people working in the field of computer sciences as its new ICT staff. Their primary task is related to the administering of SCL's Grid site AEGIS01-PHY-SCL. This state-of-the-art distributed computing platform is giving each of them a chance to conduct forefront research in several key new ICT fields. The CX-CMCS stipends of the new technical staff are being matched by funds from SCL eInfrastructure projects SEE-GRID, SEE-GRID-2 and EGEE II.

Reinforced infrastructure:

SCL's high performance computing infrastructure is organized around the AEGIS01-PHY-SCL grid site, a key part of national and regional production grid infrastructure, and an esteemed partner at the pan-European level.

The current configuration consists of 200 CPU cores with 212 GB RAM, 27 TB storage space, 40 kVA UPS, high throughput network layer 3 switches stacked to an aggregate of 206 Gbps ports. The whole configuration is stored in 5 racks and cooled by a contained 170 kBTU integrated system. The AEGIS01-PHY-SCL Grid site is logically organized into:

- **Worker nodes –** 42 quad-core nodes each with 4 GB RAM, connected through two channel-bonded Gbps ethernet interfaces to stacked layer 3 network switches.

- **Storage element –** 3 storage units each with 9 TB disk space in RAID-5 hardware configuration for data protection and integrity. Each storage unit has a quad-core configuration with 4 GB RAM.

- **Core services –** 8 dual-core servers with 4 GB RAM providing all essential Grid services that integrate the above computing and storage resources into a unified resource. In addition, AEGIS01-PHY-SCL also provides core services for national, regional and pan-European Grid infrastructures integrating all of them into a unified and user friendly resource.
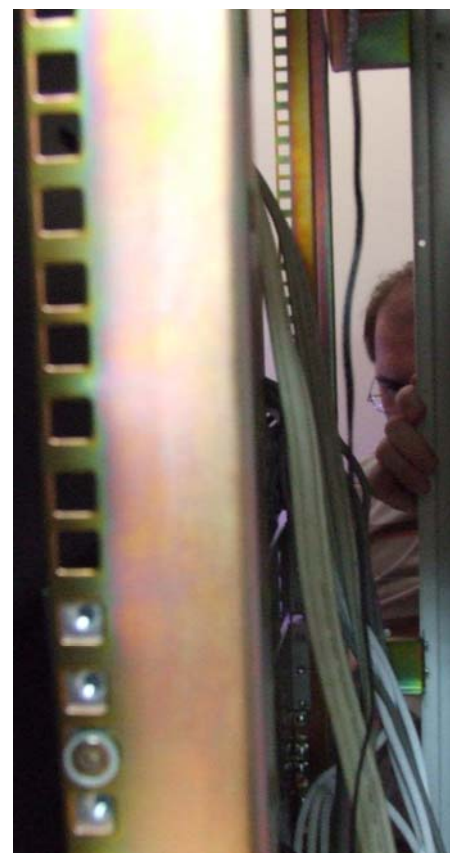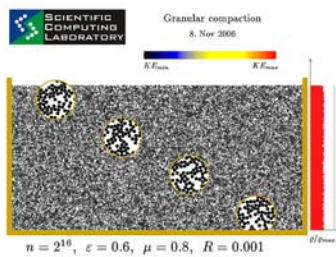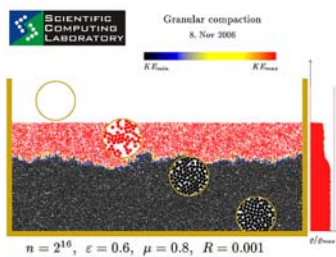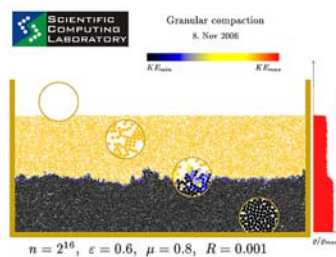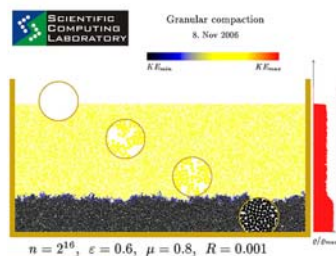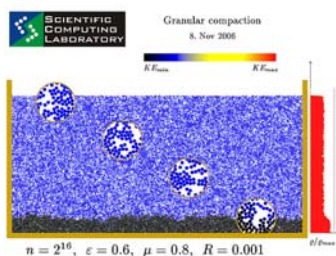
EU Commisioner Potocnik at start of CX-CMCS project: On July 14, 2006 the SCL and IPB were hosts to high level delegations from EU Directorate General for Research, headed by Janez Potocnik, Commissioner for Research, and from the Ministry of Science of Serbia, headed by Aleksandar Popovic, Minister of Science. The joint delegation included Andras Siegler, Director INCO, Giancarlo Caratti, JRC, Tania Friederichs, DG Research, Ivan Videnovic, Assistant Minister of Science, and Gradimir Milovanovic, Chairman of the National Science Council.

The main purpose of the Commissioner's visit to IPB was to get first hand information about its four laboratories that were the recepients of EU Centre of Excellence grants in the 2005 SSA call for reinforcing of research excellence in the West Balkans. Serbia's R&D centre's got 8 of the region's 10 grants, half of these went to the IPB, including the best evaluated R&D proposal in the region – CX-CMCS.

Science at SCL: Simulation of granular compaction

The figures on the left represent screen shots of the granular simulation and visualization package developed at SCL. Granular materials are large assemblies of solid macroscopic particles. Examples of such materials include sand, stones, soil, ores, pharmaceuticals, and variety of chemicals. Granular materials have wide applicability in everyday life. At the same time they behave differently than all other familiar forms of matter – solids, liquids, or gases.