ReCompSoLS
reinforcement of the centre for computational solutions in the life sciences

Project no: 043749

Project acronym: ReCompSoLS

Project title: Reinforcement of the Centre for Computational Solutions in the Life Sciences

Instrument: Specific Support Action

Activity Area: International Cooperation

Publishable Final Activity Report

Period covered: from 01/04/07 to 31/03/10

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Duration: 36 months

Project coordinator name: David Smith
Project coordinator organisation name: Ruder Boskovic Institute

Table of Contents

1 Publishable Final Activity Report

1.1 Project Execution

1.1.1 Project objectives

The primary objective of the project entitled Reinforcement of the Centre for Computational Solutions in the Life Sciences (ReCompSoLS, 043749) was to improve and reinforce the research capacities of the Centre for Computational Solutions in the Life Sciences (CompSoLS). The Centre is a multidisciplinary collaborative research venture situated at the Ruđer Bošković Institute in Zagreb, Croatia. The activities of the Centre range from bioinformatics of entire genomes to quantum-mechanical treatment of small model systems and include efforts focused on docking, proteomics, and mechanistic biochemistry.

We had proposed to achieve the reinforcement through several complementary measures.

In order to sustainably increase the human resource level of the Centre, we devised a Dynamic Recruitment Initiative, whereby, rather than simply funding graduate students for the entirety of their studies, we aimed to introduce short-term fellowships to finance the unpredictable period between the completion of undergraduate studies and the potential procurement of long-term funding by, for example, the Croatian Ministry of Science, Education, and Sport (MSES).

In order to reinforce the material resources of the Centre, we had proposed to purchase a state-of-the-art computer cluster, and associated ancillary equipment, and install it on site. Access was to be granted to all members of CompSoLS as well as selected individuals in our partner network.

To increase the integration of CompSoLS into the ERA, we proposed several activities with an international focus. In particular, we planned to organize two international workshops on the Adriatic Coast and a summer school in Zagreb aimed at bringing together the communities from the Western Balkan Countries (WBC) and Member States (MS), in our broad research area. At the same time, we envisaged a series of exchange visits with laboratories, also in the WBC and MS, designed to better educate WBC students by exposing them to high-level research environments early in their careers and to strengthen our own ties to the MS and WBC to reinforce our ability to perform high-quality cutting-edge research

It was from the position of strength, enabled by the ReCompSoLS project that we proposed to work toward our goal of increasing the uptake of Computational Life Science techniques in the WBC and improve our own integration into the ERA.

1.1.2 Contractors involved

This Specific Support Action in the area of International Cooperation was agreed with a single contractor. That contractor was the Ruder Boskovic Institute, located at Bijenička 54, 10000 Zagreb, Croatia.

1.1.3 Work performed and end results

(i) The Dynamic Recruitment Initiative (DRI)

The idea behind the DRI was to find an effective and efficient way to combat the chronic Brain Drain that is evident in Croatia. In our experience, one of the major factors contributing to the Brain Drain is the uncertain and unpredictable nature of the potentially lengthy waiting period between the time that a given student completes her undergraduate studies and the time she is granted an employment contract by the MSES (or alternative source) to begin doctoral studies. Our concept was to provide bridging finance to selected students to cover this waiting period and reduce the tendency for those students to abandon the local system in favour of more ordered labour markets in Western Europe and the USA.

Table 1. Data concerning the implementation of the DRI for the duration of ReCompSoLS

Name of Student	ReCompSoLS Contract Started	ReCompSoLS Contract Terminated	Current Status[a] (Commenced)
Karmen Čondić-Jurkić	01.05.2007	31.05.2007	MSES (01.06.07)
Vedran Lucić	01.05.2007	30.06.2007	MSES (01.07.07)
Trpimir Ivšić	15.10.2007	31.10.2008	MSES (15.10.08)
Ozren Jović	01.11.2007	31.03.2008	MSES (01.04.08)
Željka Žakić	01.12.2007	29.02.2008	MSES (01.03.08)
Tina Kokan	15.11.2007	31.03.2009	EMBO(01.04.09)
Jurica Novak	01.01.2009	30.06.2009	MSES (01.07.09)
Momir Mališ	15.07.2009	07.01.2010	MSES (08.01.10)
Matko Bošnjak	01.01.2009	31.03.2010	Waiting FP7 (01.06.10)
Antonija Tomić	01.02.2009	31.03.2010	Barcelona (01.04.10)
Goran Kovačević	01.08.2009	31.12.2009	CNSF (01.03.10)
Zoran Miličević	01.05.2009	31.03.2010	Erlangen (15.04.10)

[a] MSES means employed by the Croatian Ministry of Science, Education, and Sport. EMBO signifies employment on a project from the European Molecular Biology Organization. CNSF signifies employment on a project from the Croatian National Science Foundation.

In our opinion, the DRI proved itself to be an overwhelming success, far exceeding our initial expectations in terms of its effectiveness and impact. Our original plan saw us stand to gain a total 72 non-E.C. funded person months from a 72 person month investment through the DRI scheme. In actuality, we invested 97 person months for a return of 160. In doing this, we helped a total of twelve students as opposed to the originally planned six. We managed to secure alternate funding sources, of one form or another, for all twelve of these students, ten of whom stayed in Croatia. Only four cases were somewhat problematic in that the solutions we found were less than completely ideal (including the two brain-drain casualties). However, all four of these were a direct result of the moratorium on public employment,

introduced by the Ministry of Science Education and Sport at the beginning of 2010. We sincerely hope that this moratorium will soon be lifted and that those students with uncertain futures will find themselves with more secure positions.

(ii) Infrastructural Support

In order to reinforce our material resources of CompSoLS, we had included the purchase of a computer cluster into the ReCompSoLS project. The initial phase of the purchase was performed through a public tender, with a contract for purchase, delivery, and assembly signed on the 02.07.2007. The purchase of the required air-conditioning unit was finalized on the 29.06.2007, while the expansion to the final form of the cluster was completed on the 14.12.2007.

In a similar manner to the DRI, the cluster purchase outstripped our expectations as the computing power of the final hardware configuration significantly exceeded our initial planning, once again providing enhanced impact of the E.C. contribution to the project. In brief, the final cluster (compsols.irb.hr) consisted of a total of 56 processor cores with 124 Gb of memory and approximately 3 Tb of disk storage space.

The operating system was installed immediately after delivery. After careful system optimization and configuration of the job-scheduling system, the required software was configured, which was greatly assisted by the employment of a Technical Assistant (Petar Jager) on the 01.07.2007, through the ReCompSoLS project. The cluster performed outstandingly for the duration of the project and, apart from external power failures, the cluster has continued to operate at its full capacity since its inauguration. Figure 1 shows the cluster itself and the usage statistics for all three years of ReCompSoLS project.

01.04.07-31.03.08 *01.04.08-31.03.09* *01.04.09-31.03.10*

Figure 1. The HP ProLiant BL cluster and its usage statistics for all three years of project.

All members of CompSoLS have benefited extensively from the purchase and installation of the computer cluster in their every day work. Beyond this, however, several students and scientists from our WBC partner network regularly access and utilize the cluster. The significance of this resource to them is arguably even greater as they often have no access to a local alternative.

(iii) Exchange Visits and Associated Training Measures

An additional initiative conceived to increase the participation of CompSoLS, and indirectly the WBC in the ERA, as well as to increase the uptake of computational methodologies in the WBC, was a series of strategically timed exchange visits. In all cases, the visits were conceived to serve as training measures of one type or another.

In first year, of the project, we received visits from Jack Leunissen from Wageningen University in the Netherlands, who gave lectures as part of a Practical Bioinformatics Course – Introduction to Bioinformatics (02.07. – 05.07.2007.), coordinated by Kristian Vlahoviček. In addition, Janez Mavri, from the National Institute of Chemistry in Ljubljana, delivered a two-day course entitled "Computer Simulation of Proton Transfer in Proteins and Solutions" from the 17.10.– 18.10.2007. Professor Milena Petković from the University of Belgrade gave a course of the Construction of the Cartesian Reaction Surface Hamiltonian from 17.12.-21.12.2007. We also received two extended study visits from the MS students Kallee Karhu (21.05. – 27.07.2007) and Gireesh Krishnan (15.10 – 15.11.2007), who interacted strongly with the members of CompSoLS during their stays.

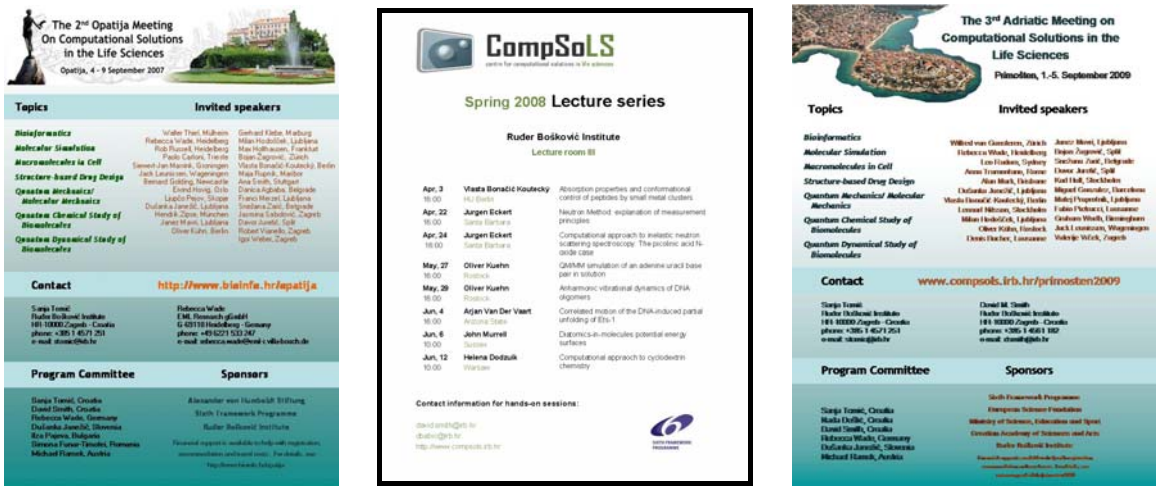

Figure 2. Posters from the workshops and a flyer used to promote the summer school.

In the second year of project, several of the visits were combined into an intensive Summer School that spanned the period from April 2008 till June 2008. The external participants in this initiative, which principally took place in spring, were: Professor Vlasta Bonacic-Koutecky, from the Humboldt University Berlin; Professors Juergen Eckert and Arjan Van Der Vaart, who visited us from their temporary base at the National Institute of Chemistry, Ljubljana, Slovenia; Professor Oliver Kuehn, from the University of Rostock; Professor Helena Dodziuk from the Institute of Physical Chemistry at the Polish Academy of Sciences; and Professor John Murrell, from the University of Sussex, Brighton, UK. With support from senior CompSoLS scientists, a series of courses were held covering: Conformational Dynamics of Peptides; Hydrogen Bonding and Hydrogen Transfer; Molecular Dynamics; Molecular Recognition; Supramolecular Chemistry; and Multidimensional Potential Energy

Surfaces, including hands-on sessions that allowed the students to become directly familiar with the techniques under discussion. The student reaction was very positive and we are very pleased with the level of uptake of the techniques presented into the students' own research.

In the third year of the project, we hosted follow-up visits from Professor Vlasta Bonacic-Koutecky, from the Humboldt University Berlin, Professor Juergen Eckert through the National Institute of Chemistry, Ljubljana, Slovenia, and Professor Milena Petković from the University of Belgrade, Serbia. Professor Leo Radom from the University of Sydney, Australia, who had been the postdoctoral host to two CompSoLS scientists, also visited us as part of a European trip. Each of these visitors gave a seminar during the course of their visit, while the more intensive local courses in the third year were provided by our own senior CompSoLS staff.

In particular, the local courses were timed to overlap with the visits from three students from the University of Mostar, in Bosna and Herzegovina. We managed to integrate these students into CompSoLS activities, including the 2nd Workshop (see below). They are a key aspect of our endeavours to encourage the uptake of computational life science solution in the WBC.

In addition to these external visits, many of the students employed through the Dynamic Recruitment Initiative, and some senior CompSoLS staff, participated in extended study stays abroad. Apart from the positive impact on local career development, these visits helped to strengthen our ties with the International School of Advanced Studies (SISSA) in Trieste, the University of Groningen, the Ludwig-Maximillians-University in Munich, the Humboldt University in Berlin, the Friedrich-Alexander-University in Erlangen-Nürnberg, the National Institute of Chemistry in Ljubljana, the University of Barcelona, and the University of Newcastle upon Tyne.

Overall, the Exchange Program was extremely successful. We reinforced the existing contacts and fostered new collaborations with scientists in the Member-States and WBC. We established a new contact network with scientists in Bosnia and Herzegovina and successfully trained graduate students working on their Ph. D theses. Several ongoing projects and applications emerged as a direct result of the ReCompSoLS exchange program. These included approved bilateral projects with Slovenia and Serbia, an application to the Alexander von Humboldt foundation to consolidate the Munich connection, an application to the Unity Through Knowledge Fund involving the the Humboldt University in Berlin and the participation in an application for a FP7-PEOPLE-2010-ITN (Marie Curie Initial Training Network), coordinated through the University of Newcastle upon Tyne.

(iv) Workshop Organization

As part of our strategy to become a focal point for the increased uptake of Computational Solutions in the Life Sciences in the WBC, and as our major dissemination events, we successfully organized two international conferences on the Adriatic coast.

The first meeting, entitled the 2nd Opatija Meeting on Computational Solutions in the Life Sciences took place in Opatija, Croatia from the 4th to the 9th of September, 2007.

Figure 3. One of the graphics used for the promotion of the Opatija conference

Altogether 83 scientists registered for that meeting, of which 75 actually participated. The most numerous were scientists from Croatia (32), followed by Serbia (10), Germany (8), Slovenia (6), Romania (4), Switzerland (3), Macedonia, Kosovo, United Kingdom and Netherlands (2 scientists from each) and Bosnia and Herzegovina, Bulgaria, Italy, Austria and Norway (1 scientist from each). Three participants from Albania registered, but were unable to attend. The participants spanned the range from diploma students (1), doctoral students (29), and postdoctoral fellows, to senior scientists. Among the participants were the vast majority of persons that we had indicated in our project proposal to be our key collaborators.

The second event, entitled the 3rd Adriatic Meeting on Computational Solutions in the Life Sciences, took place in Primošten, Croatia, from the 1st to the 5th of September, 2009.

Figure 4. One of the graphics used for the promotion of the Primošten conference

Altogether, 73 scientists participated in the meeting. The most numerous were scientists from Croatia (43), followed by Germany (4), Serbia, Slovenia, Bosnia and Herzegovina and Switzerland (3 scientists from each), Macedonia, Austria, Italy, Sweden and Australia (2 scientists from each), Kosovo, the United Kingdom, Spain and the Netherlands (1 scientist from each). Two participants from Albania initially registered, but were unable to attend. The participants covered the range from diploma students (3), doctoral students and postdoctoral fellows (almost 40 altogether) to senior scientists. Among the participants were many scientists that we had indicated in our project proposal to be our strategic collaborators.

Both conferences involved specific activities designed to make the sometimes daunting world of computational biology more accessible to the student population, especially those from the WBC. In Opatija, we held *hands-on* practial sessions where we guided the students through the actual mechanics involved in carry out the calculations. In Primošten we changed the format slightly to more informal, tutorial style, presentations with the student populations able to ask questions both about the techniques in general and specifically about problems they were having in their own research.

Apart from the positive effect of nurturing a more close-knit WBC community in computational life sciences and allowing them to make important contacts with eminent scientists from the MS, the workshops also had the desired effect of increasing the visibility of the Centre, both as a unit but also for the individuals who devoted their time and effort to

organizing the meetings. Indeed, several opportunities to deliver invited lectures at prominent international conferences can be considered a direct result of the success of Workshops 1 and 2. Indeed the concept has been so well received in the regions that our partner scientists from the National Institute of Chemistry in Ljubljana have decided to continue the biennial series and we sincerely look forward to actively participating in the 2011 event.

1.1.4 Closing remarks

Overall, we feel that the ReCompSoLS project was an outstanding success. All major objectives were achieved and the team involved in the implementation of the activities functioned very efficiently together. Indeed, due to a fortunate set of circumstance combined with lots of hard work, the impact of many of the activities undertaken turned out to far exceed expectations. The position of the Centre for Computational Solutions in the Life Sciences is very much reinforced. We will continue to strive to achieve positive results in the future, including enhanced participation in the European Research Area.

1.2 Co-ordinator Contact Details

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1.3 Publishable results

As the ReCompSoLS project did not produce any exploitable results, no publishable results from the Final Plan for Using and Disseminating the Knowledge are included.