

SCIENTIFIC REPORT

1. Scientific content of the event

Between the 17th and 19th of September 2008 INCDSB organized the explorative workshop “The Danube Delta International Research Center - from Biology to Bioinformatics” in the framework of the conference “The Diaspora in the Romanian Scientific Research” organized and sponsored by the Prime Minister's Office, ANCS and the Romanian Academy.

The research objective of this workshop was the presentation of the Danube Delta International Research Center project and attaining a forum of discussions with Romanian researchers, both working within the borders of Romania and outside of these borders, on the necessity and importance of establishing this research center. Following the debates in the workshop's initial section and the opinions heard at the panel discussion on this theme, all participants signed a Memorandum for the establishment of the Danube Delta International Research Center.

In the workshop section dedicated to this research center the following talks were presented: “The Exceptional Generic Fund of the Danube Delta” and “Bird Population Dynamics in the Danube Delta”. These papers demonstrated the importance and the thematic richness of the research that can be performed within the Danube Delta biotope.

In the workshop section entitled “Danube Delta – between Equilibrium and lack of Equilibrium” well known researchers from Romania and abroad presented on the threat that invasive species pose (developing on a case study from Great Britain and Ireland), on the effect of human impact on the lakes in Danube Delta and also on the possibility of better bio-monitoring the ecological evolution of the Danube Delta biotope by installing cellular bio-sensors and bio-markers.

At the end of the first day of the workshop, all attendants agreed on the importance of setting the foundations of the Danube Delta International Research Center. They presented suggestions on the organizational structure and the functional aspects of this center and the Romanian researchers from abroad expressed the willingness to communicate to their peers in research institutes abroad on the research opportunities on a variety of topics that will be available at this new center.

Within the workshop section entitled “From Biology to Bioinformatics” the scientific objective was to prove that modern biological research is currently conducted with data collected by bioinformatics methods. Several fundamental research papers in bioinformatics were presented such as “An Analysis of Cellular Signaling using Systems Biology”, “Elements of Structural Bioinformatics”, “Partial Correlation – a Valid Instrument?” but authors also presented papers that pointed out the implications and importance of applying methods pertaining to bioinformatics to interpret certain biological processes. The discussions following the presentation in this section led to a future collaboration between Romanian researchers and their

peers abroad who benefit from having more performant software and hardware equipments at their disposal.

Summing up, the main objective of the event – introducing the “Danube Delta International Research Center” and having everybody attending the conference sign the Memorandum for its establishment- was fully attained.

2. Information regarding the organization of the event

The Exploratory Workshop “International Center of Research Danube Delta – from Biology to Bioinformatics” – WE17 was organized by the INCDSB staff.

Initially, announcements about the organization of this event were sent to a great number of researchers from the Diaspora and from Romania, who could have been interested to participate. Information about the persons interested in this manifestation was collected and new on-line invitations were sent to the researchers in the Diaspora and to those from the country who do research in areas connected with the organized event.

After its assignation, the organization comity established the list of participants and the schedule of the workshop.

After the first contacts and the list of the invited persons were made, we realized that one of our guests from the Diaspora was on the list of another workshop as well. So that the things would not get complicated, we all agreed that the guest would stay on our list, and the people from the other workshop interested in the guest’s speech would become a part of our new list of guests. The final list of the participants was printed and then, after discussions with the guests, we established the sections of the workshop and the list of the lectures that were to be held.

The institute’s conference room is well equipped with the necessary devices for screen projections and, because of this fact, we did not have to rent a space in order to organize this event.

For the accommodation of the guests from the Diaspora we made reservations to a hotel in the center of Bucharest so that the guests could easily get to all the events that were organized.

A few days before the event, we attended the administrative aspects by acquiring all necessary products and contracting a catering firm for providing lunch during the days of the workshop.

One day before the beginning of the event, when everything was finalized and the invitations for the guests were already brought to the institute, we received the application of a person from the Diaspora who wished to attend our event. We managed, with help from UEFISCSU, to modify the schedule, but we could not update our guests list.

At the moment of their arrival at the head office of the institute, the participants were registered by the staff in the organizing comity. The guests from the Diaspora and from the Romania received all the materials that UEFISCSU had sent us (the tag, the backpack, the symposium documentation), as well as the documentation that presented the activity of INCDSB.

The institute assured, by the presence of a professional photographer, the capturing of the most important moments of the workshop (including the visit of Mr. Anton Anton, the president of ANCS).

We consider that the event was a success both scientifically and from an organizing point of view. The environment during the workshop was very agreeable and appropriate for discussions that lead to creating new contacts between the researchers from different fields.

Informational exchange between the guests from the Diaspora and the researchers from Romania was made and the discussions on the subjects presented at the workshop proved to be of interest to all the participants.

Final timetable

The Danube Delta International Research Center - from Biology to Bioinformatics

Miercuri, 17 Septembrie 2008

Proiectul “Centrul Internațional Delta Dunării”

09:30 – 10:00 **Manuela Elisabeta Sidoroff** – Prezentarea proiectului *Centrul Internațional Delta Dunării*

10:00 – 10:30 **Mihai Coroi** – *Folosirea GIS în cartografierea și analiza tipurilor de vegetație și relief de-a lungul râurilor din sudul Irlandei*

10:30 – 11:00 Pauza

11:00 – 11:30 **Alexandru Manoliu** – *Geofondul micologic de excepție al Deltei Dunării*

11:30 – 12:00 **Mircea Gogu** – *Dinamica populațiilor de pasări din Delta Dunării*

12:00 – 14:00 Pauza prânz, catering

Delta Dunării între echilibru dinamic și dezechilibru

14:00 – 14:30 **Mihai Coroi** – *Amenințarea speciilor invazive* – Studiu de caz din Marea Britanie și Irlanda

14:30 – 15:00 **Laura Parpala, Ionica Doina** – *Efectul impactului entropic asupra evoluției lacurilor din Delta Dunării*

15:00 – 15:30 **Daniela Bratosin** – *Biomonitorizarea Deltei Dunării pe baza de biomarkeri și biosenzori celulari – o necesitate de viitor cu dubla importanță*

15:30 – 16:00 Pauza

16:00 – 17:00 Masa rotundă: *Centrul Internațional Delta Dunării* – moderatori Manuela Elisabeta Sidoroff și Anca Oancea

Joi, 18 Septembrie 2008

De la biologie la bioinformatică

09:30 – 10:00 **Sorin Draghici** – *Analiza cailor de semnalizare celulară cu ajutorul biologiei sistemelor (systems biology)*

10:00 – 10:30 **Andrei Petrescu** – *Elemente de bioinformatica structurala si utilizarea lor în biochimie*

10:30 – 11:00 Pauza

11:00 – 11:15 **Voicu Boscaiu** – *Corelația parțială – un instrument fiabil?*

11:15 – 11:30 **Stefan Stefanescu** – *Compararea algoritmilor de simulare stocastica în biologie*

11:30-11:45 **Daniel Racoceanu** – Sistem Translational de gradare a cancerului mamar prin analiza autonoma a imaginilor histopatologice într-un cadru microscopic virtual

11:45 – 12:30 Masa rotunda: *Bioinformatica în România: prezent si perspective*, moderator Sorin Draghici, Liviu Badea

12:30 – 14:30 Pauza prânz, catering

Modelarea matematica a proceselor biologice

14:30 – 15:00 **Gheorghe Paun** – *Calcul cu membrane – stare curenta*

15:00 – 15:30 **Marian Gheorghe** – *Biologie computațională – modele discrete*

15:30 -16:00 Pauza

16:00 – 16:30 **Ion Ardelean** – *Modelarea respirației aerobe și a activității canalelor mecanosenzitive la bacterii folosind calculul cu membrane*

16:30 – 17:00 **Ion Petre** – *Un proiect de bio-modelare matematica: reacția celulelor eucariote la soc termic*

Presented themes

The heat shock response is an ancient, evolutionary conserved regulatory mechanism that allows the cell to quickly react to elevated temperatures. The heat shock response has been subject of active research for at least two reasons. On one hand, as it represents an exceptionally well-conserved signaling mechanism, it is a good candidate for deciphering the mechanistic principles of cellular regulatory networks. On the other hand, heat shock proteins are interesting, regardless of the regulatory aspects of the heat shock response, as they are of fundamental importance for many key biological processes in cells. Therefore, understanding the details of the heat shock response has broad ramifications for the onset and treatment of a number of diseases, including both neurodegenerative disorders, cancer, aging, and cardiovascular diseases. Despite intense research in this area and a number of models that have been presented to cover this process, a true mechanistic understanding of the heat shock response is still missing in the literature. In this paper we propose such a model, based on well-documented molecular reactions only, able to capture in mechanistic details the main aspects of the regulation. The model is able to account for the swift heat-induced transactivation of the genes encoding for heat shock proteins, the backregulation of the transcription, its return to the original level once the stress is removed, a lower response to a second consecutive heat shock.

We discuss a new, simple mechanistic model for the heat shock response, consisting of a minimum number of modules. In contrast with previous attempts to model the eukaryotic heat shock response, our model does not include modeling "blackboxes" (such as hypothesized components and biochemical reactions). We also consider present a mathematical model associated with the model and its experimental validation. For specific parameter estimation and model validation, we use both literature data, as well as new experimental data. In light of the

archetypal nature of the heat shock response, we believe that the presented minimal model should be useful as a general basis for modeling strategies of more complex cellular processes.

Ion Petre

A systems biology approach to pathway analysis

A common challenge in the analysis of genomics data is trying to understand the underlying phenomenon in the context of all complex interactions taking place on various signaling pathways. A statistical approach using various models is universally used to identify the most relevant pathways in a given experiment. In this talk, we show that despite its general adoption, this statistical analysis is unsatisfactory, and can often provide incorrect results. Using a systems biology approach, we developed an impact analysis that includes the classical statistics, but also considers other crucial factors such as the magnitude of each gene's expression change, their type and position in the given pathways, their interactions, etc. On several illustrative data sets, the classical analysis produces both false positives and false negatives while the impact analysis provides biologically meaningful results.

Sorin Draghici, Ph.D.

5. The final list of the participants

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