# FP6 INCO contract No. 026343

# CX-CMCS

## Centre of Excellence for Computational Modelling of Complex Systems



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# Deliverable D07

# CX-CMCS Brochure

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**Abstract:** Deliverable D07 – "CX-CMCS Brochure" is a public document. The deliverable includes the CX-CMCS Brochure which represents the basic document distributed during the projects Dissemination and Visibility activities

# Document Revision History

| Date | Issue | Editor | Summary of main changes |
|------|-------|--------|------------------------|
| January 22, 2007 | - | Aleksandar Bogojevic | |
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# Preface

The basic strategic objective of the CX-CMCS proposal is to transform the Scientific Computing Laboratory (SCL) into a centre of excellence, i.e. to decisively increase the quality of research conducted at SCL, and make it a preferred WB 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 has 14 staff members, and participates in several international and national projects, including FP6 project SEE-GRID and Cost action P10. SCL defines the current state of the art in high performance computing in WBC with its PARADOX cluster (64+2 processors with aggregate speed $R_{max}=0.21$ Tflops).

The proposed CX-CMCS SSA aims to reinforce research capacity at SCL by: hiring young researchers, providing of training and mobility for the research staff, and 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 (storage element, high throughput switch, and upgrade of RAM) 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 emerging GRID technology. CX-CMCS plans to set up an International Advisory Board whose expertise will help SCL develop a long term strategy and facilitate 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.

## Strategic objectives

The basic strategic objective of the CX-CMCS proposal is to transform SCL into a centre of excellence, i.e. to decisively increase the quality of research conducted at SCL, and make it a preferred WB research partner for EU institutions working in the fields of simulation of complex systems and of GRID technology.

Centres of excellence do not exist in a vacuum, however. In order for SCL to achieve and maintain a status of excellence, the proposed SSA aims to positively effect the research environment in Serbia at several levels: SCL's immediate R&D environment (the national partners in this proposal), the high performance computing segment, and the national R&D system as a whole.

## Specific objectives

The specific objectives for the current SSA proposal have been formulated through an analysis of the following key points:

- Wider developmental objectives of Serbia and Montenegro and the West Balkan region pertaining to research and development (as presented in the Action Plan adopted at the Ministerial conference in Thessaloniki in June 2003);
- Existing strengths and weaknesses at SCL an the high performance computing sector in Serbia including: professional resources, material resources, financial and organizational resources, principle impediments;
- Assessment of availability of graduate students and young researchers that could be newly employed at SCL.
- Assessment of indirect social impacts of the process of strengthening of SCL and its efficient integration into a wider European R&D effort.

The outlined analysis has resulted in the following specific objectives, each of which directly leads to a set of measurable and directly verifiable sub-objectives.


**Objective 1 – Enhance quality of R&D at SCL**

- **Sub-objective 1.1**: Set up an International Advisory Board for the new centre of excellence;
- **Sub-objective 1.2**: Establish a framework for more efficient management of research at SCL by developing a flexible, problem oriented R&D plan that will successfully integrate that research into a wider European effort.
- **Sub-objective 1.3**: Develop a specific set of benchmarks for tracking the quality of R&D at SCL, and perform a benchmarking exercise.
- **Sub**-**objective 1.4**: Devise and implement a long term strategy for achieving and maintaining research excellence.
- **Sub-objective 1.5**: Insure viability of SCL as a centre of excellence beyond the project lifetime by finding other sources of funding.


**Objective 2 – Expand and mobilize human resources**

- **Sub-objective 2.1**: Recruit and employ young researchers; develop explicit career plans for the newly employed researchers.
- **Sub-objective 2.2**: Enhance working conditions for young researchers by setting up an R&D environment at SCL that is integrated into ERA, providing challenging research problems, state of the art equipment, and enhanced mobility.


**Objective 3 – Reinforce existing S&T capacities at SCL**

- **Sub-objective 3.1**: Maintain and upgrade existing S&T equipment and high-tech infrastructure.
- **Sub-objective 3.2**: Improve the availability and reliability of SCL's computing resources, determine and implement optimal strategies for their use.


**Objective 4 – Enhance mobility and integration into ERA**

- **Sub-objective 4.1**: Network with EU, regional and national partner institutions through exchange of personnel, research results and joint numerical experiments; participate in joint RTD activities within these networks.
- **Sub-objective 4.2**: Host scientists from EU for training and research.
- **Sub-objective 4.3**: Organize training of graduate students and young researchers through short-term missions at EU institutions.


**Objective 5 – Contribute to the reinforcing of ICT capacities at the national level**

- **Sub-objective 5.1**: Reinforce the quality of research in SCL's immediate R&D environment, by strengthening their human capacity through stipends, yearly visits, and by conducting joint research activities.
- **Sub-objective 5.2**: Reinforce human capacity in Serbia's high performance computing sector by training young researchers to be employed at national research institutions and hi-tech companies.
- **Sub-objective 5.3**: Contribute to the national R&D system by developing 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.


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The three year CX-CMCS project kicked-off on July 1, 2006.  The project plans to issue the following deliverables:

| Deliverable No | Deliverable title | Delivery date | Nature | Dissemination level |
|---|---|---|---|---|
| D01 | CX-CMCS Web site | M1 | R | PU |
| D02 | Career development plan for newly employed young researchers | M2 | R | CO |
| D03 | CX-CMCS International Advisory Board | M3 | O | PU |
| D04 | Equipment tendering and procurement report | M3 | R | PU |
| D05 | Inauguration meeting report | M4 | R | PU |
| D06 | Mobility and training plan | M6 | R | PU |
| D07 | CX-CMCS Brochure | M6 | R | PU |
| D08 | 12M Progress reports | M12, M24 | R | PU |
| D09 | CX-CMCS Promotional video material | M15 | O | PU |
| D10 | Benchmark procedures for quality assessment of RTD centres of excellence | M18 | R | PU |
| D11 | SCL research quality assessment | M24 | R | PU |
| D12 | Proceedings of International dissemination workshop | M30 | R | PU |
| D13 | Strategy of long term sustainable growth of research excellence in transition | M30 | R | PU |
| D14 | Scientific computing landscape of Serbia | M33 | R | PU |
| D15 | Presentation of policy papers to decision makers | M34 | R | PU |
| D16 | Final project report | M36 | R | PU |

*Legend: R = Report, O = Other, PU = Public, CO = Confidential (only for members of the consortium incl. EC).*

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## References

[1]     Project CX-CMCS – 026343 – Annex I – Description of Work

# Executive summary

**What is the focus of this Deliverable?**

The focus of this deliverable is the presentation of the CX-CMCS Brochure, the principle document to be handed out during the project's dissemination and visibility tasks.

**What is next in the process to deliver the CX-CMCS results?**

The deliverable and workflow progress is described in the project Annex-I – Description of Work [1]

**What are the deliverable contents?**

Introduction to basic aspects of CX-CMCS dissemination and visibility effort and a brief presentation of the structure and contents of the CX-CMCS Brochure document.

**Conclusions**

The four page CX-XMCS Brochure gives the basic information-at-a-glance about the project and the Scientific Computing Laboratory. This information is principally geared to the media and to researchers working on similar areas of research as SCL. The project Brochure, however, is also useful for all other target audiences of CX-CMCS's dissemination effort.

# 1. Introduction

The present deliverable deals with a key document for the successful implementation of work package 4 of the CX-CMCS project – Dissemination and visibility. CX-CMCS puts a strong emphasis on the dissemination and visibility of the results of the performed research as well as the effort to produce a high technology centre of excellence in the WB region. To be successful in this role the dissemination and visibility work package needs to address four distinct audiences:

- EU research community;
- Research community in Serbia;
- Wider public in Serbia;
- Relevant policy makers at local and national levels.


The EU research community needs to be addressed in order to improve EU-wide visibility of SCL, to find a niche for future participation and collaboration in EU RTD programmes, to extend the number of quality RTD institutions that SCL collaborates with, to facilitate future two-way researcher mobility to and from SCL, to seek training as well as to offer training to others in the areas of our expertise, and, last but not least, to inform young researchers who have left Serbia during the nineties (brain-drain) that there exist centres of excellence in key areas of RTD that they can collaborate with and/or return to.

The Serbian research community must be made aware of the results at SCL, and in particular of the results of the CX-CMCS effort at helping it become a centre of excellence, in order to maintain the leading role of SCL, to promote high performance computing in fundamental and applied research, to promote the GRID computing paradigm and the integration of Serbia's computing capacity into the flexible virtual organization that GRID represents, to serve as an example to other quality research institutions in Serbia to modernize their research activities and integrate them more thoroughly into ERA.

Outreach to the wider public in Serbia serves just as important a role. It enhances interest in S&T in general and physics and high performance computing in particular (throughout the previous decade of wars and crisis interest in science has plummeted, as has university enrolment in the hard sciences and engineering, including computer sciences). Visibility of institutions such as SCL can widen public support for R&D by showing the public specific examples of how their research efforts benefit every day life.

The final audience the CX-CMCS project seeks to address are the relevant policy makers at national and local levels. They are extremely important if the reinforcing of quality of research at SCL is not to remain an isolated effort. CX-CMCS envisages to present policy makers with several important reports concerning the state of the scientific computing R&D sector in Serbia along with a set of recommendations regarding quality assessment and quality assurance mechanisms applicable to RTD.

These target audiences will receive information about the CX-CMCS project and the research conducted at SCL via its web site and through promotional material created by the project throughout its duration. The project will also organize an International dissemination workshop that will bring together 10 leading researchers from EU with researchers from SCL and its national partner institutions, and will publish the proceedings. The international dissemination effort will include presentations of project results at scientific conferences, as well as the participation of SCL in dissemination efforts of EU partners. CX-CMCS will also organize meetings with national partners and outreach missions of the whole SCL staff to six selected institutions in Serbia. Wider public outreach will be carried out through promotions in national and local media and the organizing of popular lectures throughout Serbia.

## 2.  CX-CMCS Brochure

The CMCS Brochure is the principle document to be used within the projects Dissemination and visibility activities. The four page colour document:

- Presents an outline of the basic vision behind the CX-CMCS project.

- Gives a brief outline of SCL's approach to scientific computing and illustrates this with two examples from the laboratory's area of expertise (efficient path integral Monte Carlo calculations; simulation and visualization of granular compaction).

- List the basic categories of planned impacts of the 3 year project for reinforcing research capacity of the Scientific Computing Laboratory at the Institute of Physics in Belgrade, including the project':

    o  Impact on technology

    o  Impact on research

    o  Social impact

    o  Impact on national RTD policy

    o  Contribution to EU policies

    o  Impacts on dissemination and exploitation of results

    o  Impact on related national and international research activities.

- Presents the two key aspects of SCL's reinforcement:

    o  Hiring of new young researchers in physics and computer sciences to work at SCL, their training and the guaranteeing of their enhanced mobility.

    o  Strengthening of SCL's key research infrastructure

- Gives information about the visit of EU Commissioner for Research and Science to the IPB at the launch of CX-CMCS project.

The following four pages are screen shots from the CX-CMCS brochure. The electronic version of the brochure is available in PDF format on the project's web site:

http://cx-cmcs.phy.bg.ac.yu/press/cx-cmcs-brochure.pdf

## 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.
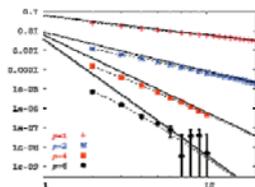
### Science at SCL: Systematic speedup of path integrals

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

**Figure 1 – Page 1 / 4 of CX-CMCS Brochure**

## 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).

**Figure 2 – Page 2 / 4 of CX-CMCS Brochure**

## 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, 18 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 6 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.
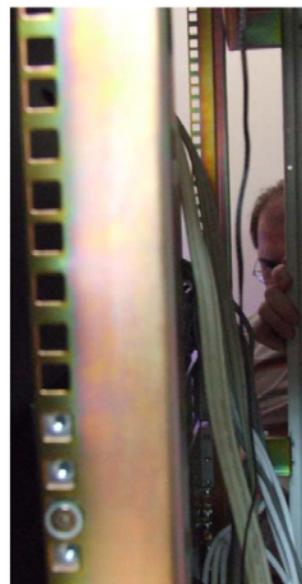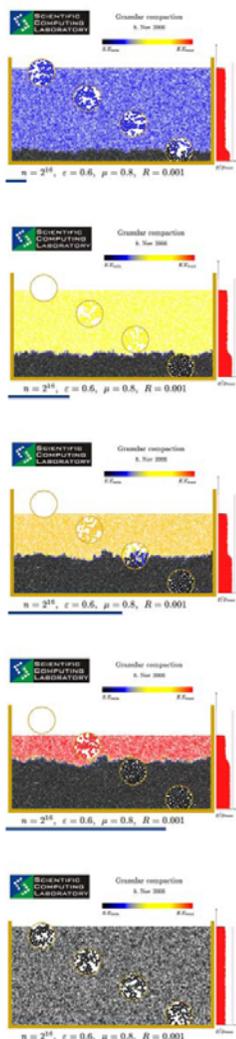




**Figure 3 – Page 3 / 4 of CX-CMCS Brochure**

**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.*

**Figure 4 – Page 4 / 4 of CX-CMCS Brochure**