Artificial Wet Neuronal Networks from Compartmentalised Excitable Chemical Media (NEUNEU)

NeuNeu Consortium
http://www.neu-n.eu

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Contents

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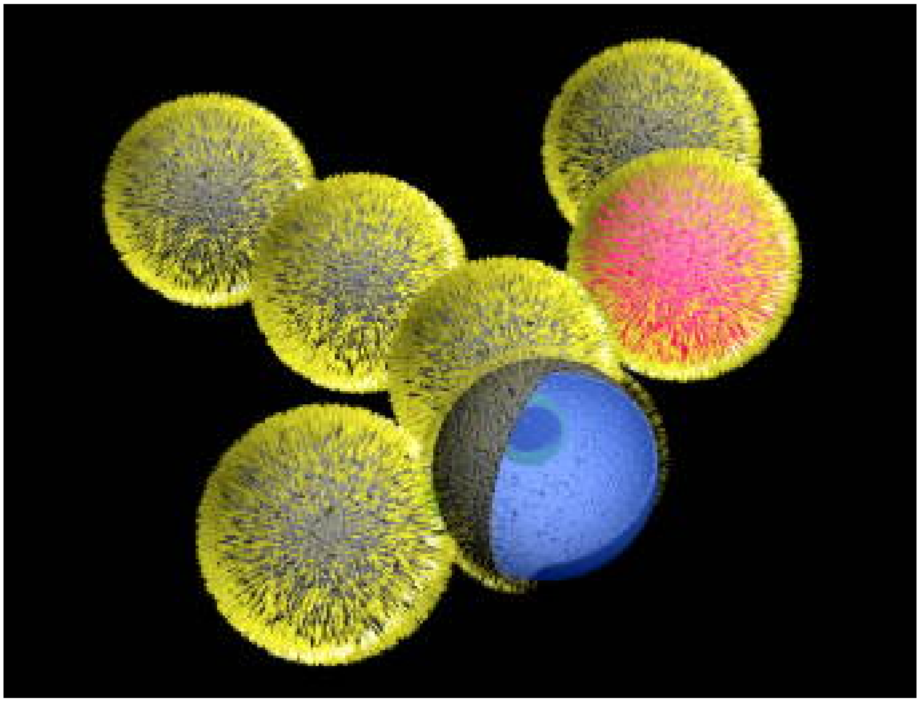
The NEUNEU research program is concerned with the development of mass-producible chemical information processing components and their interconnection into functional architectures.



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The individual supramolecular components will crudely resemble biological neurons and will be capable of excitation and self-repair. Self-organisation of organic compounds and proteins will be complemented with dielectrophoretic manipulation to fabricate small devices from interconnected supramolecular components. State-of-the-art micro- and nano-scale technologies will be exploited to take well established physico-chemical phenomena into the new context of forming a flexible and efficient substrate for a chemistry-based information technology. Through integrated modeling from component to architecture level a broad understanding of the capabilities and limitations of the implemented as well as related technologies will be established. This ambitious collaboration among computer-scientists, biophysicists, chemical-physcists, biochemists, chemical-biologists, and electrical engineers will develop the core science needed to build a future massively parallel computing infrastructure, will deliver prototype devices, and will pave the ground to harnessing bio- and nano-materials for a novel approach to cognitive computing.

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Summary description of project context and objectives

Information processing is ubiquitous in nature and functions very differently from our present computing technology (cf. Figure 1). Based on molecular components and phenomena it demonstrates that an alternate route to information processing exists. The NEUNEU project has explored this path with a minimal system that exhibits the properties (signal transmission, signal gain, self-repair) desirable for a molecular information processing architecture that harbors the potential to scale to applications. To explore the concept of performing computations with excitable media we use the Belousov-Zhabotinsky (BZ) medium. The BZ reaction is an oscillating reaction, existing far from the thermodynamic equilibrium. Though there are variations, the BZ-mixture can be prepared from potassium bromide, malonic acid, sodium bromate, sulfuric acid and ferroin as the catalyst and redox indicator.

When the system is oscillating, the indicator is continuously switching between its oxidized and reduced form, changing its color between blue and red Figures 2-12. Stirring the system leads the whole mixture to show oscillations in all parts of the reaction vessel. On the contrary, leaving the mixture relatively undisturbed in a flat Petri dish, the BZ medium generates 2D excitation wave patterns similar to those visible in the droplets in Figure 2.

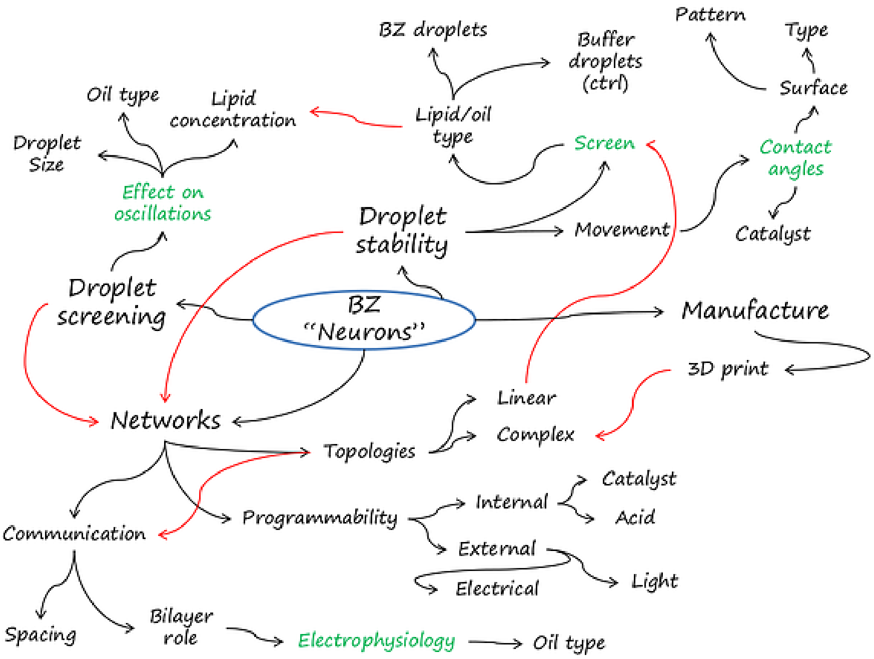


Figure 1: General overview of the computing Belousov Zhabotinsky droplet systems

To harvest the signals that are transmitted through the chemical medium for computations, continuous excitations may not always be desirable. The BZ medium, however can be prepared such that it does not spontaneously oscillate. Instead, the excitation needs to be triggered from the outside (e.g., by a silver wire) or by an already existing excitation wave. Hence we call the state of the medium "excitable" or "sub-excitatory".

Using the "sub-excitatory" condition alternatively, we can also include logic elements inside single large droplets. In this case, waves do not spread in every direction, but preserve their shape and direction as illustrated in Figure 16.

When we drop water containing BZ medium into oil, the phases do not merge and droplets form automatically. We are using microfluidics to produce droplets of smaller volumes, with higher precision, and in large quantities (Figure 2-4). Encapsulating the BZ reaction in these small droplets has the advantage of discretizing the otherwise continuously propagating excitations into precise controllable units.

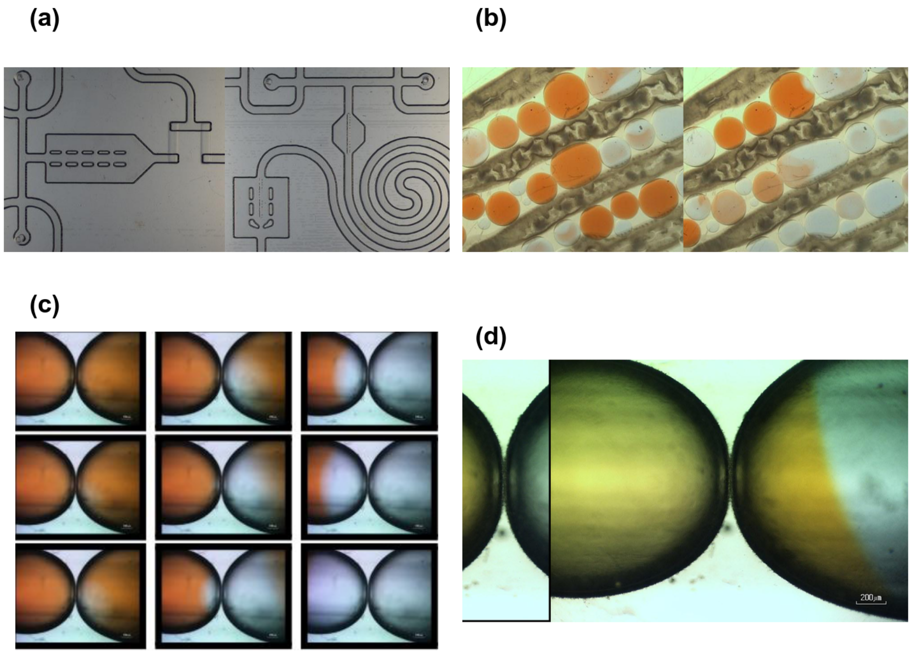


Figure 2: **(a)** Examples of microfluidic structures for generation and handling of droplets. **(b)** Manually aligned droplets of BZ-reaction medium. **(c)** Transmission of excitation from droplet to droplet. **(d):** Microscopic view of the droplet-droplet interface: an excitation just passed through. (*P. King & J. Corsi, ECS Univ. of Southampton, 2011, 2013*)

The compartmentalisation is achieved by lipid molecules contained in the oil phase. These lipids self-assemble at the surface of the droplets and stabilize the droplets against merging. Living cells are also covered with lipids, but in this case lipids assemble between two aqueous compartments and therefore form the double layer typical for biomembranes. The amphiphilic lipid molecules assembling at the border between the oil and the ionic ("water with BZ") phase, produce a lipid monolayer in our system.

When two of the droplets come into contact, the lipid monolayers coating each droplet can form a double layer similar to a biological membrane. We have found that the formation of this bilayer is important for the the exchange of chemical compounds and consequently the propagation of the BZ medium excitation from droplet to droplet.

By varying the coupling between droplets, the droplet radii, and BZ medium compositions, we have generated droplets with a wide variety of properties, such as excitability, oscillation phase length or refractory times. Controlling these properties is important to engineer droplet networks with computational capabilities as illustrated in Figures 13-17.

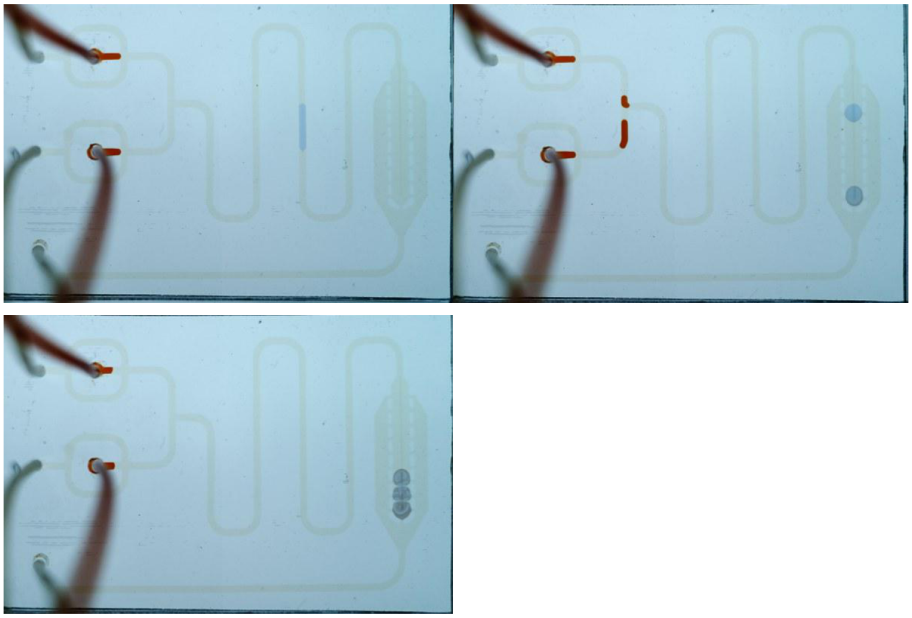


Figure 3: BZ medium is mixed on chip to create a linear array of oscillating droplets. (P. King, ECS Univ. of Southampton, 2013).

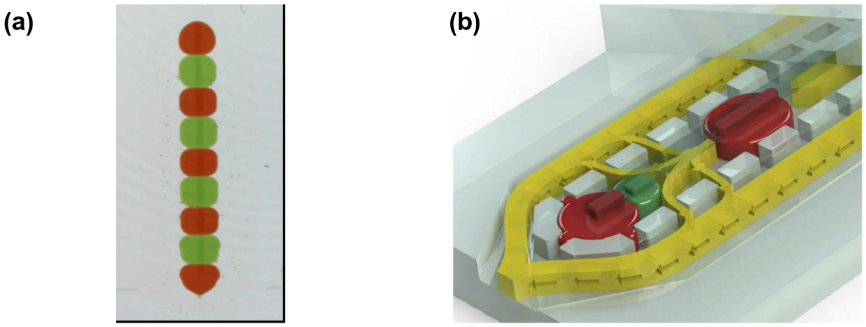


Figure 4: Droplet trap on microfluidic chip for linear droplet arrays. **(a)** Droplets filled with color die. **(b)** 3-D graphics illustrating the fluid flow. (*P. King, et al. Interdroplet bilayer arrays in microfluidic droplet traps from 3D-printed molds, 2013, submitted.*)

Work Performed and Main Results

The NEUNEU project has approached its objectives with a hierarchy of studies encompassing laboratory experiments to produce functional droplets, biophysical modeling of the chemical dynamics in the droplets, theoretical studies of droplet interactions, and computer simulation studies of complex droplet architectures.

To produce droplets that can serve as elementary components in a computing architecture three problems needed to be solved. First, a suitable chemical composition of the reaction medium in the droplets had to be determined. Second, a suitable composition of the lipid layer enclosing the droplet needed to be found. And third, a microfluidic droplet generator that can deliver fresh active droplets of a desired size is required. Work has been undertaken to tackle all three challenges. Initial experiments with large drops (3-10mm diameter) of BZ medium in oil showed that the BZ medium can function in lipid coated droplets. Observations of the temporal excitation patterns indicated that the excitation may travel directly from droplet to droplet without any pores and in special cases even without direct contact of the droplets. This result was encouraging, because the transmission of excitation from droplet to droplet is essential for a droplet-based architecture. However, it also leads to the problem of isolating droplets to prevent undesirable interactions.

o determine the conditions under which transmission of excitation can take place we made specialised reaction vessels by producing a mold on a 3D-printer for PDMS, a transparent rubber material commonly used for microfluidic chips. After some initial problems with this technique had been resolved it turned out to be a fast and flexible method to produce high-aspect ratio channels. We have demonstrated the feasibility of mixing droplets of BZ reaction media on-chip and assembling arrays of oscillating droplets of variable chemical composition and volume into linear arrays of communicating droplets.

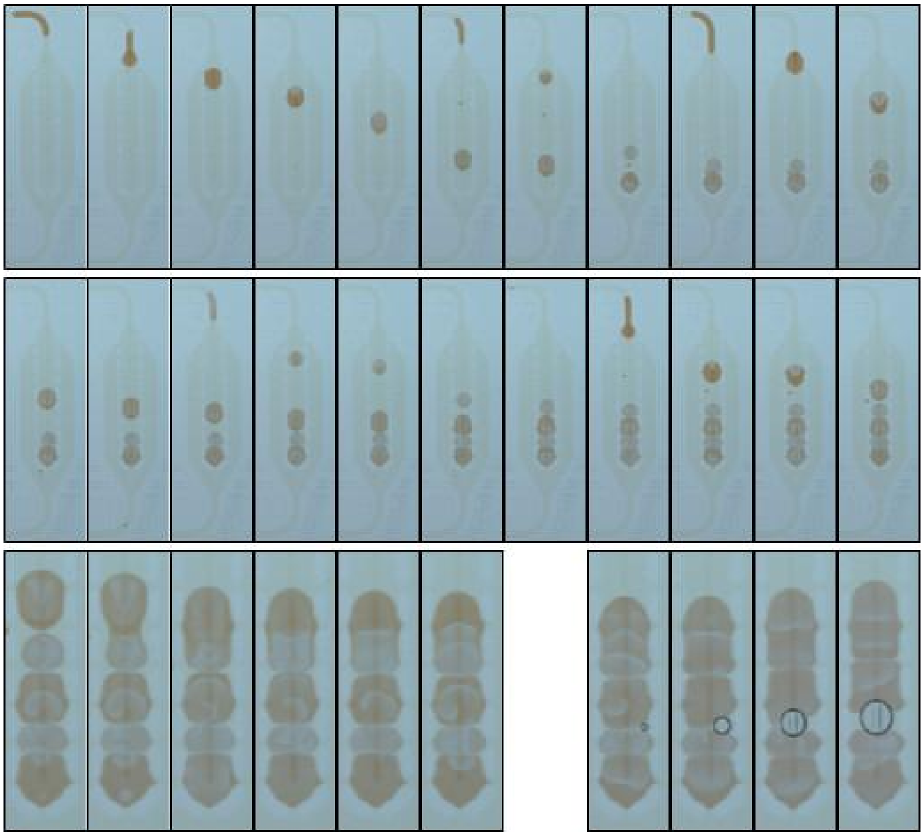


Figure 5: The volume and chemical composition of BZ droplets mixed on chip can be varied from droplet to droplet. With electrophysiological measurements we have shown that lipid bilayer membranes are formed between droplets in the chip. (P. King, ECS Univ. of Southampton, 2013).

We have also investigated the use of a variation on the BZ reaction that replaces the traditionally used malonic acid substrate with cyclohexanedione (CHD) (see Figure 10). This version of BZ does not produce gas, making it ideal for use in enclosed microfluidic chips. It also exhibits a number of unique behaviours, including strong droplet-to-droplet communication and wide excitation pulse width.

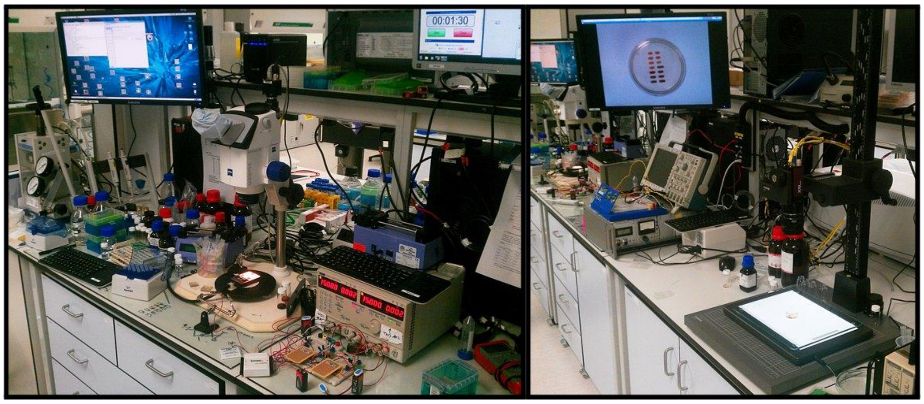
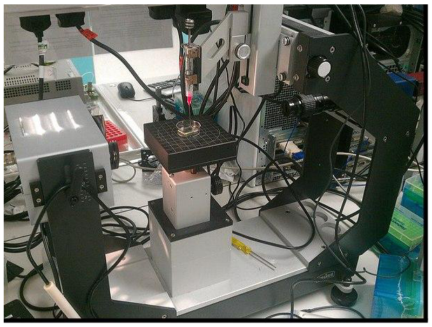


Figure 6: Experimental setup used to optically and electrically investigate the behaviour of BZ droplets. (G. Jones / P. King, Centre for Biohybrid Devices, Univ. of Southampton, 2013)



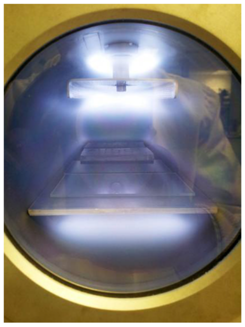


Figure 7: **Left:** Contact angle measurement setup used to study excitation induced motion of BZ-droplets. **Right**: Oxygen plasma chamber used for bonding of microfluidic chips. (G. Jones, Centre for Biohybrid Devices, Univ. of Southampton, 2013)

In order to gain control over oscillations in the droplets, we developed an optical technique that allows us to change excitability of individual droplet without affecting the neighbours. This approach requires additional catalyst, the ruthenium complex, that sensitizes the reaction to blue light. For moderate light intensities we observe increase in the period of oscillations whereas strong

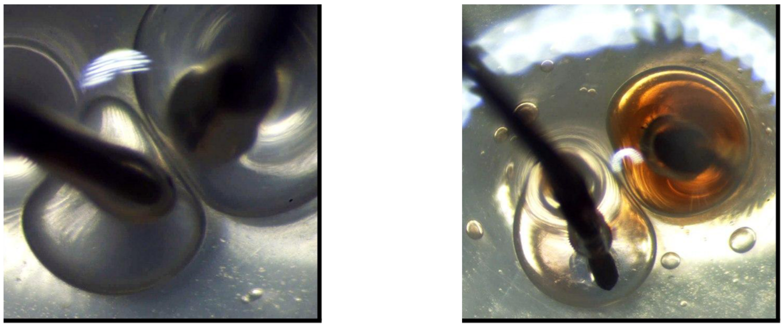


Figure 8: Probing of the droplet-droplet interface with electrical measurements (G. Jones, Centre for Biohybrid Devices, Univ. of Southampton, 2013)

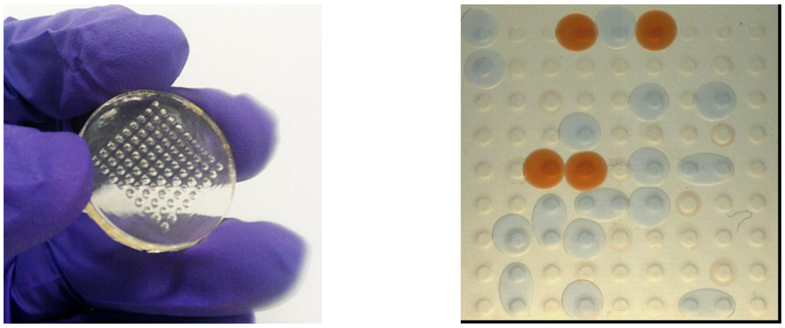


Figure 9: **(a)** Array template fabricated using 3D-printing technology and used for 2D-droplet array studies such as shown in **(b)** with droplets in different states. (G. Jones, Centre for Biohybrid Devices, Univ. of Southampton, 2013)

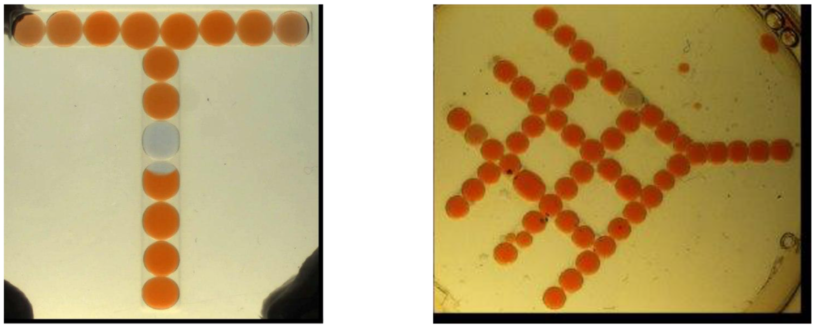


Figure 10: Creating droplets that communicate reliably and are stable against fusion proved challenging. After careful optimization of the chemical composition it was possible to construct and study arrays with over 50 droplets. (G. Jones, ECS Univ. of Southampton, 2013).

illumination can stop the oscillations completely. The light coming from high power LEDs is transferred to a specific droplet through optical fibers to limit the amount of light spreading to the surrounding.

We applied this method to study small systems of coupled BZ droplets (consisted of two or three droplets) for their potential of information storing. To build a simple, one bit memory cell two different, stable oscillatory states need to be distinguished. Here we illuminated the droplets with light strong enough to suppress oscillations and then turn it off with a specified time shift for each droplet. Activation sequences of excitations (modes) initiated this way were studied and our results indicate that only the three droplet systems have two stable rotational modes that can be used as different memory states. Moreover we demonstrated that we can change direction of the rotations a few times during one experiment.

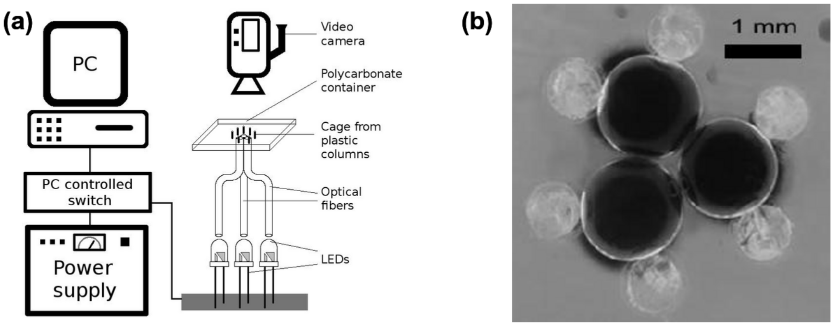


Figure 11: **(a)** The setup for experiment with coupled oscillations in a few (here three) photosensitive droplets build at ICFPAN. **(b)** Top view of three droplets trapped in a plastic columns cage. (cf. *K. Gizynski, K. et al., Light controlled oscillations of interacting Belousov-Zhabotinsky droplets, 2013. to be submitted*)

Thinking of more powerful systems for information processing, we started to study the experimental conditions in which **a 3D structure** of droplets can be generated, as illustrated in Figure 12. However, the difficulties to observe such complex systems need to be overcome. We are also able to simulate 3D droplet networks *in silico* (see Figure 13) and developed a method to derive "optimal" self-assembly strategies (Figure 14).

On the theoretical side, three simulation models have been developed for different levels of abstraction: First, a family of kinetic ordinary differential equation (ODE) models describe the chemistry of single droplets and a few connected droplets. These models are quantitative in the sense that they are fitted to experimental data.

Second, a numerical integration of the Oregonator equations simulates wave propagation within a single droplet and a collection of (so far) statically arranged droplets (Figure 16 right). With this model, we have been exploring the compu-

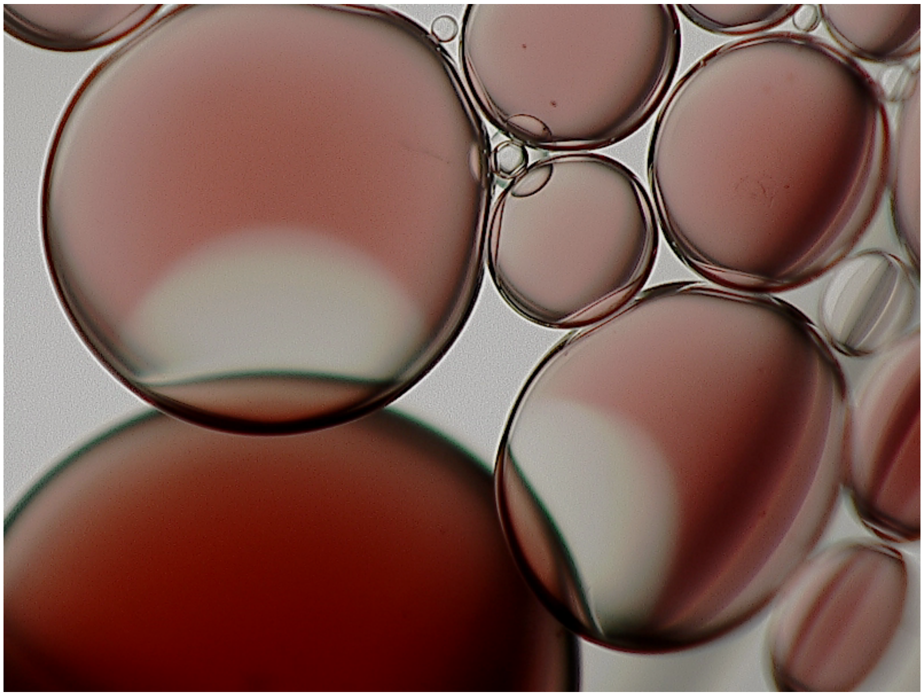


Figure 12: Excitation propagation in a 3D structure of BZ-droplets. The diameter of the largest droplet is 2 mm. The excited regions, characterized by a high concentration of oxidized catalyst, can be seen as white areas in two central droplets. The photograph was made at ICFPAN by Mr. Emilien Leonhardt from HIROX, Europe.

tational possibilities of BZ vesicles by creating key computational components, such as logic gates and arithmetic circuits. BZ excitation waves are used to represent discrete quanta of information. Validation of some of these simulations in-vitro has supported this approach to computing in BZ discs as 2D analogues of BZ vesicles (Figure 16 left).

The third simulation model abstracts away the internal spatial dynamics of a droplet and uses a state-base model allowing for efficient event-based simulations of large networks (Figure 13). Additionally, dynamical droplet structures and their self-assembly processes specified by simple rules can be simulated in 3D (up to about 500 droplets). Hence the assembly and the signal propagation can be modeled in the same framework, allowing for computation processes that control the assembly. Additionally an efficient stochastic simulator considering only the topological structure has been developed.

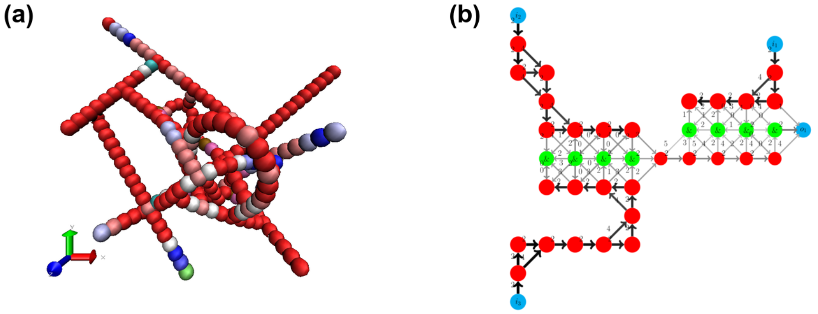


Figure 13: **(a)** Stochastic 3D simulation of a droplet network counting the number of active inputs. **(b)**Information flow in a 2-D simulated stochastic droplet network classifying a Proben1 cancer data set. Source code available at: *www.biosys.uni-jena.de*; further simulation software for droplet computers can be found on *www.neu-n.eu*

We have developed a fundamentally new way to automatically designing droplet architectures in which the signal representation needs not to be prespecified (Figure 15). E.g., it is not necessary to specify beforehand how a zero or one has to be represented. The basic idea is to couple multiple instances of the droplet network such that it has to settle down in a specific attractor, which allows to evaluate whether the network performs the computation correctly. Moreover this attractor provides also a signal encoding. We due to its feedback structure we call those networks *re-entrant networks of repeated Units (RERUN) networks* or*tautological loops*. The we use at evolution and self-organization at the same time. In that, self-organization is used to find suitable signal representations by the network itself. Evolution is used to search for suitable networks. We demonstrate *in-silico* the basic viability of this approach as well as the applicability of this approach for droplet networks

In exploring our 2D abstraction of BZ vesicles, *BZ-discs*, we managed to physically

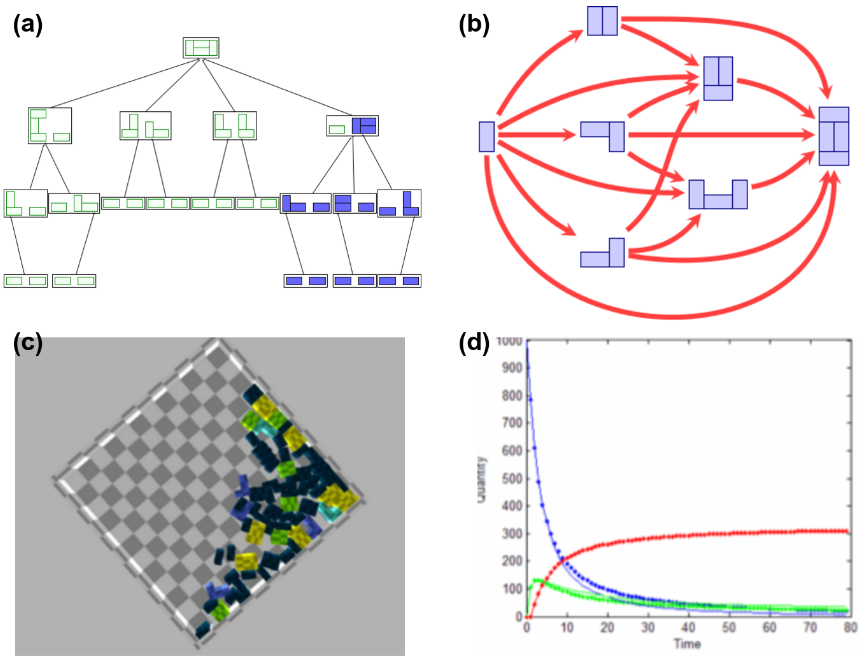


Figure 14: Illustration of our approach to select self-assembly pathways and for finding good kinetic rate constants for a self-assembly process, which we envision in future as a possible route towards fabricating complex droplet architectures. Here we assume a four component structure to be assembled. The procedure consists of an algorithm that derives all possible assembly options for a desired target structure**(a)**. Then a dynamical chemical ODE model is derived whose structure is sketched in**(b)**. The ODE model is fitted to the experimental data, here obtained from a physical simulation,**(c)**. Then global optimization is applied to find “optimal” rate constants**(d)**. (cf. *Luo, H.; Dittrich, P.; Zauner, K–P. Selecting Self-Assembly Pathways, 2013, submitted)*

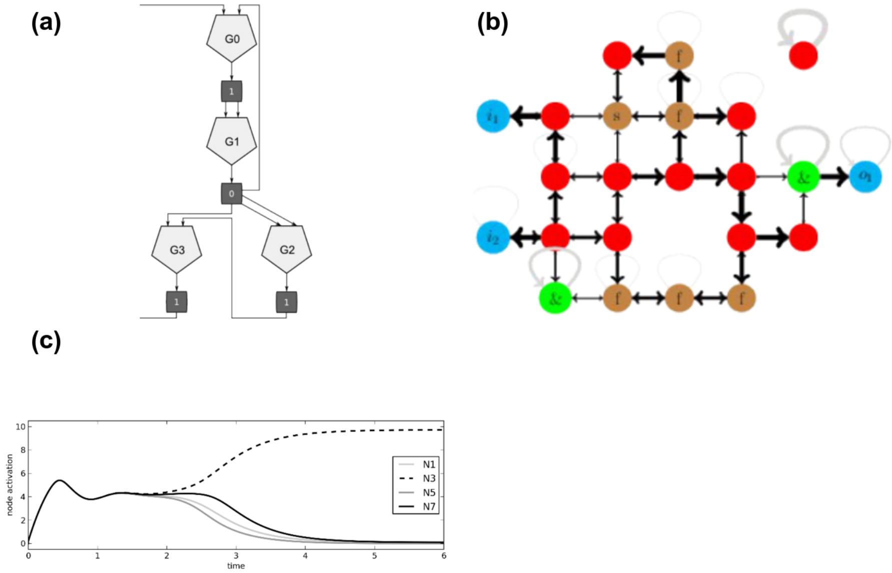


Figure 15: Example of a RERUN network **(a)** for evolving NOR Boolean function. G0, G1, G2, G3 are four instances of the same design of a computational unit, which could be for example a droplet network as sketched **(b)**. In order to test whether the droplet network is suitable for NOR calculation, we generate four copies of it (G0, G1, G2, G3) and connect them according to the RERUN network **(a)**. Then we start the system with a randomly assigned initial state and wait until an attractor is reached **(c)**. If the network is computing well (as it is here), then the distances between connections ("wires") marked with different logical values (i.e.., 0 and 1) must be large, while the distance between connections marked with the same logical value must be small (cf. *Egbert, M.; Gruenert, G.; Dittrich, P. Using Re-Entrant Networks of Repeated Units to Facilitate the Automated Design of Logic Gates in Unconventional Media: A New Method, 2013, submitted)*

implement some of our simulated designs as illustrated in Figure 16. In this composite time lapse image actual BZ-waves (monochrome left column) are shown to closely follow the simulation (colour, right column).

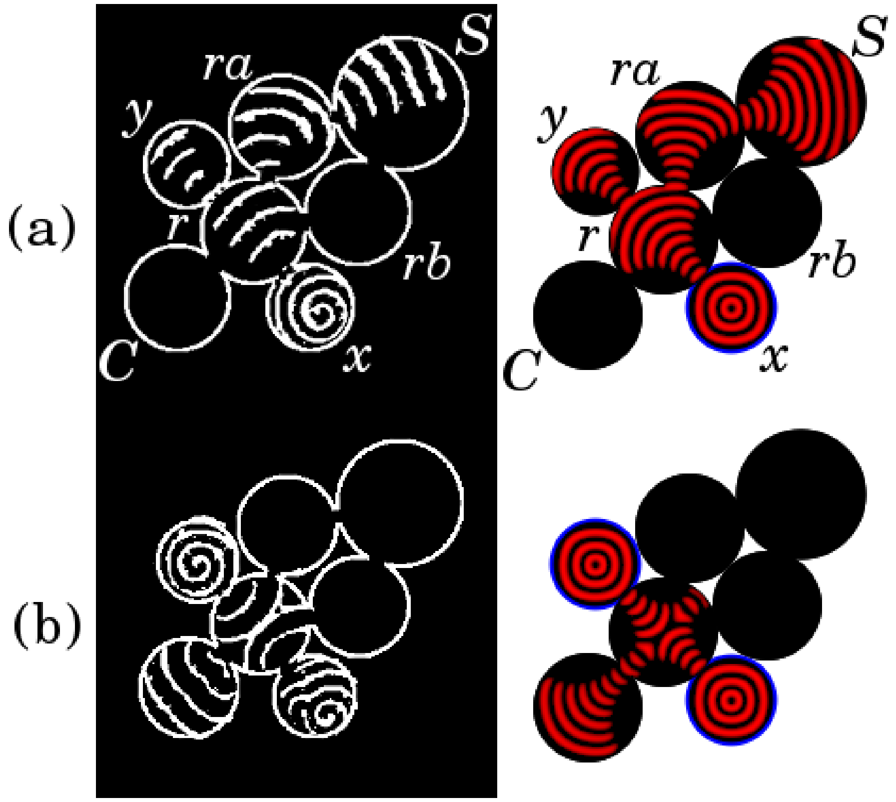
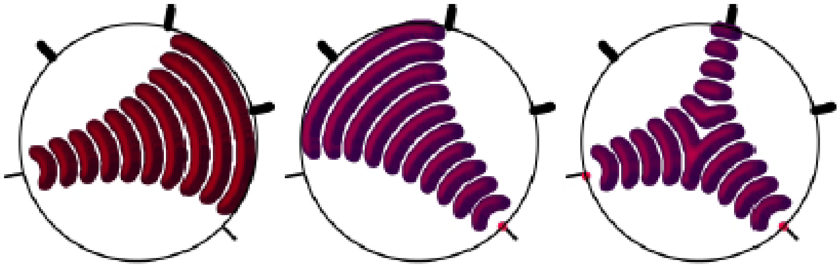


Figure 16: Elementary arithmetic circuit (1bit Half adder) created from optically transcribed BZ-discs **(left)**derived from numerical simulation**(right)**. For animation see: http://uncomp.uwe.ac.uk/holley/discs/discs.html.

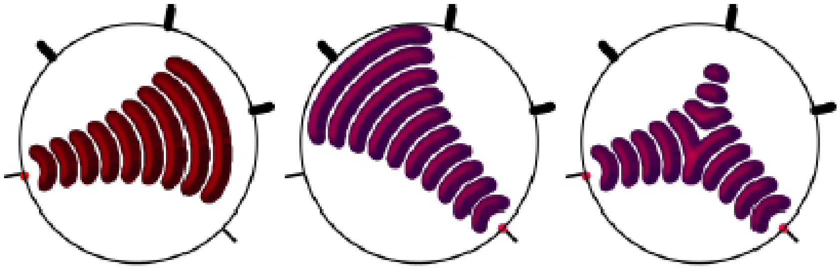
Further to our static logical and arithmetic designs with BZ-discs we have also created optically modulated polymorphic gates, where the logic function of a BZ-disc logic gate can be controlled by light intensity. In computer simulations based on the Oregonator model we demonstrate that the outcomes of inter-fragment collisions can be controlled by varying the illumination level applied to the medium. We interpret these wave fragments as values of Boolean variables and design collision based polymorphic logical gates. The gate implements operation XNOR for low illumination, and it acts as NOR gate for high illumination. As a NOR gate is a universal gate then we are able to demonstrate that a simulated light sensitive BZ medium exhibits computational universality (Figure 17).

For the design of a droplet computer we developed a fundamentally new technique



x=1, y=0 x=0, y=1 x=1, y=1

(c)$\alpha = \frac{2\pi}{3}, \phi = 0.07874$



x=1, y=0 x=0, y=1 x=1, y=1

(d)$\alpha = \frac{2\pi}{3}, \phi = 0.07875$

Figure 17: Simulated optically controlled polymorphic logic gate made from BZ-discs. The function of the BZ-logic gate can be changed depending upon light intensity. BZ-discs in each column are presented with the same inputs on (narrow lines x,y) but output function (thick lines) is altered in the bottom row by a subtle change in light intensity (theta).

that combines self-organization and evolution by tautological loops of droplet circuits. Furthermore we have developed a technique to study the information flow in droplet computers, helping the design and analysis (Figure 15(b)). Our methods do not require the signal encoding to be specified beforehand. For artificial evolution explicit as well as generative representations are used.

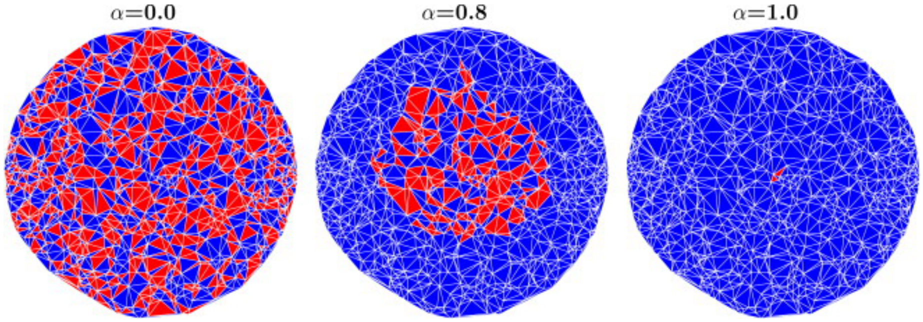


Figure 18: Example of a Delaunay triangulation automata with memory consisting of 1000 points for three different memory charges. The patterns are generated at T=100 starting a single active (red) triangle at T=0. (cf. *Alonso-Sanz/Adamatzky 2013* *http://dx.doi.org/10.1016/j.nancom.2013.10.001*)

We have developed automata models of BZ ensembles using Delaunay triangulation (DT).

DTs are formal models of Belousov-Zhabotinsky (BZ) vesicles networks. Usually lipid vesicles filled with BZ mixture are of different sizes, they do not form a hexagonal lattice as a rule. Also the vesicles can be unstable: a coalescence transforms fine-grained networks of elementary vesicle-processors into coarse-grained ensembles of non-lattice vesicular structures. When BZ-vesicles, quite possible of different sizes, are aggregated into an ensemble and tightly packed, they are represented by Delaunay triangulation. Using an automaton based approach we studied how delayed reaction/excitation of vesicles (analogous of automaton) memory might affect propagation of information/excitation in the BZ ensembles (Figure 18).

We presented a procedure of self-assembly of BZ ensembles based on growing beta-skeletons which remain connected for any (as yet specified during the growth phase), value of beta however large it is. In computational experiments we demonstrated that with an increase of beta and/or decrease of approximation accuracy, the skeletons undergo a transformation from almost regular lattices or networks to branching trees to cross-like graphs (Figure 19).

In computer experiments with cellular automata we designed theoretical tools for growing information pathways in arrays of excitable elements which self-update their excitation intervals (Figure 20). We have shown that it is possible to use principles of collision-based computing (where growing pathways collide and interact with each other) to grow non-trivial information propagation circuits.

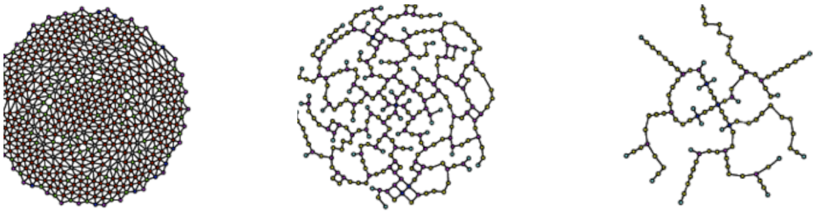


Figure 19: Examples of beta-skeleton models of BZ ensembles grown from a single seed. From [*Adamatzky, A. On growing connected beta-skeletons Computational Geometry , 2013, 46, 805 - 816*http://arxiv.org/abs/1304.1986]

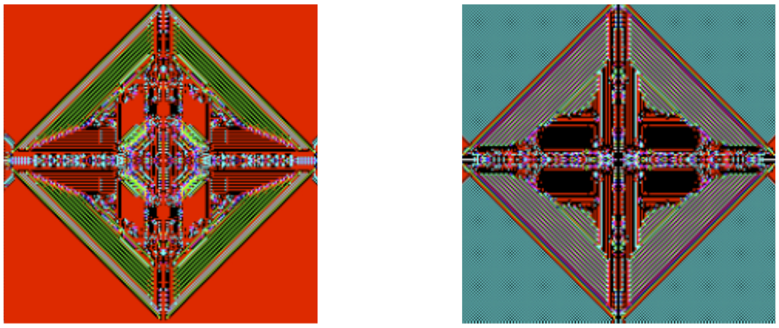


Figure 20: Dynamics of excitability imitated in two-dimensional cellular automaton. From *Adamatzky, A. On diversity of configurations generated by excitable cellular automata with dynamical excitation intervals. Int J Modern Physics C, 2012, 23 10.1142/S0129183112500854*

It is possible to implement universal routing of conductive wires by positioning seeds of growing wires, the following operations with wires are implementable: formation of stationary wires, stopping of both growing wires, formation of conductive circuit with one growing wire, reflection of wires without conductive bridging, co-orientation of both growing wires without formation of conductive bridge, symmetric reflection and multiplication without formation of conductive bridge.

Potential impact and use

Over the past three decades information technology found application in organisation, communication and increasingly in appliances. Wherever information processing could be applied, it typically revolutionised the field within two decades. The very narrow choice of available technologies for information processing, however, has so far prevented the application of information processing in many areas. The NEUNEU project expects to broaden the range of techniques and substrates available for computation. For the immediate future the concepts, methods and devices developed within the NEUNEU project will be most relevant as research tools. However, the unique challenges posed by the project (much larger droplet size than typically used in fluidic chips) have also led to the development of new techniques in the laboratory at least one of which is likely to find application in other areas on a shorter time scale: The fabrication of arrays of large inter-droplet bilayers on chip has direct use for screening bilayer permeability mediated by channel proteins or nanopores in a drug development and toxicity testing context.

The availability of chemical computing media will in the future allow for information technology that can be tightly interwoven with chemical and biochemical systems. Such wet computing architectures are complementary to conventional information technology and are expected to find applications which are not feasible with conventional technology. The control of chemical states within living cells through an information processing drug would be an example. The fine grained control of chemical reactions to enable biomolecule-like complexity in synthetic macromolecules and consequently a large range of new functional materials, would be another example.

Results

Deliverables of the project

Deliverable	Title	DueDate	Finished?
D6.1	Public Website	4/2010	yes
D2.1	Preliminary simulation program and model, in press, International Journal of Unconventional Computing (2011)	10/2010	yes
D1.1	Report about full characterization of BZ reaction in lipid-enclosed droplets	12/2010	yes
D2.2	Report on the model of interacting droplets and a simulation program	2/2011	yes
D3.1	Report on computational model for architectures composed of a moderate number of units	2/2011	yes
D5.1	Periodic management report (Year 1)	2/2011	yes
D3.2	Report for comp. model for architectures composed of large numbers of droplets	5/2011	yes
D1.2	Report about a-hemolysin facilitated BZ droplet excitation	6/2011	yes
D2.3	Report or publication on the final version of the simulation model and its experiments	8/2011	yes
D2.4	Report or publication on computation with one and two droplets	8/2011	yes
D3.3	Implementation of a computational model (software published on website)	8/2011	yes
D3.4	Report or publication on signal dynamics within many droplet systems	8/2011	yes
D4.1	Software model of synaptic connection between two BZ-droplets (published on website)	8/2011	yes
D4.2	Report of BZ-droplet network capable for classification of binary strings	1/2012	yes
D4.3	Report on computer model of a polymorphic gate implemented at a junction between two BZ-vesicles	1/2012	yes
D4.4	A catalog of communication architectures emerged in conglomerates of BZ-vesicles	1/2012	yes
D5.2	Periodic Management Report (Year 2)	1/2012	yes

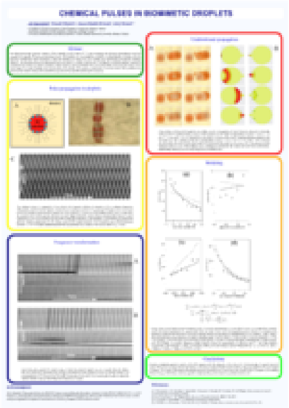
Table 1: This table lists all the milestones and reports that have to be delivered by this project. Finished reports can be downloaded from the “yes” of the finished column.

Deliverables of the project (continued)

Deliverable	Title	DueDate	Finished?
D1.3	Report about excitation propagation through multi-droplet arrays	2/2013	yes
D4.5	Software models of sorting and classification implemented in acyclic networks (published on website)	2/2013	yes
D4.6	Design of sequential logical circuits evolved Report or publication on algorithms	2/2013	yes
D4.9	Report or publication on BZ-vesicles with planar graph approach	2/2013	yes
D1.4	Report about excitation propagation through large droplet networks	10/2013	yes
D2.5	Report or publication on computation with three and more units	10/2013	yes
D3.5	Report or publication on emergence and scalability at architectural level	10/2013	yes
D3.6	Report or publication on adaptation and learning at architectural level	10/2013	yes
D4.8	Report or publication on autonomous network generation through self-organization	10/2013	yes
D6.2	Publish models/video/software on public website	10/2013	yes
D6.3	Two international workshops	10/2013	yes
D6.4	Edited volume containing selected contributions	10/2013	yes

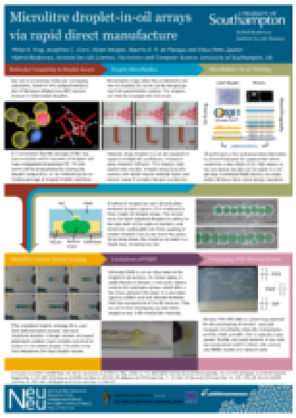
Media

Posters



CHEMICAL PULSES IN BIOMIMETIC DROPLETS

from the Conferences: Engineering of Chemical Complexity, Berlin; 20-th European Conference on Artificial Life in Paris; and FUNCDYN 2011, 4-th European Science Foundation Conference on Functional Dynamics in Praha.



Microlitre droplet-in-oil arrays via rapid direct manufacture

University of Southampton

from the Nanobiotech conference 2011 in Montreux


ECAL 11

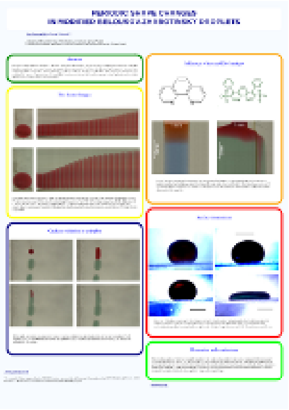
PARIS

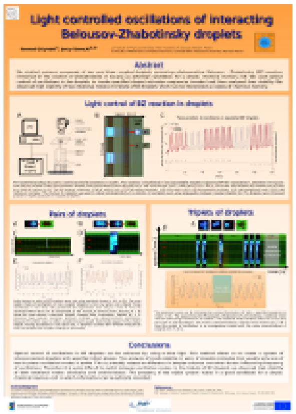
Salon de l'Argentine

Friday, August 12 afternoon

Program

from the INCUP Workshop at ECAL 2011, Paris


presented at the Gordon Conference on Oscillations and Dynamic Instabilities in Chemical Systems, Waterville, Maine USA, July 15-20.07.2012


Light controlled oscillations of interacting Belousov-Zhabotinsky droplets

Abstract

Light control of BZ reaction in droplets

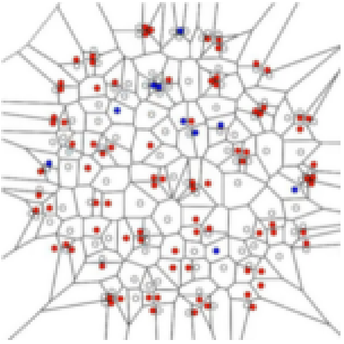
Pairs of droplets

Triplets of droplets

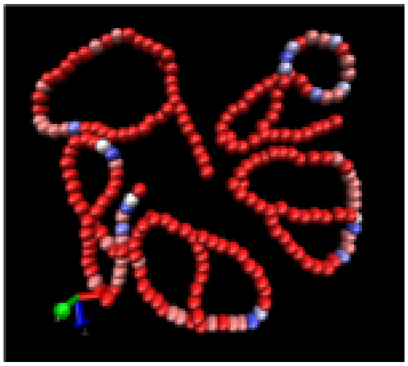
Conclusions

presented at 7th International Conference for Engineering of Chemical Complexity, Rostock 10 - 13 June 2013

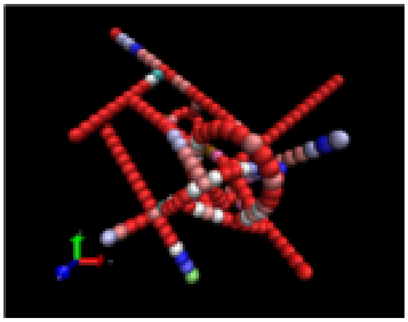
Videos



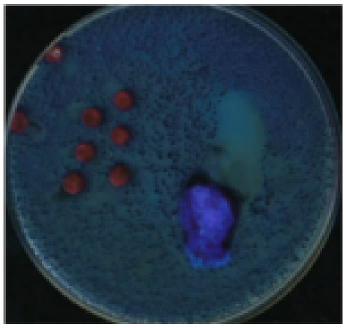
Self-organization of excitable bubbles (youtube).



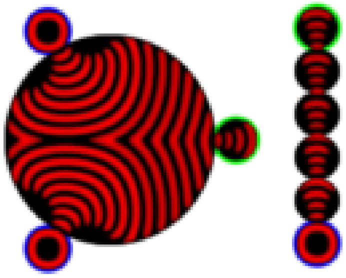
Simulation of travelling excitations in a very simple, cyclic network.



Simulation study of a simple droplet network that maximally stimulates one of the output droplet channels, counting the number of active input signals.

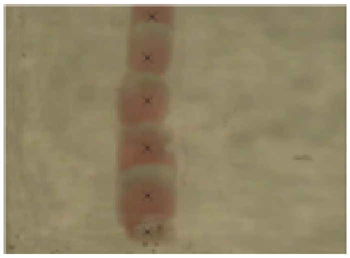


Emulsion Turing Machine (youtube), more videos can be found here.



Movies of the BZ simulations described in "(2011) Computational modalities of Belousov–Zhabotinsky encapsulated vesicles. *Nano Communication Networks*, **2**, 50–61. available: http://www.sciencedirect.com/science/article/pii/S1878778911000135 local: http://users.minet.uni-jena.de/~dittrich/prj/neuneu/pub/preprints/2011_Holley_modalities_of_BZ.pdf"

Movies of experiments described in "(2011) Logical and arithmetic circuits in Belousov-Zhabotinsky encapsulated disks. *Phys. Rev. E*, **84**. available: http://link.aps.org/doi/10.1103/PhysRevE.84.056110 local: http://users.minet.uni-jena.de/~dittrich/prj/neuneu/pub/preprints/2011_Holley_circuits_in_BZ.pdf".



Supplementory movie showing the experiment described in “ (2013) Multi-scale Modelling of Computers made from Excitable Chemical Droplets. *IJUC*, **9**, 237–266. available: http://oldcitypublishing.com/IJUC/IJUCabstracts/IJUC9.3-4abstracts/IJUCv9n3-4p237-266Gruenert.html local: http://users.minet.uni-jena.de/~dittrich/prj/neuneu/pub/deliverables/D3.2_Modelling.pdf”

```
2   2 2 2   2      
  1 2 2   2 2 0   2
  0       2 1   2  
2   2 2   2   0 1  
1   2 2 2   1   1 2
0   2 2       2 2 2
  2   2 2 1   2 2 2
2   1 1 1   0 2 2 2
    0 1 0 2 0 0 2  
  2 2 2   2 0 2 2  
```

DropSim, an event-based stochastic and deterministic simulator for droplet computers and a manual.

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Luo, H., Dittrich, P. and Zauner, K.-P. (2013) Selecting Self-Assembly Pathways. *(to be submitted to Artificial Life)*.

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Not mainly related with NEUNEU, but acknowledging NEUNEU

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Events related to the NeuNeu project

NEUNEU specific events:

28.4.2010:	NEUNEU Kickoff Meeting
28-30.9.2010:	2nd NeuNeu Meeting, Southampton
28-29.3.2011:	3rd NeuNeu Meeting and 1st Review Meeting, Brussels
24-25.11.2011:	4th NeuNeu Meeting, Warsaw
14-16.3.2012:	5th NeuNeu Meeting and 2nd Review Meeting, Southampton
14.9.2012:	6th NeuNeu Meeting, San Candido, Italy
	TODO: Add remaining meetings

Other events of possible interest:

10-21.9.2012:	1st COBRA Summer School on Biological and Chemical Information Technologies (BioChemITSchool 2012), San Candido, Italy
2.5.2013:	Information Processing with Belousov-Zhabotinsky Reaction by Prof. Jerzy Gorecki, Institute of Physical Chemistry, Polish Academy of Science (Poster)

Links

The CHEM-IT Projects

- BACTOCOM (Bacterial Computing)
- MATCH-IT (Matrix for Chemical IT)
- ECCELL (Electronic Chemical Cells)
- NEUNEU (this site)

Related Coordination Action

- COBRA

Related Projects

- ETICA (Ethical issues of emerging ICT Applications)

Local NEUNEU Sites

- NeuNeu at the University of Southampton

NEUNEU in the Press

2010:

- Heise
- Ticker Description of the Project (german)
- BBC News Article about the project
- Soton Project Announcement
- IEEE Computing Now
- TAZ article, newpaper (german)

2011:

- ERCIM News
- Lange Nacht der Wissenschaften Jena (german)

Funding

- FP7: FET Proactive Intiative: Bio-chemistry based Informatoin Technology(CHEM-IT)

FUNDING OPPORTUNITIES from the
FUTURE & EMERGING TECHNOLOGIES scheme

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