Coordination of Biological and Chemical IT Research Activities

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Second COBRA conference: Report on BioChemIT2012

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Abstract

The *2nd COBRA Workshop on Biological and Chemical Information Technologies* (BioChemIT2012) was held on 6th September 2012, as part of the 11th International Conference on Unconventional Computation & Natural Computation. The objectives of BioChemIT2012 were to provide a forum to present and discuss the latest advances of Bio/Chem IT research and to contribute to the development of the COBRA C^{hem}B^{io}IT Roadmap. It was attended by about forty people and eleven papers were presented illustrating the breadth of work in the field from wet lab work to computer simulations. A plenary lecture was given by Professor Susan Stepney on; *'Sub-symbolic artificial chemistries'*. A panel session on Technology Governance and Roadmapping was introduced by a presentation from Dr. Jane Calvert about her involvement in the writing of the UK Government's Synthetic Biology Roadmap for the UK and the role of roadmapping. Professor John McCaskill, presented an early draft of the COBRA C^{hem}B^{io}IT Roadmap for Biological and Chemical Information Technology which was followed by discussion.

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1. Overview

The BioChemIt2012 workshop was very popular and was attended by about forty people, at times there was standing room only. Eleven papers were presented illustrating the breadth of work in the field from wet lab work to computer simulations. Presenters ranged from well established researchers to very early career researchers.
The plenary lecture was given by Professor Susan Stepney, Director of the York Centre for Complex Systems Analysis (YCCSA), on; *'Sub-symbolic artificial chemistries'*. The interesting and stimulating lecture outlined work carried out in the Centre developing an Artificial Chemistry and was followed by a lively discussion.

The day concluded with a panel session on Technology Governance and Roadmapping introduced by a presentation from Dr. Jane Calvert. Dr. Calvert, who is a member of Innogen; the Centre for Social and Economic Research on Innovation in Genomics and is based at the University of Edinburgh, spoke about her involvement in the writing of the UK Government's Synthetic Biology Roadmap for the UK and the role of roadmapping.

Professor John McCaskill, lead on the development of the COBRA roadmap, presented an early draft of the COBRA C^{hem}B^{io}IT Roadmap for Biological and Chemical Information Technology. A lively discussion about both the role of roadmapping in general and more particularly the scope and meaning of the COBRA roadmap followed.

2. Date and Location

The *2nd COBRA Workshop on Biological and Chemical Information Technologies* (BioChemIT2012) was held on 6th September 2012, as part of the 11th International Conference on Unconventional Computation & Natural Computation 2012 (UCNC '12) which took place at the Fundamental Computer Science Laboratory of the University of Orléans.

3. Objectives

The objectives of BioChemIT2012 were to provide a forum to present and discuss the latest advances of Bio/Chem IT research and to contribute to the development of the COBRA C^{hem}B^{io}IT Roadmap. The workshop was intended to advance the interaction, exchange, and communication between Bio/Chem IT research groups and projects so building a scientific community and providing input for the COBRA C^{hem}B^{io}IT Roadmap.

The workshop included invited lectures, contributed talks and a panel discussion session on the COBRA C^{hem}B^{io}IT Roadmap. This allowed the project to gather important information from the community, as well as offering an opportunity for participation in the development of this important document.

4. Organisation

BioChemIT2012 was organised as part of the 11th International Conference on Unconventional Computation & Natural Computation 2012 (UCNC '12) which took place at the Fundamental Computer Science Laboratory of the University of Orléans. This series of

international conferences is devoted to all aspects of unconventional computation and natural computation, theory as well as experiments and applications. These conferences were previously named Unconventional Models of Computation (UMC) from 1998 to 2002 and then Unconventional Computation (UC). For the 11th edition, the conference became Unconventional Computation and Natural Computation (UCNC).

A page was created on the COBRA website with the information about the Workshop: www.cobra-project.eu/biochemit2012_call.html containing a call for abstracts and linked with the Conference Website: http://www.univ-orleans.fr/lifo/events/UCNC2012/index.php for registration. Registration was handled by the UCNC '12 organisers.

Two invited speakers were organized: Professor Susan Stepney, Computer Science, University of York gave the plenary lecture; *Sub-Symbolic Artificial Chemistry*, and Dr Jane Calvert, Innogen; the Centre for Social and Economic Research on Innovation in Genomics at the University of Edinburgh talked about her experience of working on the UK Synthetic Biology Roadmap; *Governing and imagining the future: reflections on the UK synthetic biology roadmap* which set the scene for the panel discussion. Professor John McCaskill also gave a presentation on the COBRA C^{hem}B^{io}IT Roadmap to initiate the discussion.

Eleven abstracts were accepted for presentation from a range of researchers at different stages in their careers and covering different aspects of the field. It was also agreed with the editors of the MIT Press journal Artificial Life that the authors of selected abstracts would be invited to submit full papers to a special issue of the journal to be compiled after the workshop. The call for papers associated with this has been issued.

The program committee was made up of:

- Martyn Amos (Manchester Metropolitan University)
- John McCaskill (Ruhr-Universität Bochum)
- Steen Rasmussen (Syddansk Universitet)
- Irene Poli (Università Ca' Foscari di Venice)
- Peter Dittrich (Friedrich-Schiller-Universität Jena)

5. Programme

5.1 Programme

Time	Title	Presenter(s)
08:45	08:45 Arrival and welcome	Martyn Amos
09:00	Evolutionary search in engineered bacterial population.	Benes *et al.*
09:20	Engineering multicellular logic through conjugation.	Göni-Moreno
09:40	Optimizing for open-ended complexity in simulated prebiotic evolution	Lui *et al*.
10:10	Towards MicroBRAIN	Ieropoulos *et al*.
10:30	Break	
10:50	Neural isomorphisms of adaptive Belousov Zhabotinsky encapsulated vesicles	Holley *et al*.
11:10	Autonomous droplets: From neurons to muscles	Jones et al.
11:30	Selecting self-assembly pathways	Luo *et al*.
11:50	Selective propagation of Belousov-Zhabotinsky waves in milliscale channels	Abraham *et al*.
12:10	*De novo* automated design of RNA logic circuits	Landrain *et al*.
12:30	Lunch	
14:00	Plenary lecture: Sub-symbolic artificial chemistries	Stepney
15:00	SimSoup: Molecular structures designed for network memory and evolution	Gordon-Smith
15:20	MICREAgents: Microscale Chemically Reactive Electronic Agents	McCaskill *et al.*
15:40	Break	
16:00	Panel/discussion session: Governing and imagining the future: reflections on the UK synthetic biology roadmap Presentation on the COBRA C^{hem}B^{io}IT Roadmap Discussion	Dr Jane Calvert, Professor John McCaskill

Abstracts from the presentations can be downloaded from http://www.cobra-project.eu/abstract2012/.

5.2 Plenary Lecture from Professor Susan Stepney

Sub-symbolic artificial chemistries

Susan Stepney, Department of Computer Science, University of York

Abstract:
Artificial Chemistries (AChems) are often suggested as a suitable basis for the rich behaviour and dynamics needed to underpin Artificial Life systems. However, traditional AChems have their limitations, often requiring ad hoc programming extensions to encompass new behaviours. Here I describe our work on sub-symbolic AChems, which overcome some of these limitations, potentially providing a uniform approach to developing systems exhibiting unbounded novelty in silico.
Slides from the lecture can be viewed at http://www.cobra-project.eu/docs/Presentation-SusanStepney.pdf

5.3 COBRA C^{hem}B^{io}IT Roadmap discussion

5.3.1 Invited Lecture from Dr Jane Calvert

Governing and imagining the future: reflections on the UK Synthetic Biology Roadmap.
Jane Calvert, Centre for Social and Economic Research on Innovation in Genomics, University of Edinburgh

Slides from the lecture can be viewed at http://www.cobra-project.eu/docs/Presentation-JaneCalvert.pdf

Notes from lecture
The aim of roadmaps is to shape people's behavior through a particular view of the future – roadmaps are performative. They work best for technologies where progress is incremental and for which applications are predictable, this is not the case for emerging technologies.

'*Weave a picture if the future that attempts to galvanize actions in the present'*, McDowell, 2012

They contain the idea of a road, why one road?

- shared purpose to make things happen
- but a single view can dominate
- downplays uncertainties
- narrow group informing discussion
- a road map (real) is not linear, there are multiple paths
- should think more in terms of multiple paths

Roadmaps should not be one-offs, should be ongoing and adaptive and updated.

The UK Synthetic Biology Roadmap aims to accelerate economic growth by stimulating and supporting business-led innovation, synthetic biology needed a roadmap because it is a key emerging technology. The group was already setup and running before the social and ethical issues were added into discussion. Initially data was collected on the synthetic biology

community. Participants were asked in workshops about their short, medium and long-term expectations in the field. The community building function of the workshops was also important. A vision and recommendations were produced, not really a roadmap, it says very little about science, it is more about products and industry. The emphasis is on the economic, reflecting the driving force behind the creation of the roadmap. The production of roadmap is not the end of process but the beginning. It is necessary to have engagement with wide groups including supposed end users.
The Synthetic Biology Roadmap says little about the science compared to the COBRA pre-roadmap vision.

Grand challenges are tools '*for mobilising an international community of scientists towards predefined global goals'*, Brooks et al. 2009. The advantage of a grand challenge is that it can incorporate many different types of research. Almost by definition they have significant social dimensions. Taking as an example personal fabrication from the COBRA document; moving away from mass production to personal fabrication. Is there really a demand? Who wants it? Societal impact, jobs etc.? Throw away mentality?

Discussion of the future is important because it has real effects in the present.

Discussion

- Visions contain value judgements so people were asked questions about the nightmare scenarios as well.
- Just because something is technologically possible does not mean that it is desirable for everyone in every circumstance.
- The Synthetic Biology Roadmap is very generic, is there more detail below this? No, it is very generic, so is it even a roadmap or more a report (a tourist guide) than a roadmap?
- How speculation becomes reality, the future becomes concrete through current activities, discussion like this (the Synthetic Biology Roadmap).

5.3.2 Draft COBRA ChemBioIT Roadmap for Biological and Chemical Information Technology

Presented by Professor John McCaskill, COBRA lead on Roadmap development

Notes from presentation

The primary/first input to the roadmap came from the survey conducted by Steen Rasmussen. Participants were largely people known already to the project; 85 participants, across a range of activities. They were asked for key publications and projects in the area in survey this information was then used to expand the list. This gave a particular focus to start the roadmapping process. This was necessary as Chemical and Biological Information Technology means so many different things to different people. It is necessary to adopt a coherent perspective on the way forward to enable progress so starting from inspired by life scenario to get coherence;

'*Life is a self-sustained chemical system capable of undergoing Darwinian evolution*.'
G. F. Joyce, 1994

The litany;
In stark contrast with current computer technology biological cells compute in construction using molecular and spatial information in order to organise, power, sustain, repair, move, communicate, reproduce, protect and evolve themselves robustly, and from simple and scarce materials and energy resources in their complex environments.

Mastery and adaptation of this programmable self production technology with novel chemicals, novel information, novel architecture, novel environments and novel objectives will lay the basis for the sustainable biocompatible and personalised intelligent device construction and sustainable engineering of the future.

Current Executive Summary of Roadmap;
To develop by 2024 a portfolio of emerging ChemBioInfoFab Technologies that allow humanly configured, autonomous control of massively parallel information processing and ongoing fabrication in macroscopic artefacts with molecular scale precision, that are sufficiently generic and complex to serve as a toolkit for good solutions to a diverse range of technical challenges/problems.

On-going fabrication is what sets this apart from normal information processing. It is very general in terms of applications but specific in the way in which the information technology interacts with the Chem and Bio to produce the new functional activity. In the COBRA realm diagram, items in more overlapping sets are more relevant. This field is not just trying to replicate the biosphere but to create a humanly manageable technology, trying to move to the intersection of all four elements (chemistry, biology, fabrication, IT), developing humanly manageable technology at the intersection of all four spheres.

In the roadmap the aim is to develop a list of less than 12 core technologies that are sufficiently close to the overarching objectives, this will summarise large swathes of scientific and technological activity. The initial list is a stimulus constructed by John McCaskill rather than a consensus list. It is divided into *illustrative* sub-bullets rather than *defining* sub-bullets. The list will be expanded, reshuffled and sorted and passed to an international panel to thresh out a more detailed roadmap for the sub-bullets. Metrics need to be identified to see how these areas relate to each other and how they fit together. They will be arranged in terms of progress towards the goal, there are difficulties comparing different elements in terms of progress towards the goal.
Ideally all the technologies would be multi-scaled, robust, flexible, evolvable, autonomous, complex, sustainable and self-constructing but also programmable and controllable, however many of these things are antagonistic to one another. Would like to be able arrange these so can the direction that people are shifting in this can be seen. Impact on society will be included.

This is not the final product, there is much more to do, not yet ready to engage with the public. At this stage still formulating the scope of the roadmap, need to agree on an overarching objective, agree on a list of component areas and threads that we might want to structure it with. Then a panel of those working in the field together with representatives from other sides of the community including social scientists will be invited to participate in threshing out a roadmap document. The first draft following for feedback from this group and the COBRA team will be posted publicly on the web and comments invited.

5.3.3. Discussion of Roadmap

Involving the public;

- There is no such group as ‘the public’.
- Should look for people who have a specific interest in specific applications.
- Can’t address the public at large, most people not interested in what you are doing.
- Have to take those who are actually interested, interested amateurs. (e.g. DIYBio)
- One of the aims of this is to make technology personal, to empower individuals to create technology, DIY technology is a key component.
- This will help to resolve negative images associated with computer science, to challenge the dominant image of computer science.
- It will be useful to engage the bio-hacker community both as potential users of the technology and to help with expectation management because interested amateurs act as evangelists for a new area, they can be an influential voice in their communities.
- This is very goal-orientated, looking for tool-kits to do things, rather than asking how it works. Hackers may also be more interested in how it works.

Other roadmaps;

- The ICT Roadmap is very technological, it defines technical things that need to be achieved and proposes candidate technology, it gives an indication at what point candidate technologies should be approved or eliminated, it doesn’t say what it is going to be used for. There are different types of roadmaps for different types of technologies. To create that sort of roadmap for BioChemIT is harder to do that as there is not such a consensus, a consensus about what BioChemIT achievements would need to be in place would be necessary, this is partly the role of the metrics being developed.
- The semi-conductor industry roadmap is also not a single axis but basically it is computation and quantity dominated. Intertwining with fabrication and autonomy issues makes for a more complex metric. A metric can be formulated which allows progress to be gauged. There is a relatively clear vision that as in biology there is a molecular scale detailed structure participating in locally autonomous / semi-autonomous orchestrated activity up to very large scale.

Dimensions/metric:

- If vision is ecological, evolutionary technology with advantages of biology but under human control can create a quantitative roadmap which is similar to the semi-conductor roadmap and really quantify progress.

- This is a multi but not infinite -axis entity so need to work out the significant/relevant axes. One of the things that came up in the morning was that open-ended evolution suggests a creativity axis. Most of the technologies are not even evolvable let alone open-endedly evolvable. There are many dimensions of evolvableness.
- What is missing here (also missing from the semi-conductor roadmap) is a reference to anything like intelligence. Why not? Depends if you want to grasp the hydra that is intelligence. How is it defined?
- Also missing from a technological standpoint is cost.

- Some quantitative measure on axes would be helpful.

Sustainability:

- What does sustainable mean in this context? Many things, but it does contact with the ecological idea of sustainable, not consuming resources, not clogging up the environment, not causing insurmountable problems in another sector, involves resources.
- Are sustainable and self-constructing the same axis or a different axis? Clearly separate concepts, they overlap here because of resource utilisation, self-construction need to be sustainable, it's about the metabolic component of self-construction. Self-construction is on as a facet of sustainability.
- Might not want self-construction to be sustainable, because of proliferation, that is a different axis, programmable/controllable axis.

ChemBioIT specific:

- It is interesting to look at and highlight what is specific for ChemBio rather than conventional ICT; fast, efficient. Where ChemBio ICT would be different from conventional ICT.
- Only speed and efficiency are heavily pursued in hardware side of conventional ICT, robustness and flexibility is talked about but it is usually talked about in the context of we can't do it properly and we can't do it properly and we have to look at biology to teach us how to do it.

Life:

- If we look at this diagram and put life on it programmable and controllable is in the middle and everything else is out on the edge. Depends what you are looking at, if talking about construction then life is pretty good at making complex entities.
- If we take life and add programmability do we have what we want?
- Life is good at construction but not good at abstract computation maybe.
- Not looking at turning life into technology but at making technologies come alive, actual life as it is vs. abstract life with all its potential and ramifications. Does this mean that there are more axes that need to be there to distinguish what trying to do here achieve from life? Because if life has nearly done it and if it doesn't actually capture what is wanted that implies there might be some other axes that are needed.
- Life does have some sort internal programmable control, there huge gaps in our understanding of that.
- Would like to see suggestions for additional axes on the metric.
- Diagram for conventional life and diagram for conventional ICT would also make useful comparison to highlight key differences.

John McCaskill issued an invitation to those present to participate in the roadmapping exercise? Details of the proto-roadmap will be circulated. of proto-roadmap.

6.0 Participants

Participants who signed in to the workshop:

Chinnu ABRAHAM	University of Southampton
Martyn AMOS	Manchester Metropolitan University
Kerstin ANDERSSON	Karlstad University, Sweden
Masashi AONO	RIKEN Advanced Science Institute
David BENEŠ	Silesian University in Opava, Research Institute of the IT4 Innovations Centre of Excellence
Jane CALVERT	University of Edinburgh
Maurits DE PLANQUE	University of Southampton
Ada DIACONESCU	Télécom Paris Tech, CNRS LTCI
Andre ESTEVEZ-TORRES	CNRS, Marcoussis
Mohammad-hadi FOROUGMAND-ARAABI	University of Tehran
Marian GHEORGHE	University of Sheffield
Angel GONI MORENO	Manchester Metropolitan University
Chris GORDON-SMITH	SimSoup
Gerd GRUENERT	University Jena
Julian HOLLEY	University of the West of England
Ioannis IEROPOULOS	Bristol Robotics Laboratory
Natasha JONOSKA	University of South Florida
Istvan KENYERES	Organica Water Inc.
Hwi KIM	Korea University
Philip KING	University of Southampton
Matthew LAKIN	University of New Mexico
Thomas LANDRAIN	Institute for Systems and Synthetic Biology
Leong Ting LUI	University of Nottingham
Hanjie LUO	University of Southampton
Béatrice MARQUEZ-GARRIDO	European Commission
Giancarlo MAURI	Università Milano-Bicocca
John MCCASKILL	Ruhr-Universität Bochum
Amanda MINNICH	UNM
Makoto NARUSE	National Institute of Information and Communications Technology
Yusuke OGURA	Osaka University
Kazunari OZASA	RIKEN
Arjun RALLAPALLI	Duke University
Darko STEFANOVIC	University of New Mexico
Susan STEPNEY	York Centre for Complex Systems Analysis, University of York
Jun TANDA	Osaka University
Naoya TATE	The University of Tokyo
Margaret TAYLOR	Manchester Metropolitan University
Lance WILLIAMS	University of New Mexico
Klaus-Peter ZAUNER	University of Southampton

7.0 Photographs of BioChemIT12

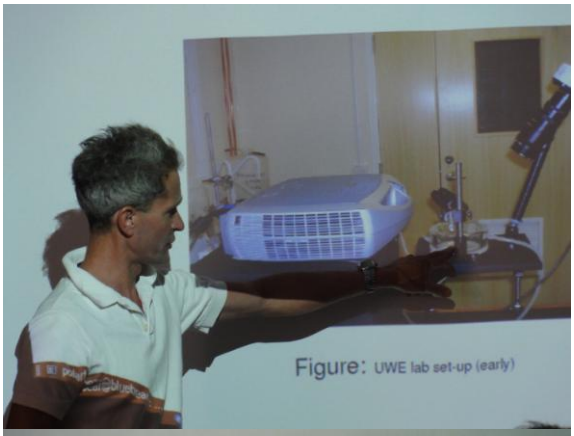
Figure: UWE lab set-up (early)


Scaffold: