



Coordination of Biological and Chemical IT Research Activities

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BioChemIT2012

Report on first COBRA Summer School

WP3 D3.2

Jan. 22nd, 2013 Version 1



Abstract

The 1st COBRA Summer School on Biological and Chemical Information Technologies (BioChemIT2012) was held from September 9th, 2012, until September 22nd, 2012, in San Candido/Innichen, Southern Tyrol, Italy. The objective of the BioChemIT2012 summer school was to provide a state-of-the-art presentation of the field of novel unconventional biological and chemical information technologies, teach related skills to the students, and provide a stimulating environment for fruitful interdisciplinary interactions and discussions. Thirteen multinational and multidisciplinary lecturers presented talks, discussions, practical exercises and a laboratory course. Twenty-one students from several continents with different backgrounds attended the summer school and participated also in a poster session and workgroups with self-proposed topics.

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1. Date and Location

The 1st COBRA Summer School on Biological and Chemical Information Technologies (BioChemIT2012) was held from September 9th, 2012, until September 22nd, 2012, in San Candido/Innichen, Southern Tyrol, Italy.

2. Objectives

The objective of the BioChemIT2012 summer school was to

1. provide a state-of-the-art presentation of the field of novel unconventional biological and chemical information technologies, that is, novel biological, chemical and hybrid (mems) computational substrates,
2. teach related skills that widen the competences of the students to construct and study such novel technologies, and
3. provide a stimulating environment for fruitful trans disciplinary interactions and discussions.

3. Committees and Organization

A website was created with the information about the summer school:

<http://www.cobra-project.eu/summerschool.html>

The program booklet containing the program, lecturer CVs and lecture abstracts is available here:

<http://www.cobra-project.eu/docs/SummerSchoolBooklet.pdf>

The **program and student selection committee** was formed by the following scientific board:

- Peter Dittrich (FSU Jena, program chair)
- Martyn Amos (MMU, Manchester)
- John McCaskill (RUB Bochum)
- Irene Poli (UNIVE, Venice)
- Steen Rasmussen (FLINT, Odense)

Responsible for venue management and travel **organization** were:

- Irene Poli (UNIVE, Venice, organization chair)
- Debora Slanzi (UNIVE, Venice)

- Matteo Borrotti (UNIVE, Venice)
- Agnese Boscarol (UNIVE, Venice)

Student **registration** and admission as well as **program booklet** preparation:

- Gabi Escuela (FSU Jena)
- Martin Engler (FSU Jena)

The **website** was maintained by:

- Margaret Taylor (MMU)

4. Program and Participants

The school ran for two weeks. Approximately 50% of the school's schedule was devoted to lectures provided by experts. The other 50% of the time was reserved for working groups that students formed at the beginning of the school.

The content of the program ranges from theory (e.g. unconventional computing paradigms, theoretical results) over computer simulation and programming to courses focusing on lab and experimental issues.

4.1. Lecturers and Supervisors

The following lecturers (in order of appearance) contributed to the summer school:

- Harold Fellermann (University of Southern Denmark, Odense)
- Jasmin Fisher (Cambridge University)
- Tetsuya Yomo (Osaka University)
- Klaus-Peter Zauner (University of Southampton)
- Jerzy Górecki (Polish Academy of Sciences, Warsaw)
- Maurits de Planque (University of Southampton)
- Philip King (University of Southampton)
- Irene Poli (University Ca'Foscari, Venice)
- Ángel Goni Moreno (Manchester Metropolitan University)
- Pasquale Stano (University of Roma Tre)
- Norman Packard (European Center for Living Technology, Venice)

- Steen Rasmussen (University of Southern Denmark, Odense)
- Peter Dittrich (Friedrich Schiller University, Jena)

The following additional support staff (in alphabetical order) attended the summer school:

- Matteo Borotti (University Ca'Foscari, Venice)
- Martin Engler (Friedrich Schiller University, Jena)
- Debora Slanzi (University Ca'Foscari, Venice)

4.2. Program

The summer school took place from Sep. 9th, 2012 until Sep. 22nd, 2012 with the first as well as the last day reserved for travel and Sep. 16th for an extracurricular excursion. Most lectures were scheduled in the morning and the afternoon reserved for workgroup meetings.

The lectures included talks, discussions, practical exercises and a laboratory course. To familiarize the participants and lecturers with the research topics of the audience, a poster session was held. Workgroups were formed by students with self-proposed topics and the results were discussed at the end of the summer school.

The program, lecturer CVs and abstracts were also made available in the summer school program booklet, which was distributed at the beginning of the summer school and can be downloaded at <http://www.cobra-project.eu/docs/SummerSchoolBooklet.pdf>

Lectures and informal activities took place at:

	9:00 – 10:30	11:00 – 12:30	14:00 – 15:30	16:00 – 17:30
Mon, 10th	Opening, Overview	Getting to know each other	<i>Compartments in Biochemical Information Technology</i> Harold Fellermann	Poster Session
Tue, 11th	<i>Executable Biology</i> Jasmin Fisher	<i>Constructive Approach to Life's Characteristics</i> Tetsuya Yomo	Workgroup Formation	
Wed, 12th	<i>Constructive Approach to Life's Characteristics</i> Tetsuya Yomo	<i>Executable Biology</i> Jasmin Fisher		
Thu, 13th	<i>Informed Matter: The Confluence of Information Processes and Material Science</i>	<i>Compartments in Biochemical Information Technology</i> Harold Fellermann Klaus-Peter Zauner		
Fri, 14th	<i>Reaction-Diffusion Computing</i> Jerzy Gorecki			
Sat, 15th	<i>Microscale BioChemIT Devices – Applications and Fabrication</i> Maurits de Planque	<i>Informed Matter: The Confluence of Information Processes and Material Science</i> Klaus-Peter Zauner	<i>Make your own microfluidic chip!</i> <i>Practical lab excercise</i> Philip King, Maurits de Planque, Klaus-Peter Zauner	
Mon, 17th	<i>Evolutionary Design of Experiments</i> Irene Poli	<i>On Genetic Logic: Design, Modeling and Simulation</i> Angel Goni-Moreno		<i>Liposome Technology for Minimal Cells, Synthetic Communication, Smart Drug Delivery</i> Pasquale Stano
Tue, 18th	<i>Liposome Technology for Minimal Cells,</i>	<i>Applied Experimental Design</i>		<i>Living Technologies and Bottom-up Protocells</i>

	<i>Synthetic Communication, Smart Drug Delivery</i>	Norman Packard		Steen Rasmussen
Wed, 19th	Pasquale Stano			
	<i>Applied Experimental Design</i>	<i>On Genetic Logic: Design, Modeling and Simulation</i>	<i>Living Technologies and Bottom-up Protocells</i>	
	Norman Packard	Angel Goni-Moreno	Steen Rasmussen	
Thu, 20th	<i>Liposome Technology for Minimal Cells, Synthetic Communication, Smart Drug Delivery</i>	<i>Organization-Oriented Chemical Computing</i>		
	Pasquale Stano	Peter Dittrich		
Fri, 21st	Presentation of Workgroup Results	Discussion, Open Problems	12:00 Summer School Closing	

Legend:

Lecture	Informal activity
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4.3. Abstracts

Harold Fellermann

The role of Compartments in Biochemical Information Technology

Supramolecular compartments, such as vesicles, play a vital role in biology as well as in many ChemBio-ICT applications. Compartments can encapsulate various chemicals, and thus concentrate or separate reactants. In addition, their surfaces can be decorated with functional molecules such as membrane proteins, anti-bodies, etc., that can greatly modify their behavior. This allows compartments to become agent-like entities in ChemBio-ICT applications.

In the first lecture, we will discuss the properties of biochemical compartments and how these can enable and enhance biotechnological functionality beyond the traditional mindset of well-stirred tank reactors. We will introduce state-of-the-art modeling approaches from computational physics that allow us to investigate self-assembly as well as static and dynamic properties of supramolecular compartments.

In the second lecture we will continue our investigation of compartmentalization and encapsulation, but this time from a logical point of view: rather than understanding compartments as assemblies of individual molecules, we now see them as agents on their D3.2

own right. To this end, we will present modeling frameworks (e.g. the brane calculus) that allow us to describe compartments as interacting complex objects.

The presentation will draw on examples from several ChemBio-ICT projects that our research group is currently pursuing in both theory and experiment.

Jasmin Fisher

Executable Biology

The decade of genomic revolution following the human genome's sequencing has produced significant medical advances, and yet again, revealed how complicated human biology is, and how much more remains to be understood. Biology is an extraordinary complicated puzzle; we may know some of its pieces but have no clue how they are assembled to orchestrate the symphony of life, which renders the comprehension and analysis of living systems a major challenge. Recent efforts to create executable models of complex biological phenomena - an approach we call Executable Biology - entail great promise for new scientific discoveries, shedding new light on the puzzle of life. At the same time, this new wave of the future forces computer science to stretch far and beyond, and in ways never considered before, in order to deal with the enormous complexity observed in biology. This lectures series will provide an introduction to Executable Biology, through various success stories in using formal methods (e.g., Boolean/Qualitative Networks, compositional state-machines) to tackle specific biological questions, and visualization and modeling tools designed for biologists to model cellular processes in a visual-friendly way.

Tetsuya Yomo

Constructive Approach to Life's Characteristics

What makes lives different from others? Natural cells evince phenomena more ordered than a simple assembly of molecules. There is a gap between living and non-living worlds. Only once the transition over the gap has ever occurred, which is the origin of life. In the first lecture, I would explain some experiments to construct and evolve a cell-like model from molecules to address the following questions: Why must the complicated reaction network have been confined into micro-scaled environments? What conditions are required for the simple assembly of bio-molecules to take Darwinian evolution?

Another characteristic of life is stochasticity. With the same genetic background and the same inputs from environments, organisms sometimes behave more stochastically or less precisely than machines. In terms of accuracy or efficiency, life is far behind machine. In the second lecture, focusing on the gene expression in cells, I would address the questions: What causes the cells fluctuate their gene expression? Does the fluctuation give cells some flexibility to environmental changes? What advantage has maintained the fluctuation at the cost of low efficiency in the course of evolution?

Klaus-Peter Zauner

Informed Matter: The Confluence of Information Processes and Material Science

The 19th century brought about an understanding of energy for the molecular level. The 20th century saw rapid progress in the manipulation of matter enabling the purposeful design of

organic molecules, and the advent of biochemistry. The latter opened the view on marvelously sophisticated macromolecules and supra-molecular structures - but offered no path to enter this design space. It is for the 21st century to complement the achievements of the past with the application of information processes at the molecular scale. When this hurdle can be tackled, however, the technology impact will rival the advent of organic chemistry.

To make the complexification of matter exhibited by nature amenable to engineering, it will be necessary to mimic the molecular level information processes employed by organisms to fabricate and maintain their molecular machinery. Living systems are peculiarly organised inhomogeneous arrangements of the very same matter that forms the remaining dead universe. Their highly organised state can be sustained only by active maintenance which in turn necessitates the processing of information – life without computation is inconceivable. Conversely, the proficiency with which single-cell organisms maintain their living state under adverse conditions and severe constraints in energy and material indicates the efficiency that may be achieved through the direct use of the physical characteristics of materials for computation.

This course will explore the dual role of molecular information technology as a facilitator for the synthesis of complex materials and as a resource for computational power.

Jerzy Górecki

Reaction-Diffusion Computing

There are many ways in which the time evolution of a medium where chemical reactions proceed can be used for information processing. During my lecture I will consider a spatially distributed medium, characterized by concentrations of reagents involved represented by functions of space and time. The reagents interact locally via chemical reactions. They can also migrate in space and influence the time evolution in the neighborhood. I will assume that the diffusion of molecules is responsible for migration and so the time evolution of the considered medium can be described by a set of parabolic differential equations where the local terms model the chemical kinetics and the differential operators describe diffusion. The research on information processing with such a medium is called the reaction-diffusion computing¹.

The key question is how to interpret the natural time evolution of the medium defined by reagents involved in the language of information. I will show that there are many alternatives. The choice depends of the properties of the medium. For example if we consider an excitable chemical kinetics then the straightforward method of information coding is related to the presence of excitation at a given point of the medium at a selected time. It can be assumed that an excitation pulse represents the symbol 1 and its absence the symbol 0. Within such representation we can introduce the binary logic, gates and operations on strings. It can be shown that a universal computer can be made with an excitable chemical medium. The realization of information processing operation simplifies if the medium has an intentionally introduced geometrical structure of regions characterized by different excitability levels. We show that in information processing applications the geometry plays an equally

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Adamatzky A, De Lacy Costello B et al. (2005) Reaction-Diffusion Computers. Elsevier Science

important role as the dynamics of the medium and allows one to construct devices that perform complex signal processing operations even for a relatively simple kinetics of the reactions involved. I will review a number of chemical realizations of simple information processing devices like signal diodes, logical gates or memory cells and we show that by combining these devices as building blocks the medium can perform complex operations like for example counting of arriving excitations. If time allows I will discuss information processing potential of a medium composed of droplets containing an oscillating chemical reaction.

The ideas of chemical reaction-diffusion computing can be translated to other physical systems showing similar properties. The solid analog of wet chemistry is the medium composed of carriers in specially prepared semiconductors.

Maurits de Planque

Microscale BioChemIT Devices: Applications and Fabrication

Studying, or perhaps more appropriately for BioChemIT, implementing chemical or biochemical reactions or bacterial cultures in small volumes has many advantages. Microliter volumes obviously require much less chemicals than conventional milliliter reaction chambers such as cuvettes or Petri dishes, enabling efficiency savings when dealing with costly biomolecules. Furthermore, multiple reactions or environmental conditions can be evaluated simultaneously in an array of isolated microwells. However, these small reaction chambers can easily be connected to each other in various 2D patterns, giving rise to a heterogeneous reaction medium. Such compartmentalization makes it possible to mimic some key concepts of biological information processing, for example the threshold-modulated pulse propagation between neurons in the brain.

The fabrication of microscale wells and channels is based on well established methods from the IC industry, most notably lithography with UV light. With the relatively recent development of 'soft' lithography variations, in which a micropatterned master is used to cast an inverse copy of an elastomeric polymer, the fabrication process can also be performed in a standard laboratory rather than a clean room facility. For small reaction chambers evaporation should be avoided, hence it is usually necessary to bond the micropatterned substrate to a flat layer, typically glass because of its chemical compatibility and optical transparency. To fill the device or to introduce different chemicals at various stages of the reactions, microfluidics are also required. All these methods will be explained with an emphasis on practical issues such as the smallest and largest dimensions that can be realized with a given technique.

Philip King, Maurits de Planque and Klaus-Peter Zauner

Introduction to PDMS microfluidics: Make your own microfluidic chip

There will be an opportunity to gain hands-on experience with soft lithography: creating an elastomeric replica from a micropatterned master mold and bonding this replica to a glass substrate to define microchannels and microchambers that are visualized with a colored solution. This exercise illustrates miniaturization approaches to BioChemIT. It also shows that soft lithography-enabled microfluidic experiments can be performed in any laboratory and do not require special equipment.

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Irene Poli

Evolutionary Design of Experiments

Several areas of experimental research are characterized by large sets of parameters that can affect the result of the experimentation: the rich libraries of compounds now available, the different ways one can create compositions, and the great variety of laboratory protocols produces an extreme large number of parameters that scientists must control in developing their experiments. In this lecture we will address the problem of designing high dimensional experiments with the evolutionary approach based on statistical models. This approach can search information in huge spaces achieving the “intelligent data” (data with information) with a very limited amount of resources.

More specifically we will consider:

1. The design of experiments: randomization, replication, blocking.
2. Factorial designs and response surface methodology
3. The high dimensional experimental search space
4. The evolutionary approach to the design
5. The evolutionary model-based design of experiments

Ángel Goni Moreno

On Genetic Logic: Design, Modeling and Simulation

The engineering of logic functions into living cells is of growing interest and forms the basis of the emerging field of synthetic biology. Following a direct analogy with conventional electronic logic, we can engineer genetic devices with Boolean logic behaviors. Although still in its infancy, genetic logic gates represent a promising route to the future implementation of more complex systems to be applied in ecology or medicine. The design, modeling and simulation of biological systems are fundamental steps to the engineering of robust and reliable genetic devices. Many internal features of a specific system are only discovered and understood by performing a strong mathematical analysis. Thus, to have control over simulation tools can lead to a much faster and precise development of synthetic biology as well as other biological disciplines.

Pasquale Stano

Liposome Technology for Minimal Cells, Synthetic Communication and Smart Drug Delivery

1. Lipid vesicles as cell models: Preparation, properties, characterization
 - Chemistry and physics of amphiphilic molecules
 - Liposome technology
2. Minimal cells: from origin of life to synthetic biology

- Self-organization phenomena in the life's origin on the Earth
- The bottom-up approach to the construction of synthetic cells

3. Synthetic cells capable of communicating with natural cells? A bio-ICT tool for basic and applied research

- Lipid vesicle as drug carrier: the state of the art in drug delivery
- Towards the development of synthetic communication between synthetic and natural cells

Peter Dittrich

Organization-Oriented Chemical Computing

All known life forms process information on a bio-molecular level. This kind of information processing is known to be robust, self-organizing, adaptive, decentralized, asynchronous, fault-tolerant, and evolvable. Computation emerges out of an interplay of many decentralized relatively simple components (molecules). Therefore it appears attractive to consider chemical information processing as part of novel hybrid intelligent systems.

However, it turned out that in accordance with Conrad's trade off principle, programming a chemical computer appears to be difficult and novel techniques are required that help to bridge the micro-macro gap between reaction rules and resulting behavior. In this lecture we will focus on chemical computing in which the computation can be explained as a qualitative change in the composition of molecular species. For this case, chemical organization theory can be applied to predict the potential behavior of a chemical program. The basic idea is to explain the process of computation as a transitions between chemical organizations, which are closed and self maintaining sets of molecular species.

The lecture will enable the students to apply the respective method by following a concrete example including practical exercises.

4.4. Participants

A total of thirty-eight students applied for participation in the summer school, each application received a scoring based on the student's qualification and appropriate research discipline. Four students were rejected; seven students could not attend due to various reasons. All students applied and were eligible for a scholarship, covering half-board and attendance fee.

4.4.1. List of Participants

The following participants (in order of application date) attended the summer school:

- Peter Banda (Computer Science, USA)
- Emiliano Altamura (Material Chemistry, Italy)
- Martin Ullrich (Chemical Engineering, Czech Republic)

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- Lee Yiling (Bioinformatics, Malaysia)
- Ong Hui San (Molecular Biology, Malaysia)
- Borys Wrobel (Molecular Biology, Poland)
- Mazlina Ismail (Bioinformatics, Malaysia)
- Noor Munyati Othman (Microbiology, Malaysia)
- Nocolò Mazzucco (Nanomedice, Italy)
- Gabriele Sponchia (Chemistry, Italy)
- Tengku Yasmin Yusof (Microbiology, Malaysia)
- Nur' Ain Ishak (Bioinformatics, Malaysia)
- Riccardo Marin (Material Science, Italy)
- Gerd Gruenert (Bioinformatics, Germany)
- Stephan Richter (Bioinformatics, Germany)
- Adam Gorczynski (Chemistry, Poland)
- Chinnu Merin Abraham (Electronics Engineering, UK)
- Martin Elstner (Chemistry, Germany)
- Özlem Özkan (Medical Informatics, Turkey)
- Lidia Yamamoto (Computer Science, Belgium)
- Marta Fik (Chemistry, Poland)

4.4.2. Workgroups

The following workgroup topics were formulated by students initiative.

- 1. Evolution of structures, simulation of dividing cells, local communication**
 - Which computations can be performed by these structures?
 - Evolution of structures, evolving an implicit representation vs. an explicit representation
- 2. Rubiks Cube project**
 - Computer simulation and algorithms
 - Wetlab implementation: requirements of the molecules, organization and control
 - Factors influencing structure formation, energy and bonds
- 3. Review of the state of the art of fabricating protocells**
 - Applications of protocells, targeted protocell movement
 - Artificial Cells as reporting system for expression
- 4. Self-assembly in DNA and self-cleaving RNA**
 - Conformational dynamics
 - Kinetics in RNA/DNA computing
- 5. Evolution of modularity**
 - e.g. protein domains, incl. simulations
- 6. Molecular Dynamics on Clusters/GPU**
 - Unstructured artificial chemistries, mass action, state
 - Differences between molecular dynamics and “real” quantum mechanics
- 7. Artificial Chemistries**

- How to map program primitives to artificial chemistries?
- How to solve problems with artificial chemistries?

4.4.3. Testimonials

A report of one participant's experience can be read here:

http://www.cobra-project.eu/summerschool_experience.html

An anonymous survey was conducted at the end with three questions to the participants about the summer school. A summary of the very positive answers follows.

What would you keep?

- All the didactic material
- The workgroups
- Number of students
- Duration of the summer school
- Multidisciplinary talks, open discussion sessions, "open-table-ness"
- content of the lectures, overview of computational science and BioChemIT, "benchmark" problems of biochemical computing
- International experience and opportunity, diversity of participants background
- Relaxed atmosphere with a lot of free time for working groups and discussion
- The location, remarkable small city
- Common housing
- Extracurricular trips
- Funding for young researchers
- Everything

What would you change?

- More experiments, practical activities
- Group supervisors for workgroups, more feedback on workgroup results, intermediate presentations
- More balanced workgroups by students expertise
- Bridge Theory vs. Experiment
- Students presentations on research and cultural background

- More interaction between lecturers and students (questions from students the next day or lecturers stay around after talk)
- Afternoon lectures, keep lectures to morning
- Self-organized dinner

Other comments

- For me it was really a very nice experience. I've tried to think of possible suggestions and things to change, but nothing came to my mind. Keep it as it is... and thank you!!!
- The summer school was very well organized. I think that everyone enjoyed the time spent here. Just one observation: The last mail with "technical" information about trip and other stuff arrived a little bit late.
- Practical or exercise sessions were very successful, continue on this direction
- Advertise some logistics more explicitly, for example, bring warm clothes, hiking shoes, etc.
- Wonderful place to have a school!
- Please invite / include us (Natural Computing Lab, University of Malaya) in future activities
- Personally, I think all of things here is PERFECT – accommodation, food, speakers, lectures, peoples and others. It should be held for next time and more frequently.
- Try to encourage MSc and PhD students to take part in discussion – special discussion panels for students, I was really fond of the stay here!, great organization
- Totally enjoyed this Summer School!

4.5. Pictures

Photographs from the Summer School are available here:

<http://www.cobra-project.eu/docs/SummerSchoolImages.pdf>

BioChemITSchool 2012 Program



COBRA

Coordination of Biological and Chemical IT Research Activities





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COBRA Directory

Project Management



Martyn Amos

Leader of BACTOCOM,
COBRA coordinator



John McCaskill

Leader of ECCell,
roadmap coordinator



Steen Rasmussen

Leader of MATCHIT,
stakeholder consultation
coordinator



Peter Dittrich

Leader of NEUNEU,
community development
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Irene Poli (ITA)

Co-Director,
European Center for
Living Technology

BioChemITSchool 2012

Organisers

Matteo Borrotti

Agnese Boscarol

Martin Engler

Gabi Escuela

Debora Slanzi

Margaret Taylor

Disclaimer

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14:00 - 15:30	16:00 - 17:30	18:00 - open end
	Welcome Pizza Party	
<i>Compartments in Biochemical Information Technology</i> Harold Fellermann	Poster Session	
Workgroup Formation		
Student's Presentation		
<i>Make your own microfluidic chip</i> Philip King, Maurits de Planque, Klaus-Peter Zauner		

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Fri, 21st	Presentation of Workgroup Results	Discussion, Open Problems
		12:00 Summer School Closing

14:00 - 15:30

16:00 - 17:30

18:00 - open end

Hiking

*Liposome Technology for
Minimal Cells, Synthetic
Communication, Smart
Drug Delivery*
Pasquale Stano

*Living Technologies and
Bottom-up Protocells*
Steen Rasmussen

*Living Technologies and
Bottom-up Protocells*
Steen Rasmussen



Harold Fellermann

University of Southern Denmark

Dr. Harold Fellermann is currently a post-doc at the Center for Fundamental Living Technology (FLinT) which is located at University of Southern Denmark. The group's main scientific mission is to assemble the components of minimal living systems, ultimately protocells, bottom up from inorganic and organic components. The long-term technological vision is to develop the foundation for a living technology characterized by robustness, autonomy, energy efficiency, sustainability, local intelligence, self-repair, adaptation, and self-replication, all properties current technology lack, but living systems possess. In 2009 he obtained a Ph.D. at the University of Osnabrück, Germany. In 2006 he was a Research Fellow for Modelling in Systems Ecology at the UFZ Center for Environmental Research, Dept. Ecological System Analysis, Leipzig. From 2004 to 2007 he was a Research Fellow for Modelling on Artificial Life at the Complex Systems Lab, Universitat Pompeu Fabra, Barcelona, Spain, the Los Alamos National Laboratory, New Mexico, USA and the European Center for Living Technology, Venice, Italy. He received the VVO-Award for outstanding work in support of research & academia in 2000.

The Role of Compartments

in Biochemical Information Technology

Supramolecular compartments, such as vesicles, play a vital role in biology as well as in many ChemBio-ICT applications. Compartments can encapsulate various chemicals, and thus concentrate or separate reactants. In addition, their surfaces can be decorated with functional molecules such as membrane proteins, anti-bodies, etc., that can greatly modify their behaviour. This allows compartments to become agent-like entities in ChemBio-ICT applications.

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The presentation will draw on examples from several ChemBio-ICT projects that our research group is currently pursuing in both theory and experiment.



Jasmin Fisher

Microsoft Research Cambridge & Cambridge University

Dr. Jasmin Fisher is one of the founders of the field of Executable Biology and a leader in the area of formal methods in biology. Over the past decade, she has been pioneering the study on usage of program analysis techniques for the analysis of biological models. Her research focuses on the construction and analysis of executable models that mimic aspects of biological phenomena in order to better understand complex biological systems. She is mainly interested in processes of cell fate determination and signalling networks operating during normal development and cancer.

She currently is a researcher at Microsoft Research Cambridge in the Programming Principles and Tools group as well as Affiliated Lecturer in the Cambridge Systems Biology Centre & Department of Biochemistry at University of Cambridge. Her research includes theoretical projects (i.a. formal modelling languages designed specifically for biological systems) as well as applied projects (i.a. predictive modelling of *C. elegans* vulval development, computational analysis of segmentation in *Drosophila* embryogenesis).

She received her PhD in Neuroimmunology from the Weizmann Institute of Science in Rehovot, Israel in 2003.

Executable Biology

The decade of genomic revolution following the human genome's sequencing has produced significant medical advances, and yet again, revealed how complicated human biology is, and how much more remains to be understood. Biology is an extraordinary complicated puzzle; we may know some of its pieces but have no clue how they are assembled to orchestrate the symphony of life, which renders the comprehension and analysis of living systems a major challenge. Recent efforts to create executable models of complex biological phenomena - an approach we call Executable Biology - entail great promise for new scientific discoveries, shedding new light on the puzzle of life. At the same time, this new wave of the future forces computer science to stretch far and beyond, and in ways never considered before, in order to deal with the enormous complexity observed in biology. This lectures series will provide an introduction to Executable Biology, through various success stories in using formal methods (e.g., Boolean/Qualitative Networks, compositional state-machines) to tackle specific biological questions, and visualization and modelling tools designed for biologists to model cellular processes in a visual-friendly way.



Tetsuya Yomo

Osaka University

Prof. Tetsuya Yomo is a Professor at the Osaka University and a Project Leader of Dynamical Micro-scale Reaction Environment Project (ERATO, JST). The main research topics of his group are complex systems, experimental evolution, artificial cells, and artificial symbiosis. Currently, he is experimentally synthesizing artificial life, investigating genetic networks for cell differentiation and symbiosis to understand fundamental rules behind biological complex systems.

Prof. Yomo received his Ph.D. in Engineering from Graduate School of Engineering, Osaka University in 1991. He was appointed as Assistant Professor at Faculty of Engineering, Osaka University in 1991, then served as an Associate Professor (1998-2002) and later moved to Graduate School of Information Science and Technology, Osaka University and was appointed as a Professor in 2006. He has won a number of awards including the Zuckerkandl Prize by Journal of Molecular Evolution in 2002.

Constructive Approach to Life's Characteristics

What makes lives different from others? Natural cells evince phenomena more ordered than a simple assembly of molecules. There is a gap between living and non-living worlds. Only once the transition over the gap has ever occurred, which is the origin of life. In the first lecture, I would explain some experiments to construct and evolve a cell-like model from molecules to address the following questions: Why must the complicated reaction network have been confined into micro-scaled environments? What conditions are required for the simple assembly of bio-molecules to take Darwinian evolution?

Another characteristic of life is stochasticity. With the same genetic background and the same inputs from environments, organisms sometimes behave more stochastically or less precisely than machines. In terms of accuracy or efficiency, life is far behind machine. In the second lecture, focusing on the gene expression in cells, I would address the questions: What causes the cells fluctuate their gene expression? Does the fluctuation give cells some flexibility to environmental changes? What advantage has maintained the fluctuation at the cost of low efficiency in the course of evolution?



Klaus-Peter Zauner

University of Southampton

Dr. Klaus-Peter Zauner is a Senior Lecturer in the Science and Engineering of Natural Systems Group of the School of Electronics and Computer Science at the University of Southampton. He was born in Stuttgart, soldered together a Sinclair ZX81 as his first computer and went on to study Biochemistry at the University of

Tuebingen. Intrigued by Nature's molecular scale information processing mechanisms he left Tuebingen in 1992 for Detroit to join Michael Conrad's Biocomputing Group - at the time one of the very few places with research in molecular computing and likely the first computer science group with its own wet-laboratory. Under Michael Conrad's mentorship he worked on conformational computing and enzymatic computing. Klaus-Peter received his Ph.D. in computer science from Wayne State University, Detroit in 2001. He started his academic career as a Visiting Assistant Professor at Wayne State University, then returned to Europe in 2002 to work with Peter Dittrich in the Bio Systems Analysis Group at the University of Jena, before taking up a Lectureship at the University of Southampton in 2003. He leads a team that works across the boundaries of (bio-)chemistry, electronics, microfluidics, and software to make the complexification of matter part of future chemistry and engineering. He was a Microsoft Research European Fellow, recipient of a Leverhulme Research Leadership Award, and is a founding editor of the International Journal of Unconventional Computing. Klaus-Peter is collaborating nationally and internationally to shape the direction of this nascent research field.

Informed Matter

The Confluence of Information Processes and Material Science

The 19th century brought about an understanding of energy for the molecular level. The 20th century saw rapid progress in the manipulation of matter enabling the purposeful design of organic molecules, and the advent of biochemistry. The latter opened the view on marvellously sophisticated macromolecules and supra-molecular structures - but offered no path to enter this design space. It is for the 21st century to complement the achievements of the past with the application of information processes at the molecular scale. When this hurdle can be tackled, however, the technology impact will rival the advent of organic chemistry.

To make the complexification of matter exhibited by nature amenable to engineering, it will be necessary to mimic the molecular level information processes employed by organisms to fabricate and maintain their molecular machinery. Living systems are peculiarly organised inhomogeneous arrangements of the very same matter that forms the remaining dead universe. Their highly organised state can be sustained only by active maintenance which in turn necessitates the processing of information - life without computation is inconceivable. Conversely, the proficiency with which single-cell organisms maintain their living state under adverse conditions and severe constraints in energy and material indicates the efficiency that may be achieved through the direct use of the physical characteristics of materials for computation.

This course will explore the dual role of molecular information technology as a facilitator for the synthesis of complex materials and as a resource for computational power.



Jerzy Górecki

Polish Academy of Sciences

Prof. Jerzy Górecki's research focuses on chemical informatics. His interests are unconventional computing with nonequilibrium chemical medium, computational chemical kinetics, large scale microscopic computer simulations of chemical systems far-from-equilibrium and stochastic effects in chemical systems.

He is a professor at the Institute of Physical Chemistry at the Polish Academy of Sciences and since 2007 also associate professor at the Department of Mathematics and Computer Science at the Cardinal Stefan Wyszyński University, Warsaw. He received his Ph.D. at the Institute of Physical Chemistry, Warsaw in 1984 and his D.Sc. at the Department of Mathematics and Physics, Jagiellonian University, Cracov in 1994. He is internationally well connected with past research assignments at the Department of Chemistry at the University of Manchester, UK (1986-1988), the Department of Chemistry, McGill University, Montreal, Canada (1991), the Institute of Molecular Science, Okazaki, Japan (1991-1992) and short research visits to Japan (Tokyo Institute of Technology, International Christian University in Mitaka and Kyoto University) and to Italy (La Sapienza, Roma).

He authored over 100 papers and is a member of the Editorial Board of the International Journal of Unconventional Computing.

Reaction-Diffusion Computing

There are many ways in which the time evolution of a medium where chemical reactions proceed can be used for information processing. During my lecture I will consider a spatially distributed medium, characterized by concentrations of reagents involved represented by functions of space and time. The reagents interact locally via chemical reactions. They can also migrate in space and influence the time evolution in the neighborhood. I will assume that the diffusion of molecules is responsible for migration and so the time evolution of the considered medium can be described by a set of parabolic differential equations where the local terms model the chemical kinetics and the differential operators describe diffusion. The research on information processing with such a medium is called the reaction-diffusion computing [1].

The key question is how to interpret the natural time evolution of the medium defined by reagents involved in the language of information. I will show that there are many alternatives. The choice depends of the properties of the medium. For example if we consider an excitable chemical kinetics then the straightforward method of information coding is related to the presence of excitation at a given point of the medium at a selected time. It can be assumed that an excitation pulse represents the symbol 1 and its absence the symbol 0. Within such representation we can introduce the binary logic, gates and operations on strings. It can be shown that a universal computer can be made with an excitable chemical medium. The realization of information processing operation simplifies if the medium has an intentionally introduced geometrical structure of regions characterized by different excitability levels. We show that in information processing applications the geometry plays an equally important role as the dynamics of the medium and allows one to construct devices that perform complex signal processing operations even for a relatively simple kinetics of the reactions involved. I will review a number of chemical realizations of simple information processing devices like signal diodes, logical gates or memory cells and we show that by combining these devices as building blocks the medium can perform complex operations like for example counting of arriving excitations. If time allows I will discuss information processing potential of a medium composed of droplets containing an oscillating chemical reaction.

The ideas of chemical reaction-diffusion computing can be translated to other physical systems showing similar properties. The solid analog of wet chemistry is the medium composed of carriers in specially prepared semiconductors.

[1] Adamatzky A, De Lacy Costello B et al (2005) Reaction-Diffusion Computers. Elsevier Science



Maurits de Planque

University of Southampton

Dr. Maurits de Planque's main research interests are bio-nanoscience and bio-nanotechnology, including biosensors. He routinely collaborates with a wide range of scientists and engineers, from theoreticians to molecular biologists and clean room experts. He hosts engineers who are interested in biomedical applications of nanotechnology as well as bioscientists who are keen to gain experience with nano- and microfabrication or high-resolution microscopies.

He currently works as Life Sciences Interface Lecturer in ECS, Southampton, UK.

After obtaining a PhD in biophysics and a first degree in (bio-)chemistry in Utrecht, Netherlands, he worked as a postdoctoral fellow in Melbourne and in Oxford.

Microscale BioChemIT Devices

Applications and Fabrication

Studying, or perhaps more appropriately for BioChemIT, implementing chemical or biochemical reactions or bacterial cultures in small volumes has many advantages. Microliter volumes obviously require much less chemicals than conventional milliliter reaction chambers such as cuvettes or Petri dishes, enabling efficiency savings when dealing with costly biomolecules. Furthermore, multiple reactions or environmental conditions can be evaluated simultaneously in an array of isolated microwells. However, these small reaction chambers can easily be connected to each other in various 2D patterns, giving rise to a heterogeneous reaction medium. Such compartmentalization makes it possible to mimic some key concepts of biological information processing, for example the threshold-modulated pulse propagation between neurons in the brain.

The fabrication of microscale wells and channels is based on well-established methods from the IC industry, most notably lithography with UV light. With the relatively recent development of 'soft' lithography variations, in which a micropatterned master is used to cast an inverse copy of an elastomeric polymer, the fabrication process can also be performed in a standard laboratory rather than a clean room facility. For small reaction chambers evaporation should be avoided, hence it is usually necessary to bond the micropatterned substrate to a flat layer, typically glass because of its chemical compatibility and optical transparency. To fill the device or to introduce different chemicals at various stages of the reactions, microfluidics are also required. All these methods will be explained with an emphasis on practical issues such as the smallest and largest dimensions that can be realized with a given technique.



Irene Poli

University Ca'Foscari, Venice

Prof. Irene Poli is professor of Statistics at the University Ca'Foscari of Venice and CoDirector of the European Centre for Living Technology (ECLT). She leads a research group on statistical design of experiments and data analysis for combinatorially complex high dimensional problems, developing a new approach to design and modelling based on the concept of evolution.

After graduating from the University of Pavia, she pursued postgraduate research at Imperial College of Science and Technology of London (UK), and later at the Centre for Non-linear Science, Los Alamos National Laboratory and the Santa Fe Institute (NM, USA). Her major research interests have been in Bayesian nonparametric inference, nonlinear time series models, predictive neural networks, evolutionary computation and more recently in evolutionary design of experiments and modelling.

She is Fellow of the New York Academy of Science, of the Bernoulli Society, of the Royal Statistical Society and of the Italian Statistical Society. Currently she is member of the Science Board of ECLT, of the Doctoral Program of the School of Advanced Studies in Venice and of the Doctoral School of Statistics in Padova. She is also a component of the Scientific Committee of CIVEN, a university network devoted to the research in the field of nanotechnologies.

She collaborated and coordinated several large interdisciplinary and international research projects, including the EU integrated project in IT: Programmable Artificial Cell Evolution (PACE). Currently she is the coordinator of the Fondazione Venezia project: Designing Informative Combinatorial Experiments (DICE) at ECLT, and also coordinator of MIUR project "Evolutionary Experimental Designs". She published over 100 papers, and co-authored three books.

Evolutionary Design of Experiments

Several areas of experimental research are characterized by large sets of parameters that can affect the result of the experimentation: the rich libraries of compounds now available, the different ways one can create compositions, and the great variety of laboratory protocols produces an extreme large number of parameters that scientists must control in developing their experiments. In this lecture we will address the problem of designing high dimensional experiments with the evolutionary approach based on statistical models. This approach can search information in huge spaces achieving the “intelligent data” (data with information) with a very limited amount of resources.

More specifically we will consider:

1. The design of experiments: randomization, replication, blocking.
2. Factorial designs and response surface methodology
3. The high dimensional experimental search space
4. The evolutionary approach to the design
5. The evolutionary model-based design of experiments



Ángel Goñi Moreno

Manchester Metropolitan University

Dr. Ángel Goñi Moreno's research interests range from Artificial intelligence to Systems Biology. He is currently a researcher at the Novel Computation Group (NCG-MMU), School of Computing, Mathematics and Digital Technology, Manchester Metropolitan University, UK. The group's research focuses on the development of new methods and techniques for efficiently solving important scientific and industrially relevant problems, the development and performance analysis of novel and/or advanced computing systems, the development of computational methods based on natural/self-organizing systems, and fundamental underlying theory.

In 2010 he obtained a Ph.D. in Computer Engineering with his doctoral thesis being in the field of Bacterial Computing and a M.Sc. in Artificial Intelligence. He previously worked at the Natural Computing Group at Universidad Politécnica de Madrid (UPM), Spain with research focussing on the fields of DNA Computing and Computational Biology.

On Genetic Logic

Design, Modeling and Simulation

The engineering of logic functions into living cells is of growing interest and forms the basis of the emerging field of synthetic biology. Following a direct analogy with conventional electronic logic, we can engineer genetic devices with Boolean logic behaviours. Although still in its infancy, genetic logic gates represent a promising route to the future implementation of more complex systems to be applied in ecology or medicine. The design, modelling and simulation of biological systems are fundamental steps to the engineering of robust and reliable genetic devices. Many internal features of a specific system are only discovered and understood by performing a strong mathematical analysis. Thus, to have control over simulation tools can lead to a much faster and precise development of synthetic biology as well as other biological disciplines.



Pasquale Stano

University of RomaTre

Dr. Pasquale Stano's research focuses on the physico-chemical properties of vesicles and other compartments, and their use as cell models.

He currently is a member of the Dept. of Biology of the University of RomaTre. He is a member of the International Liposome Society and of the Italian Society of Pure and Applied Biophysics (SIBPA). Currently he is involved in the Minimal Cell project (see CentroFermi) and on new approaches for understanding the origins of macromolecules in prebiotic conditions.

He received his scientific education in chemistry at the University of Pisa, Italy. In his thesis he worked on the design and synthesis of heterotopic Schiff base ligands and relative nickel and copper supramolecular complexes, and studied the kinetics of transamination on these substrates. He joined Prof. Pier Luisi's research group at the ETH Zürich in 2002, working on the liposomal drug delivery of camptothecin derivatives, in a collaboration with the Italian pharmaceutical company Sigma-Tau in Pomezia (Roma). From 2003 on he was working on the properties and reactivity of vesicles, DNA condensation in reverse micelles, matrix effect and self-reproduction of vesicles, and on the AmB interaction with sterol containing vesicles. In 2004 he moved to the Dept. of Biology of the University of RomaTre.

In 2007, he has co-edited a special issue of *Origins of Life and Evolution of Biospheres* on "Basic Questions about the Origins of Life (proceedings of the 4th Course of the International School on Complexity - Erice - 1-6 October 2006)".

Liposome Technology

for Minimal Cells, Synthetic Communication and Smart Drug Delivery

1. Lipid vesicles as cell models: Preparation, properties, characterization
 - Chemistry and physics of amphiphilic molecules
 - Liposome technology
2. Minimal cells: from origin of life to synthetic biology
 - Self-organization phenomena in the life's origin on the Earth
 - The bottom-up approach to the construction of synthetic cells
3. Synthetic cells capable of communicating with natural cells? A bio-ICT tool for basic and applied research
 - Lipid vesicle as drug carrier: the state of the art in drug delivery
 - Towards the development of synthetic communication between synthetic and natural cells



Norman Packard

European Centre for Living Technology

Dr. Norman Packard has worked in the areas of chaos, learning algorithms, predictive modeling of complex time series, statistical analysis of evolution, artificial life, and complex adaptive systems. He is now focusing on the development of evolutionary chemistry in programmable microfluidic technology. Long-range applications of this technology include the fabrication of artificial cells from non-living material, and their programming for useful functionality.

He is the Director of the European Centre for Living Technology. He currently works at the US branch of the company (ProtoLife Inc.) in San Francisco, California after co-founding ProtoLife S.r.l., an Italian company based in Venice, Italy, which applies machine learning techniques to the design of experiments (DoE) for high throughput experiments in biotechnology.

Packard holds a B.A. from Reed College (1976) and Ph.D. in Physics from University of California at Santa Cruz (1983). After post-docs at IHES (Bures-sur-Yvette) and IAS (Princeton), he joined the physics department at the University of Illinois, Urbana-Champaign in 1987, where he became an associate professor before leaving to become a co-founder of Prediction Company in 1991. There he served as CEO from 1997 to 2003, then as chairman of the board of directors until 2005, when the company was bought by UBS. From 2004-2008, Packard was involved in PACE (Programmable Artificial Cell Evolution), developing and applying the techniques of ProtoLife. As part of the PACE project, Packard participated in the founding of ECLT (the European Center for Living Technology), where he has served as director, and as a member of the Center's Science Board.

Packard has had a long-standing involvement with the Santa Fe Institute, currently serving on its external faculty.

Steen Rasmussen

University of Southern Denmark

Prof. Steen Rasmussen has pioneered approaches, methods, and applications for self-organizing processes in natural and artificial systems: abstract self-programmable matter, molecular dynamics (MD) lattice gas simulations for molecular self-assembly, mesoscale simulation tools, rational and evolutionary protocell design, disaster mitigation and decision support systems based on collective intelligence, as well as novel simulations for large-scale socio-technical systems.



He is currently the Head of the Center for Fundamental Living Technology (FLinT), a Research Director at the Department for Physics and Chemistry at University of Southern Denmark, External Research Professor at the Santa Fe Institute, USA, as well as Principle Investigator for the upstart of the Initiative for Society, and Policy (ISSP) in Denmark. Further, he is the co-director on the European Union sponsored Programmable Artificial Cell Evolution (PACE) project, and he was one of the founders of the Artificial Life movement in the late 1980s. He is currently on the Science Board for the European Center for Living Technology in Venice, Italy, which he is a co-founder of in 2004.

He was previously the Team Leader for the Self-Organizing Systems team at Los Alamos and a Guest Professor at University of Copenhagen (2004-5). He was heading the Los Alamos Protocell Assembly (LDRD-DR) project and the Astrobiology program (origins of life) at Los Alamos developing experimental and computational protocells and Cell-Like Entities, with USAF as a co-sponsor. He was the Chair of the Science and Engineering Leadership Team (SELT) for 2001-2002 in the Earth and Environmental Science (EES) Division at LANL. He co-developed the Transportation Simulation System (TRANSIMS), which is now implemented by the USA Department of Transportation. He co-directed the Urban Security Initiative at LANL, developing an integrated simulation framework for urban systems as well as web-based disaster mitigation tools, which were implemented in the May 2000 Cerro Grande Wildfire where 20.000 people were evacuated. He was also part of the original Los Alamos team on Critical Infrastructure Protection, to be implemented by the US Department of Homeland Security.

In 1988 he received the “P. Gorm-Petersens Mindelegat” award in the presence of Her Majesty the Queen, Magrethe II of Denmark, the 2004 the Los Alamos Achievements Award for Excellence and the 2005 World Technology Network Reward.



Peter Dittrich

Friedrich Schiller University, Jena

Dr. Peter Dittrich is a private lecturer associated with the Chair of Bioinformatics at the Institute of Computer Science, in the Friedrich Schiller University of Jena, Germany. He leads the junior Bio Systems Analysis Group, which is also member of the Jena Centre for Bioinformatics. Dittrich's research interests include:

Systems Theory, Systems Analysis and Optimization, Computational Systems Biology, Artificial Life, Artificial Chemistries, Origin of Life, and Unconventional Computing. In 1995 Dittrich was part of the first group that developed an in-silico chemical controller for an autonomous robot. At that time they also suggested chemical programs for hyper-cyclic associative memory, parity checking, sorting, and prime number computation. In 2001 he received the Dr. rer. nat degree from the Department of Computer Science at the University of Dortmund. Since 2004, Dittrich's Jena group has been working in national and international research programs, as for example, in the framework of the german priority program "Organic Computing", and in the European Commission projects: ESIGNET (Evolving Cell Signaling Networks in Silico) and NEUNEU (Artificial Wet Neuronal Networks from Compartmentalised Excitable Chemical Media). Notably, his group developed a theory of chemical organizations that provides a new promising tool to construct, analyse, and understand complex dynamical reactions networks and in particular, chemical programs.

Organization-Oriented Chemical Computing

All known life forms process information on a bio-molecular level. This kind of information processing is known to be robust, self-organizing, adaptive, decentralized, asynchronous, fault-tolerant, and evolvable. Computation emerges out of an interplay of many decentralized relatively simple components (molecules). Therefore it appears attractive to consider chemical information processing as part of novel hybrid intelligent systems.

However, it turned out that in accordance with Conrad's tradeoff principle, programming a chemical computer appears to be difficult and novel techniques are required that help to bridge the micro-macro gap between reaction rules and resulting behavior. In this lecture we will focus on chemical computing in which the computation can be explained as a qualitative change in the composition of molecular species. For this case, chemical organization theory can be applied to predict the potential behavior of a chemical program. The basic idea is to explain the process of computation as a transitions between chemical organizations, which are closed and self-maintaining sets of molecular species.

The lecture will enable the students to apply the respective method by following a concrete example including practical exercises.



Philip King

University of Southampton

After studying for a BSc in Biological Sciences with specialisation in Microbiology at Warwick University in 2005, Philip completed a PhD investigating the microfluidic applications of microstereolithography as a member of the Sensors Research Laboratory, also at Warwick University.

He is currently working on the Artificial Wet Neuronal Networks from Compartmentalised Excitable Chemical Media (NEUNEU) EU project. The aim of the project is to create networks of individual droplets containing an excitable chemical media e.g. Belousov Zhabotinsky reaction mixture, where the progress of excitation waves through the droplet arrays can be used for computation.

Towards this goal he carries out research into macro-scale (0.5-3.0 mm diameter) droplet generation systems. Progress has been accelerated by the use of additive layer manufacture (a.k.a. rapid prototyping, 3D printing) techniques for the rapid turnaround of precision-engineered moulds for subsequent use with PDMS, a ubiquitous microengineering casting material. A particular area of interest for him is the passive control of droplets using the shape of the fluidics, aided by electrically actuated techniques such as electrowetting. Parallel work has been carried out into the fine-tuning of the chemical media for use in our systems.

Introduction to PDMS microfluidics

Make your own microfluidic chip

There will be an opportunity to gain hands-on experience with soft lithography: creating an elastomeric replica from a micropatterned master mold and bonding this replica to a glass substrate to define microchannels and microchambers that are visualized with a colored solution. This exercise illustrates miniaturization approaches to BioChemIT. It also shows that soft lithography-enabled microfluidic experiments can be performed in any laboratory and do not require special equipment.

