Hungary-Serbia
IPA Cross-border Co-operation Programme

Jó szomszédok a közös jövőért

A MAGYAR TUDOMÁNY ÜNNEPE

Magyar Tudomány Ünnepe 2010

Határok nélküli tudomány

KIHÍVÁSOK ÉS LEHETŐSÉGEK
A TUDOMÁNYTERÜLETEK HATÁRÁN

Modellezés az élettudományokban

2010. december 3. péntek

Szeged, SZAB-székház nagyterem

az SZTE Orvosi Fizikai és Orvosi Informatikai Intézet,
Bolyai Intézet és az Újvidéki Egyetem Matematikai és Informatikai Intézet,
MTA Szegedi Akadémiai Bizottság Matematikai és Fizikai Szakbizottság,
Orvostudományi Szakbizottság és Gyógyszerészeti Szakbizottság
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9 50 Megnyitó

10 00 *Bari Ferenc*
(SZTE Orvosi Fizikai és Orvosi Informatikai Intézet)
A mikrokeringés modellezése

10 25 *Szappanos Balázs*
(MTA SZBK Biokémiai Intézet)
Nagyléptékű anyagcserehálózatok modellezése

10 50 *Kerényi Ádám*
(MTA SZBK Bioinformatikai Csoport)
Bakteriális kommunikáció és kooperáció

11 15 Szünet

11 40 *Mándity István*
(SZTE Gyógyszerkémiai Intézet)
β-Peptid foldamerek önrendeződésének sztereokémiai és oldallánctopológiai szabályzása

12 05 *Tóth János*
(BMGE Matematikai Intézet)
Részletes egyensúly a kiralitás modelljeiben

12 30 *Karsai János*
(SZTE Orvosi Fizikai és Orvosi Informatikai Intézet)
Számítógépes modellezés a Mathematica szoftverrel: fajok területért folyó versengésének sejtautomata modelljei

12 55 Ebédszünet

14 00 *Bakonyi Tamás*
(SZIE Állatorvos-tudományi Kar, Járványtani és Mikrobiológiai Tanszék)
Nyugat-nílusi vírus okozta járvány Magyarországon

14 25 *Solymosi Norbert*
(MTA-BCE „Alkalmazkodás a Klímaváltozáshoz" Kutatócsoport)
Bayes-i epidemiológiai modellek

14 50 *Oroszi Beatrix*
(Országos Tisztifőorvosi Hivatal)
A matematikai modellezés lehetséges helye és szerepe a fertőző betegségek epidemiológiájában Magyarországon

15 15 *Röst Gergely*
(MTA-SZTE Analízis és Sztochasztika Kutatócsoport)
Determinisztikus járványterjedési modellek

15 40 Szünet

16 00 *Dénes Attila*
(SZTE Bolyai Intézet)
Tanganyika-tavi halpopulációk dinamikája

16 25 *Knipl Diána*
(SZTE Bolyai Intézet)
Korspecifikus influenza vakcinálási stratégiák

16 50 *Szimjanovszki Irma*
(SZTE Orvosi Fizikai és Orvosi Informatikai Intézet)
Fajok területfoglalásának modellezése

17 15 Zárás

Ferenc Bari

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MODELING OF MICROCIRCULATION-BRAIN IN THE FOCUS

The presentation focuses the cerebral microcirculation that responds to a plethora of different stimuli, both physical and chemical, at a variety of time scales, and by a great variety of pathways. No any existing models of the brain circulation have the scope or flexibility to deal with the complexities which arise in many medical situations. One the other hand, simplified models are used to demonstrate the ways a healthy brain circulation responds to changes in a variety of stimuli, including systemic arterial pressure, blood CO_2 levels, blood oxygenation, and functional activity of the brain. The model I would like to present provides basic insight to the regulation of cerebral microcirculation and is usable in courses of different levels of medical education.

Balázs Szappanos

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MODELING LARGE-SCALE METABOLIC NETWORKS

A major goal of systems biology is to relate genome sequence to cellular behaviour. It has recently become possible to reconstruct cell-scale metabolic networks of microbes using available genomic, biochemical and physiological data. These reconstructions are not only databases of the metabolism of a certain organism, but they can also be used to predict quantitative phenotypic effects, e.g. those of gene knockouts and gene additions. One way to do this is to convert the metabolic network reconstruction into a model which contains all known reactions of an organism in a mathematically computable fashion. We present a basic overview of the computational tools to simulate large-scale metabolic networks along with some applications in basic and applied research.

Ádám Kerényi

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BACTERIAL COMMUNICATION AND COOPERATION

Multispecies microbial consortia are a major form of life that includes examples of medical significance such as the gut flora, opportunistic pathogens living in hospital environments, bacterial-fungal consortia present in dental cavities etc. The stability of such consortia is poorly understood and is generally discussed in terms of species-specific mechanisms. On the other hand, there is a growing body of evidence that there are general stability criteria for polymicrobial consortia. Experimental and theoretical studies indicate that some species are capable of stable, long-term collaboration while non-cooperating cheat mutants can cause a local collapse of the community. These simple mechanisms provide a protection against unwanted mutations and environmental challenges so they may serve as guidelines for developing defense strategies against mixed microbial infections.

István Mándity

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TAILORING B-PEPTIDE FOLDAMERS BY BACKBONE STEREOCHEMISTRY

Foldamers, the non-natural self-organizing biomimicing systems show similar properties to the proteins, e. g. they have a tendency to fold into the specific periodic compact structures. The most thoroughly studied representatives of this field are the β-peptides consisting of β-amino acids. The prevailing 3D structure of a foldamer is determined by many factors, such as the stereochemistry, the residue type, the side-chain topology and chemistry, etc.

Based on the backbone stereochemistry, binary geometrical descriptors were devised in order to gain a simplified representation of the stereochemical building blocks governing formation of the secondary structure of peptidic foldamers. Analysis of the bitstreams of the known β-, α- and α/β-peptide secondary structures demonstrated clear relationships between the bit pattern and the preferred self-organization type. Data on the *de novo* designed foldamers demonstrate that the helices complying with the rules adopt novel biomimetic helices in solution (Fig. 1).

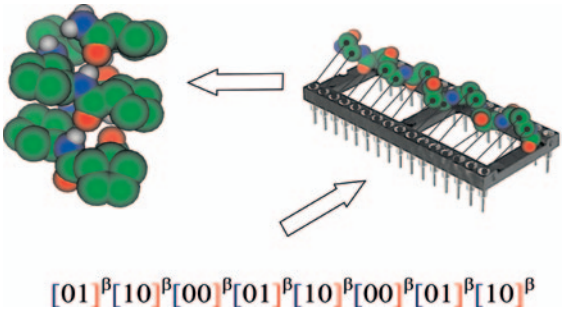

Figure 1. The *de novo* design methodology

Our results nevertheless suggest an interesting analogy: the peptidic foldamer chain acts as an analog computer executing the commands encoding the sequence of stereochemical building blocks. In this way, the proposed binary codes can be regarded as the basic instruction set in the assembly language of the peptidic foldamer sequences as analog computers.

János Tóth

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DETAILED BALANCE IN THE MODELS OF CHIRALITY (INVESTIGATING THE DYNAMICS OF BIOLOGICAL MODELS USING THE *MATHEMATICA* PACKAGE REACTIONKINETICS)

Starting from a special model of chirality we show how the mathematical theory of formal reaction kinetics and the program package based on it can be utilized when analyzing the variations of models. The speciality of the package is that it highly utilizes the advantages of Mathematica,

- it automatically writes down and numerically solves the kinetics differential equation,
- it can also simulate the usual stochastic model,
- it calculates the graph-theoretic and linear algebraic quantities which allow to deduce statements on the qualitative behavior of the concentration of the different species.

Barabás, B.; Tóth, J.; Pályi, G.: Stochastic aspects of asymmetric autocatalysis and absolute asymmetric synthesis, *J. Math. Chem.* 48 (2) (2010), 457–489.

Sipos, T.; Tóth, J. ; Érdi, P.: Stochastic simulation of complex chemical reactions by digital computer, I. The model, *React. Kinet. Catal. Lett.* 1 (1) (1974), 113–117.

Tóth, J.; Szili, L.; Zachár, A.: Stability of polynomials, *Mathematica in Education and Research* 7 (2) (1998), 5-12.

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COMPUTER-AIDED MODELING WITH *MATHEMATICA*: MODELING THE FIGHT OF SPECIES FOR TERRITORY WITH CELLULAR AUTOMATA

Simulation is the only effective tool for the study of several problems in biomedical modeling. Hence, computing and visualization tools became unavoidable. There are several – either general or special -computer software programs available designed for different kind of problems, such as Mathematica, Maple, Matlab, Modelica, Anylogic, etc.
In our talk, we consider stochastic cellular automata as tools in ecological research. After a short introduction to cellular automata, we briefly study the spatio-temporal development of some single species territory-based models. Then we consider competition of several species fighting for territory. We can find simulations can give us a lot of information on special properties such as aggregation, diffusion, role of neighbors in colonization of empty cells or extinction of the species from a cell.

Tamás Bakonyi

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WEST NILE VIRUS ENDEMIC IN HUNGARY

The West Nile virus is a world-wide distributed flavivirus, which is the causative agent of the disease "West Nile fever". This disease is characterized by fever, meningitis and encephalitis. The natural hosts of the virus are typically wild birds. The virus is transmitted between susceptible hosts by blood-sucking insects, predominantly culicid mosquitoes (arbovirus). The virus is maintained in the nature by the wild bird – mosquito cycle, but incidental mammal hosts may also get infected. Clinical disease is usually observed in humans and in horses. Although most infections remain subclinical, neuroinvasive WNV strains may cause lethal encephalitis.
A WNV strain emerged in the USA in 1999, and within five years spread all over the North-American continent. Several studies were focused on the characterisation and modeling of the spread of the virus in the susceptible host populations.
In Hungary the first WNV cases were diagnosed in 2003. In 2004, an exotic, lineage 2 virus strain emerged in the South-eastern region of Hungary, and caused encephalitic cases in birds of prey. Within a few years the

virus established itself in the region, and an explosive geographic spread was observed in 2008. Besides wild birds, lethal encephalitic cases were diagnosed in horses and in a sheep. Several human encephalitic illnesses were also reported. The virus was dispersed in all regions of Hungary, and was also spread to the Eastern parts of Austria. Subsequent outbreaks were diagnosed in the epidemic seasons of 2009 and 2010. In 2010 the lineage 2 strain also emerged in North-east Greece, with several human outbreaks and causalities.
Mathematical modeling might be a useful tool to estimate the risk of virus infections, and to predict epidemiological processes. In the case of WNV, several factors influence the extent and intensity of the seasonal epidemics. Besides climate and weather (temperature, humidity, and precipitation), the number and abundance of amplifying hosts, competent vectors, susceptible hosts, and suitable habitats should be taken into consideration. Human activity may also influence the spread of the agent.
Basic research is needed to identify the data collection methods and intensity, which could provide sufficient information for the reliable modeling of WNV epidemiological processes in Hungary.

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BAYESIAN MODELS IN EPIDEMIOLOGY

In many scientific or practical problems it is an important task to manage the uncertainty in variables, parameters of interest. Beside the frequentist approach Bayesian methods for statistical analysis, modeling are being increasingly used in different research fields (e.g. life or social science) to handle uncertainty. In quantitative epidemiology it is also a crucial object to make probability statements about parameters related to diseases, infections in populations.
In the talk, we present some main differences between frequentist and Bayesian approaches with examples from the area of veterinary epidemiology. By the examples we show some neglected viewpoints should be highlited for people working with population based health-related problems.

Beatrix Oroszi

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THE PLACE AND ROLE OF MATHEMATICAL MODELLING IN THE EPIDEMIOLOGY OF COMMUNICABLE DISEASES IN HUNGARY

Mathematical models are one of the most important types of epidemiological models. The roles of modern outbreak analysis and modelling in public health decision making is increasingly recognised. Models have benefit of making assumptions explicit and being testable.
During the presentation the author will describe the three main areas, where mathematical modelling is generally applied in epidemiology; defining optimal control strategies, predicting future numbers of cases and better understanding of disease occurrence patterns. Examples coming from the modelling of pandemic influenza 2009 and other diseases, and from the design and evaluation of intervention programs, such as vaccination, will demonstrate some of the main applications of mathematical modelling in public health.
Advanced analysis and modelling is useful to assist in public health policy making at strategic and tactical levels, however, there are some difficulties in the application of the results and predictions in the practical field work and in decision making.

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DETERMINISTIC MODELS IN MATHEMATICAL EPIDEMIOLOGY

We give a general overview of compartmental models used in mathematical epidemiology. Such models are typically formulated as a system of differential equations. We introduce the basic concepts, such as reproduction numbers and final size relations, and show how one can build the model structure based on the transmission mechanisms and other important features of a given disease and how to incorporate various intervention strategies. Advanced modeling often requires the application of infinite dimensional dynamical systems, typically due to heterogeneity (when a population is structured by age, size, spatial position or any relevant characteristics) or time delays.

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DYNAMICS OF FISH POPULATIONS IN LAKE TANGANYIKA

This is a joint work with Professors László Hatvani and László L. Stachó. We investigate a population dynamical model initiated by László Stachó. This model describes the change of the amount of two fish species – a carnivore and a herbivore – living in Lake Tanganyika. The model consists of two parts: the development of the population during a year is described by a non-autonomous system of differential equations while the reproduction at the end of each year is described by a discrete dynamical system. We showed that the equilibrium of the limit equation of our system is a globally eventually uniform-asymptotically stable point of the non-autonomous system. In the proof we use linearization, the method of limit equations and Lyapunov's direct method. We also show some results about the behaviour of the whole system with the discrete part of the reproduction and about a slightly modified system where the growth of the vegetation left on its own would be exponential.

Diána Knipl

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MODELLING THE STRATEGIES FOR AGE SPECIFIC VACCINATION SCHEDULING DURING INFLUENZA PANDEMIC OUTBREAKS

The *A(H1N1)v* is a subtype of inuenza A virus which appeared in March 2009. Finding optimal policies to reduce the morbidity and mortality for inuenza pandemics is a top public health priority. Using a compartmental model with age structure and vaccination status, we examined the effect of age specific scheduling of vaccination during a pandemic infuenza outbreak, when there is a race between the vaccination campaign and the dynamics of the pandemic. Our results agree with some recent studies on that age specifcity is paramount to vaccination planning. However, little is known about the effectiveness of such control measures when they are applied during the outbreak. We found that without reallocating any vaccines between age groups, the best scheduling scheme can decrease the overall attack rate by up to 10%. We demonstrate the importance of early start of the vaccination campaign, since ten days delay may increase the attack rate by up to 6%. Taking into account the delay between developing immunity and vaccination is a key factor in evaluating the impact of vaccination campaigns. We provide a general framework which will be useful for the next pandemic waves as well. The applicability of our population dynamic model is demonstrated for the first wave of *A(H1N1)v* in Hungary.
At last, we give a brief insight into the possibilities of developing the model with the help of integro-differential equations.

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MODELING THE COMPETITION OF SPECIES FOR TERRITORY

We consider territory-based population dynamics models and investigate the spread of species and their competition for territories where the change of the occupied territory is examined instead of the number of individuals. All of species can occupy empty patches and some (or all) of them can occupy patches that are already occupied by others. The latter phenomenon is called overcolonization. In case of two species we can suppose that there is no interaction between species. In this case only boundary equilibria exist. In other case some hierarchical relations are assumed between populations, so interior equilibrium exists which is globally asymptotically stable. The model of general overcolonization is less studied since the analysis is extremely difficult. We show that the output of the species' fight depends on the initial conditions (interior equilibrium exists however it is not globally asymptotically stable). Finally, we consider even more general models in which the colonization and extinction rates depend on the environment in different ways. In real life both the coloniziation capability and the extinction can depend on the neighborhood (or density) of the atomic patches. The behavior of such models is much more complicated. We consider different cases in which neighbors can strengthen or even weaken each other. Our results are illustrated by realtime demonstrations in *Mathematica*.

Good neighbours creating common future

IPA Cross-border Co-operation Programme HU-SRB/0901/221/088

TEACHING MATHEMATICS AND STATISTICS IN SCIENCES: MODELING AND COMPUTER-AIDED APPROACH

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