



# 2011

### **Deliverable Report**

D8.2 MATCHIT Co-organized Workshop (M18) & D8.4 Updated MATCHIT Web (M24)

Matrix for Chemical IT (MATCHIT)

#### **D8.2 MATCHIT Co-organized Workshop (M18)**

In 2011 participants from the MATCHIT Consortium co-organized three European workshops:

- 1. A session at FET11 the European Future Technologies Conference and Exhibition. Science beyond Fiction in Budapest
- 2. A workshop on Biological and Chemical Information Technologies in France
- 3. A COST Meeting on systems Chemistry in Denmark.

## 1. Session at FET11: The European Future Technologies Conference and Exhibition. Science beyond Fiction

Biological and Chemical Information Technology: Bottom-Up Chemistry and Synthetic Biology

Biological and chemical information technology (bio/chem IT) is one of the most vibrant and important emerging research domains in recent years, especially with the growth of research into systems and synthetic biology, artificial cells, chemical information processing, micro-electromechanical systems, nanotechnology and artificial intelligence. This session will present scientific results in the field, focusing on bottom-up chemistry and synthetic biology. Particular attention will be paid to bio/chem IT outside Europe, through the presentation of our plenary speaker.

#### **Speakers**

Plenary speaker: Farren Isaacs, Yale University, USA

Short presentations were also be given by representatives of the current core COBRA project:

- Steen Rasmussen, University of Southern Denmark, Denmark
- John McCaskill, Ruhr University, Bochum, Germany
- Peter Dittrich, Friedrich Schiller University, Jena, Germany
- Martyn Amos, Manchester Metropolitan University, UK

Session organizer: Martyn Amos, Primary affiliation: Manchester Metropolitan University, Manchester, UK. Position: Reader in Novel Computation

#### 2. COBRA Workshop on Biological and Chemical Information Technologies

The 1st COBRA Workshop on Biological and Chemical Information Technologies (BioChemIT2011) was held on 8th August, 2011, as part of the European Conference on Artificial Life (ECAL2011). The meeting was hosted by the Cité Internationale Universitaire de Paris, in France. ECAL is a high-level, biennial conference on the simulation and synthesis of living systems, and has been running since 1991.

The central objective of BioChemIT was to provide a forum to present and discuss the latest advances of Bio/Chem IT research. The workshop was intended to foster interaction, exchange and communication between Bio/Chem IT research groups and projects. It was also designed to contribute to community building, and to provide input to the community consultation activities of COBRA.

Topics within the scope of the workshop included: biological/chemical information technologies; molecular and chemical computing; protocells and synthetic cells; molecular robots; integration of information processing with (bio-)chemical production; nano-bio-info interface; cellular engineering, artificial neurons, and programmable information chemistry; unconventional computing substrates.

#### **Organization**

The workshop was advertised via a dedicated page on the main project website (http://www.cobra-project.eu/biochemit2011.html), and also on the main ECAL site (http://www.ecal11.org/workshops/#biochemit).

Invited lectures were given by S. Frantisek (Institute of Chemical Technology, Prague, Czech Republic) and S. Kernbach (Universität Stuttgart, Germany). We accepted ten abstracts for oral presentation, including contributions from all four COBRA constituent projects (BACTOCOM, ECCell, MATCH-IT and NEUNEU).

All abstracts are available at http://www.cobra-project.eu/abstracts (individual abstracts are also linked in the programme details, below).

The workshop program committee was formed as follows:

- Martyn Amos (Manchester Metropolitan)
- John McCaskill (RUB Bochum)
- Steen Rasmussen (Odense)
- Harold Fellerman (Odense)
- Jerzy Gorecki (Warsaw)
- Angel Goni-Moreno (Manchester Metropolitan)
- Uwe Tangen (RUB Bochum)
- Thomas Maeke (RUB Bochum)
- Gunter von Kiedrowski (RUB Bochum)
- Irene Poli (University Ca' Foscari of Venice)
- Patrick Wagler (RUB Bochum)
- Klaus-Peter Zauner (Southampton)
- Andy Adamatzky (Univ. West of England)
- Peter Dittrich (FSU Jena)
- Maurits de Planque (Southampton)
- Christian Tschudin (Basel)

#### **Programme**

The workshop was held as a full-day session on Monday 8th August, from 09:00 to 18:30. The programme was as follows:

#### Time

09:00 Welcome

09:15 Invited lecture - Stepanek Frantisek: Challenges and opportunities in the engineering of chemical robots

10:15 Chu: Noise-speed-code trade-offs in gene computers

10:45 Goni-Moreno/Amos: Design of a genetic branch predictor

11:15 Coffee break

11:30 Corsi et al.: BZ oscillations inside lipid-enclosed droplets

12:00 Holley et al.: Computational explorations in BZ mediated geometric vesicle transcriptions

12:30 Lui et al.: Towards an in silico and in vivo Turing Test for Chells

#### Time

13:00 Lunch

14:30 Invited lecture - Serge Kernbach: Chemo-ICT and microrobotics: achieving collective intelligence

15:30 King *et al.*: Towards on-chip on-demand microfluidic production and manipulation of droplets for chemical computing

16:00 Tangen: On the external programming of a self-referential evolving microcontroller system

16:30 Coffee break

16:45 Chaplin *et al.*: Implementing conventional logic unconventionally: photochromic molecules as registers and logic gates

17:15 McCaskill: Spatially interfaced Chem-IT: towards electronic chemical cells

17:45 Rasmussen: ICT and chembio-based replication

18:15 COBRA discussion session

18:30 Close

The invited lectures were as follows:

#### Challenges and Opportunities in the Engineering of Chemical Robots

Frantisek Stepanek, Institute of Chemical Technology, Prague, Czech Republic http://www.chobotix.cz

Classical robots are electro-mechanical machines designed to carry out mainly mechanical tasks in the macroscopic world, such as repetitive manipulation with heavy objects, welding, etc. If we want to miniaturise robots so that they can interact with objects at the 1-10 micrometer lengthscale (such as single-cell organisms), a simple scale-down of macroscopic machines using MEMS technologies is not feasible, due to increased effects of colloidal interactions (Brownian motion, capillarity, van der Waals forces, etc.). Hence, the aim of our work is the design and synthesis of so-called chemical robots, which we conceive as internally structured particles in the 1's-10's m size range that can freely move in their environment, selectively exchange molecules with their surrounding in response to a local or external stimulus, chemically process those molecules and either accumulate or release the product. In this talk, the following aspects will be covered: (i) architecture and design

strategies of chemical robots; (ii) fabrication methods for the synthesis of internal compartments, outer shells, and entire bodies of chemical robots, with special focus on the use of responsive polymer composites and ink-jet technology; (iii) characterisation of the chemical robot's structure and properties; and (iv) use of chemical robots for the controlled release of a chemical payload and their interaction with biological substrates (site-specific targeting). Current and future application areas of chemical robots will be reviewed and challenges for further research outlined.

#### Chemo-ICT and microrobotics: achieving collective intelligence

Serge Kernbach, Universität Stuttgart, Germany

Miniaturization of microrobotics and advances in chemo-ICT technologies create new challenges for convergence of mechatronic and chemical autonomous systems. Elements of both systems are characterized through very simple "agents", which possess rudimentary sensing, actuation and communication capabilities. However, current and potential applications require a certain degree of intelligent functionality and behavior in these systems, which can be achieved primarily in collective way by utilizing principles of swarm intelligence. This talk gives an overview over the field of microrobotics and intelligent MEMS devices and discussed several approaches of achieving global awareness and intelligent collective behavior in such limited systems.

#### **Participants**

Approximately 30 participants attended the workshop, of whom 25 signed their name on the official register:

- Amos, Martyn (Manchester Metropolitan, UK)
- Chaplin, Jack (University of Nottingham, UK)
- Chu, Dominique (University of Kent, UK)
- Corsi, Josephine (University of Southampton, UK)
- De Planque, Maurice (University of Southampton, UK)
- Dittrich, Peter (University of Jena, Germany)
- Flamm, Cristoph (University of Vienna, Austria)
- Goñi-Moreno, Angel (Manchester Metropolitan, UK)
- Gordon-Smith, Chris (SimSoup)
- Gorecky, Jerzy (Institute of Physical Chemistry, PAN, Warsaw, Poland))
- Grünert, Gerd (University of Jena, Germany)
- Holley, Julian (University of the West of England, Bristol, UK)
- Kernbach, Serge (Universität Stuttgart, Germany)
- King, Philip (University of Southampton, UK)
- Korza, Lukasz (Cardinal Stefan Wyszynski University, Warsaw, Poland)
- Kreyssig, Peter (University of Jena, Germany)
- Lenaerts, Tom (Université libre de Bruxelles, Belgium)
- Lui, Leong Ting (University of Nottingham, UK)
- McCaskill, John (Rühr University Bochum, Germany)

- Packard, Norman (European Center for Living Technology, Venice, Italy)
- Rasmussen, Steen (Fundamental Living Technology (FLinT), University of Southern Denmark)
- Reynaert, Bryan (Universidad Católica, Chile)
- Szymanski, Jan (Institute of Physical Chemistry, PAN, Warsaw, Poland)
- Stepanek, Frantisek (Institute of Chemical Technology, Prague, Czech Republic)
- Tangen, Uwe (Ruhr-University Bochum, Germany)
- Zauner, Klaus-Peter (University of Southampton, UK)

#### **Publication**

After the workshop, a call for papers was issued, inviting contributions to a special issue of *BioSystems* dedicated to the meeting.

#### 3. COST Meeting on Systems Chemistry (WG3 - CM0703)

December 8-10, 2011 the Center for Fundamental Living Technology (FLinT) at University of Southern Denmark hosted a COST Meeting on Systems Chemistry (WG3 - CM0703) with 25 participants. Pierre-Alain Monnard from SDU was the main organizer.

The meeting was the second meeting of the workgroup 3 of the COST action CM0703 "Systems Chemistry". The meeting was held by the FLinT center at the University of Southern Denmark (SDU) on its campus of Odense, Denmark, and organized by Pierre-Alain Monnard (local organizator) and Peter Walde (WG3 leader). It was a useful and stimulating gathering with 9 short presentations of representers of the workgroup members (6 on 9/12 and 3 on 10/12), and by 3 special lectures given by post-doctoral researchers from FLinT Eva Bönzli, Maik Hadorn and Harold Fellermann followed by 2 invited lectures by DAMBIC center representatives (Jonathan R. Brewer and Christoffer Lagerholm, both SDU, ½ lecture each) and Ole G. Mouritsen (MemPhys, SDU). The workgroups were represented by Robert Pascal (Université Montpellier, F), Andrea Grotzky (ETH Zürich, CH), Bart Jan Ravoo (Universitat Münster, GER) Fabio Mavelli (Università di Bari, IT), Pierre-Alain Monnard (SDU, DK), Paolo Carrara and Pasquale Stano (Università degli Studi di Roma Tre, IT), and Emiliano Altamura (Università di Bari, IT).

There were extensive discussions about possible collaboration and various aspects of the different research presented. A visit of the recently created DaMBIC (Danish Molecular Biomedical Imaging Center) was also organized (<a href="http://www.dambic.dk">http://www.dambic.dk</a>) to present the facilities to the participants as this center carries out research in imaging technologies that could be useful for them.

Thanks to the SDU infrastructure the meeting could be run very efficiently with low costs. Overall, the meeting was successful without any problems.