Welcome to

Emergence in Chemical Systems 4.0

June 22, 2015

Dear Colleagues,

On behalf of the local organizing committee and The Complex Systems Group at the University of Alaska Anchorage, I'd like to welcome you to Anchorage, Alaska and the Emergence in Chemical Systems 4.0 Conference (ECS 4.0) during June 22 – 27, 2015.

This international conference seeks to bring together theorists and experimentalists on topics related to Pattern Formation, Morphogenesis, Emergence, Hierarchies, Self-Construction of Complex Chemical Structures and Systems, Systems Chemistry, Growth Theory, Hydrodynamics and the Formation of Precipitation Structures, Chemical Networks, Chemical Gardens, Protocells and Origin of Life.

Your participation in this event is valuable. This conference will provide the opportunity for scientists and those from other research fields to exchange ideas, learn about what others are doing and meet and discuss mutual research interests.

Held on the campus of the University of Alaska, Anchorage (UAA), ECS 4.0 will provide you with a highly rewarding educational and networking experience for all plus introduce you to the scenic wilderness of Alaska.

Alaska is a place that you have to see at least one in your lifetime. It has 100,000 glaciers, 50 active volcanos (since 1760), more than 3,000,000 lakes, 30,000 grizzly, 100,000 black, and 4700 polar bears and more bald eagles than any other state combined. Our population of 710,231 allows us an unparalleled 1.3 people per square mile. I encourage you to take this opportunity to explore the many facets of Anchorage and to experience the unique Alaskan culture.

On behalf of the local organizing committee, I thank you for travelling from far and near to attend this event.

Jerzy Maselko

Dr. Jerzy Maselko
ECS 4.0 Conference Director

Emergence in Chemical Systems 4.0

Conference Information

Organization and Support

Local Organizing Committee

Dr. Jerzy Maselko, jmaselko2@uaa.alaska.edu

Dr. Jim Pantaleone, jtpantaleone@uaa.alaska.edu

Dr. Martin Cenek, mcenek@uaa.alaska.edu

Dr. Kenrick Mock, kjmock@uaa.alaska.edu

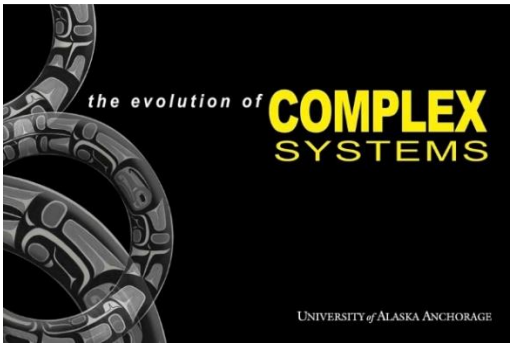
John Dede, jqdede@uaa.alaska.edu

Debora Summers, dmsummers@uaa.alaska.edu

Stephanie Ahern, srahern@uaa.alaska.edu

Tina Veldkamp, tmveldkamp@uaa.alaska.edu

With the Support of



Meeting Site

UAA UNIVERSITY of ALASKA ANCHORAGE

3211 Providence Drive
Anchorage, AK 99508

Meeting Registration

Gorsuch Commons Lobby (open 24hrs)
3700 Sharon Gagnon Ln
Anchorage, AK 99508

Monday:	2:00 pm – 8:00 pm
Tuesday:	7:00 am – 9:00 am

Fine Arts Building Lobby
3640 Alumni Drive
Anchorage, AK 99508

Wednesday:	8:30 am – 9:00 am
Thursday:	8:30 am – 9:00 am
Friday:	8:30 am – 9:00 am

Sessions

All sessions will be held in the Fine Arts Building, Rm. 150.

A guide will be at Gorsuch Commons Tuesday 8:30 am to lead you to the Fine Arts Building (lecture hall). If you need assistance or require transportation please let us know. Walking distance is about 0.75 km and will take about 10 minutes.

Schedule

The Conference Schedule can be found in your registration packet or online at http://www.cse.uaa.alaska.edu/chemicalemergence4/schedule.html.

UAA Map

A campus map is included in your registration packet or online at https://www.uaa.alaska.edu/map/.

Transportation

People Mover is the local Anchorage bus service (http://www.muni.org/departments/transit/peoplemover/Pages/default.aspx). Timetables, schedules, maps and a bus tracker are all available at this site.

Visiting Alaska

Alaska is an amazing state and we encourage you to take this opportunity to explore the wilderness, culture, and people. The Anchorage Convention and Visitors Bureau (http://www.anchorage.net) has a wealth of information available to visitors. Please review their Visitors Guide (enclosed with your registration material) or contact them to explore the many opportunities available to you. Between hiking, biking, fishing, cruises, flightseeing, wildlife viewing, shopping, museums, dining, and much more, there is an opportunity for everyone!

Meals

Meals (if not purchased during registration) may be purchased in the Gorsuch Commons cafeteria.

- Breakfast is 7:00 am - 8:45 am
- Dinner is 5:30 pm - 7:00 pm

Any special dietary needs may be directed to Bruce Bryan, General Manager, Food Service, Alaska Airlines Center, at 907-786-7883 (bruce.bryan@nmsusa.com) or Abigail Chaney, Catering Coordinator, at 907-751-7492 (Abigail.Chaney@nmsusa.com).

Lunch (included in the conference registration) will be in the Integrated Science Building (ISB) atrium.

A list of local dining establishments, many within walking distance, can be found in your registration packet.

We encourage you to join us for the **Midnight Sun Barbeque** (included in registration) Tuesday evening from 10:00 pm – 1:00 am at the Alaska Airlines Center -Varsity Sports Grill. We have over 20 hours of daylight this time of year! Come experience the midnight sun while viewing the mountains from the Varsity Sports Grill mezzanine. A guide will be at Gorsuch Commons Tuesday 9:45 pm to lead you to the Alaska Airlines Center.

The Conference **banquet** will be held Wednesday evening at the **Anchorage Museum** (https://www.anchoragemuseum.org/). If you have not already done so, reserve your tickets. The museum entrance fee and transportation is included in the cost. A bus will leave from the Gorsuch Commons at 6:00 pm.

Oral Presentations

All sessions will be held in the Fine Arts Building, Rm. 150.

Video projection of presentations/slides at Fine Arts 150 is operated through an integrated system that does not allow the connection of speakers' personal computers. Instead, you will be required to upload your presentation file(s) in the system by means of USB flash drive before your session. Technical assistance will be available for uploading, checking/converting your files. If you have any special technology requests during the conference, please contact Cedar Cussins (cdcussins@uaa.alaska.edu, 907-786-4890).

Presentations may be uploaded during Monday's registration or by the following deadlines. Morning speakers should see the computer operator in the lecture room (Fine Arts Bld. 150) no later than 8:30 am to download your presentation. Afternoon speakers please see the computer operator no later than 12:30 pm.

Accepted file formats

PPT, PPTX (Microsoft Powerpoint), PDF (Adobe Reader), files will be read on an MS-Windows platform. Any embedded or related media should be of standard image formats (JPG, BMP, GIF) and video (WVM) formats.

Macintosh users

Macintosh formats are not supported by the system. Your presentation file(s) must be fully compatible with MS-Windows environment, especially all included attached media files. Please check your presentation in a Windows environment. Please contact Cedar Cussins (cdcussins@uaa.alaska.edu, 907-786-4890) if you have any questions about the use of Macintosh systems during the conference.

Messages for Conference Participants

In case of emergencies during the conference family, friends, and colleagues may leave a message for conference participants at 907-351-1227. Debora Summers will ensure the message is relayed to the conference participant.

Hospitality Questions?

Student volunteers (local) will be available to answer questions during your stay in Anchorage. They will be available during registration, session breaks and lunch. Look for name tags that say "Ask me, I'm local!"

Smoke-free Policy

UAA has a comprehensive smoke-free policy. Therefore there is no smoking of any tobacco products in any of the UAA buildings and premises in the U-Med district.

Emergence in Chemical Systems 4.0

List of Participants/ Abstracts

Gonen Ashkenasy

Ben-Gurion University of the Negev, Israel

Emerging Oscillations and Bifurcation in Synthetic Replication Networks

Like many other open systems in nature, living organisms are replete with rhythmic and oscillatory behavior at all levels, to the extent that oscillations have been termed as a defining attribute of life. Additionally, living organisms contain internal circadian clocks that produce rhythms of a 24 hour cycle. Recently, we have started to investigate an important challenge in contemporary systems chemistry, that is, to synthetically construct "bottom-up" molecular networks that display such complex behavior. Towards this aim, we utilize catalytic replication networks, which have already served to study emergent phenomena in complex mixtures.1-2 In the first part of this talk, I will describe the kinetic behavior of small networks of coupled oscillators, producing various functions such as logic gates, integrators, counters, triggers and detectors. These networks are also utilized to simulate the connectivity and network topology observed for the Kai-proteins circadian clocks from the S. elongatus cyanobacteria, thus producing rhythms whose constant frequency is independent of the input intake rate and robust towards concentration fluctuations.3 Then, in the second part, I will disclose our experimental results, showing for the first time that the replication process can also lead to bistability in product equilibrium distribution. We believe that these recent studies may help further reveal the underlying principles of complex enzymatic processes in cells and may provide clues into the emergence of biological clocks.

1 Z. Dadon, N. Wagner, G. Ashkenasy, Angew. Chem. Int. Ed. 2008, 47, 6128-6136.
2 Z. Dadon, M. Samiappan, A. Shahar, R. Zarivach, G. Ashkenasy, Angew. Chem. Int. Ed. 2013, 52, 9944-9947.
3 N. Wagner, S. Alasibi, E. Peacock-Lopez and G. Ashkenasy, J. Phys. Chem. Lett. 2015, 6, 60.

R. Dean Astumian

The University of Maine, USA

Enhanced Diffusion, Chemotaxis, and Pumping by Active Enzymes: Progress toward an Organizing Principle of Molecular Machines

Active enzymes diffuse more rapidly than inactive enzyms. This phenomenon may be due to catalysis-driven conformational changes that result in "swimming" through the aqueous solution. Recent additional work has demonstrated that active enzymes can undergo chemotaxis toward regions of high substrateconcentration, whereas inactive enzymes do not, and, further, that active enzymes immobilized at surfaces can directionally pump liquids. I will discuss these phenomena in light of Purcell's work on directed motion at low Reynold's number and in the context of microscopic reversibility. The conclusions suggest that a deep understanding of catalytically driven enhanced diffusion of enzymes and related phenomena can lead toward a general organizing principle for the design, characterization, and operation of molecular machines.

Tamás Bánsági Jr.

University of Sheffield, UK

The urea-urease raction: dynamic behavior and applications

The rate-pH dependence of enzyme-catalysed reactions in membranes was proposed as a possible source of dynamical behaviour including bistability, oscillations and waves in biology; however, a robust experimental example of such a system is still lacking. Recent investigations with the urea-urease reaction suggest this reaction may provide such an example. In alginate beads the reaction has shown bistability in pH, and is of great potential

for materials applications: cure-on-demand frontal formation of hydrogel with heal-on-demand ability and quorum sensing driven film formation.

David Baum

University of Wisconsin, USA

Selection before the protocell

Many current models for the origin of life envisage the spontaneous origin of a simple protocell that could then undergo evolution by natural selection. These models have been motivated, at least in part, by the assumption that a bounded, replicating entity is the smallest unit capable of evolution by natural selection. However, modern multilevel selection theory removes boundaries as a prerequisite for adaptive evolution in cases where some factor other than a bounding membrane maintains long-term proximity of potential cooperators (such as members of autocatalytic metabolic networks). Under such a model, heterogeneous chemical mixtures adsorbed onto mineral surfaces have the potential to spontaneously form local autocatalytic sets that can then evolve adaptively. Assuming abundant free energy and replenishment of food resources, the resulting surface protoplasm would be expected to complexify over time based upon selection for an improve ability to displace inhibitory molecules from the surface and to more quickly colonize new exposed surfaces. This last factor can readily explain the origin of protocells. Surface protoplasm that released propagules would more readily colonize distant minerals surfaces. Furthermore, propagules that could grow and divide in the water column without a mineral surface would be able to colonize more effectively. Thus, if life-like chemical processes begin on mineral surfaces, we should expect selection for colonizing ability to eventually result in the emergence of growing and dividing protocells. This model invokes a greater role for selection than protocell first models, and also suggests a new class of experiment in which we impose selection for surface-colonizing ability and measure response to this selection as an indicator of life-like processes.

Mark Bedau

Reed College/Portland State, USA

Pragmatic pluralism about emergence

Discussions today of emergence in science and philosophy are often marked by “the emergence war”—the debate among competing views about the one true view of emergence. These emergence wars are often acrimonious and divisive, and ultimately unproductive. We should replace the emergence war with a pragmatic and pluralistic quest for all the kinds of emergence that actually help explain the some aspect of the real world. I illustrate and defend pragmatic pluralism by applying it to four important kinds of emergence: strong, weak, nominal, and door-opening emergence.

Yuagsheng Cao

Peking University, China

The free energy cost of accurate biochemical oscillations

Oscillation is an important cellular process that regulates timing of different vitallif e cycles. However, in the noisy cellular environment, oscillations can be highly inaccurate due to phase fluctuations. It remains poorly understood how biochemical circuits suppress phase fluctuations and what is the incurred thermodynamic cost. Here, we study four different types of biochemical oscillations representing three basic oscillation motifs shared by all known oscillatory systems. We find that the phase diffusion constant follows the same inverse dependence on the free energy dissipation per period for all systems studied. This relationship between the phase diffusion and energy dissipation is shown analytically in a model of noisy oscillation. Microscopically, we find that the oscillation is driven by multiple irreversible cycles that hydrolyze the fuel molecules such as ATP; the number of phase coherent

periods is proportional to the free energy consumed per period. Experimental evidence in support of this universal relationship and testable predictions are also presented.

Irene Chen

UC Santa Barbara, USA

Noise and evolution in the RNA World

Einstein famously claimed that 'God does not play dice with the universe.' However, chance can enter prebiotic RNA evolution in several ways. I describe our work on understanding the role of chance during the emergence and evolution of functional RNA and during the spread of genetic innovations.

Geoff Cooper

University of Glasgow, UK

Bridging the gap between polyoxometalate microtubes and classical chemical gardens

Chemical gardens are a great example of a self-organising nonequilibrium chemical system that creates complex structures. We have previously shown microtube growth and membrane formation from polyoxometallate (POM) crystals but these are inverted with respect to classical chemical gardens, in that POM fragments are anionic and tube growth involves their aggregation in a bulk solution containing cations. Now we have bridged the gap with classical chemical gardens and demonstrate microtube growth from a fully inorganic system where modified POM materials are used as both anion and cation.

René Doursat and Jonathan Pascalie

Complex Systems Institute, France

Morphogenetic Engineering in Synthetic Biology: Programming the emergence of collective shapes in simulated colonies of microorganisms.

Synthetic biology is a rising discipline promoting the standardized manufacturing of biological components without natural equivalents. Most works there are currently focused on the individual bacterium as a chemical reactor. Our project, SynBioTIC, addresses a more complex challenge: "shape engineering", which concerns the "redesign" of natural morphogenesis. Using realistic agent-based simulations of bacterial mats, we experiment with fundamental mechanisms able to generate collective behaviors typical of a cell assembly, such as homeostasis, self-repair, and development of complex structures. In this context, we propose a hybrid methodology, "staged evolutionary engineering of development" (SEED), in which human mediation is used as a tool for exploration and as a means of setting and refining evolutionary goals.

Tom Froese

Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México, Mexico

Motility at the origin of life and the evolution of the genome

Traditionally, there has been a dispute about whether metabolism or replication came first during the origin of life. Yet both of these approaches are in implicit agreement that the first forms of life were basically passive. That shared assumption has begun to be challenged by a new generation of metabolism-first approaches, emphasizing that movement and adaptive behavior could have played an important role right from the start (1-3). I introduce this theory of a behavior-based origin of life and consider how it can help to inform our thinking about the origins of the genetic system.

1. T. Froese, N. Virgo, T. Ikegami, Motility at the origin of life: Its characterization and a model. Artificial Life 20, 55-76 (2014).
2. M. M. Hanczyc, Metabolism and motility in prebiotic structures. Philosophical Transactions of the Royal Society B: Biological Sciences 366, 2885-2893 (2011).
3. M. D. Egbert, X. Barandiaran, E. A. Di Paolo, Behavioral metabolution: The adaptive and evolutionary potential of metabolism-based chemotaxis. Artificial Life 18, 1-25 (2012).

Jerzy Gorecki

Polish Academy of Science, Poland

Strategies of training for unconventional computing devices operating with a nonlinear chemical or biochemical medium

Emergence in a nonlinear system can be seen as an equivalent to a talent in a human population. It is gifted by Almighty to a few, but still the rest of people can contribute to civilization because their skills are enhanced by training. In my presentation I consider an equivalent approach applied to classifiers operating with a chemical information processing medium. I consider a network of lipid-covered droplets containing a solution of reagents of Bielousov-Zhabotinsky reaction. The droplets are immersed in an organic phase and they can exchange information coded in excitation pulses. The networks of droplets can be automatically generated in microfluidic reactors. I show how the information flow in a droplet medium can be tracked. The concept of mutual information between the classification problem and time evolution of the medium can be used to select the best strategy of medium training for a particular classification task. I demonstrate that the same medium can solve different problems with a high reliability, after a specific training is applied. The presented strategy of training, based on information theory, is generic and can be adopted to different physical, chemical or biological media that exhibit a complex time evolution.

Elizaveta Guseva

Stony Brook University, USA

Origins of biopolymers: mechanisms of sequence selection

How living systems arose prebiotically from random physico-chemical processes is a longstanding question. When did undirected chemical reactions begin to capitalize on fitness and undergo Darwinian evolution? Many origins-of-life studies are post-informational (postbiotic), i.e. focusing on processes that happen after there is already a molecular code and an ability to propagate "self". Here, in contrast, we are focusing on the transition from prebiotic to postbiotic. We are interested in how polymers with random sequences may lead to informational polymers with particular sequences, which then dominate the population. To study sequence-structure properties of informational copolymers we use HP lattice model -- a successful polymer-folding model of hydrophobic (H) and polar (P) monomers. Using sequences and structural information from the HP-model we have found conditions under which a set of certain sequences dominates the population with time. We use direct stochastic simulations of the dynamic models of the polymerization to figure out how sequence structure and aspects of the different dynamic models determine the structure and behavior of the emerged cooperative sets of the polymers. We find that some sequences become autocatalytic for accelerating the syntheses of others.

Helen Hansma

University of California at Santa Barbara, USA

Muscovite Mica, Mechanical Energy, Potassium, Crowding, and Life's Origins

Muscovite mica has many advantages as a site for life's origins [HHansma 2010 J Theor Biol & HHansma 2013 J Biol Struct Dynamics]. Mechanical energy from moving mica sheets appears to be feasible for organic syntheses, based on new research in mechanochemistry. Could this mechanical energy also facilitate electron transfers needed

for reductive molecular syntheses? Crowding was probably necessary at life's origins [HHansma OLEB 2014]. Results will be presented about the effect of potassium ions between Muscovite mica sheets on the polymerization of amino acids. Potassium ions hold Muscovite mica sheets together and are present in all living cells at high concentrations. Potassium ions are an order of magnitude better than sodium ions in the polymerization of an amino acid [Dubina, et al. 2013 OLEB]. Muscovite mica samples are now being investigated for their ability to facilitate Carbonyl-Di-Imidazole-induced peptide formation, by Prof. M Dubina and his research team at St. Petersburg Academic University of Russia.

Christine He

Georgia Tech, USA

Overcoming Strand Inhibition with Viscous Environments

Nucleic acid replication is a fundamental process in living systems, but understanding its prebiotic origins has been an elusive problem. While extant life utilizes complex molecular machinery to carry out nucleic acid replication in a step-wise fashion, a major challenge in the origins of life field is identifying a simpler, prebiotic replication mechanism. A significant bottleneck in demonstrating continuing rounds of replication is a phenomenon known as strand inhibition, where the favorability of forming a long duplex prevents separation of the single-strands for sufficient time to allow monomer/oligomer binding and ligation.
We propose addressing the problem of nucleic acid strand inhibition by employing highly viscous solvents to control the annealing rates of long templates and monomers/oligomers. In a viscous environment, DNA mobility is slowed in a length-dependent manner, so that long DNA strands (such as template and copy strands) are kinetically trapped; meanwhile, monomers or short oligomers can diffuse quickly and bind to their complementary targets on the templates. Template duplex formation is further slowed by the formation of intramolecular secondary structure on the template single strands.
Based on these thermodynamic and kinetic effects, we hypothesize that thermal cycling in a viscous environment can be used to drive sustained rounds of nucleic acid self-replication. In this work, we use DNA as a model informational polymer to demonstrate that a deep eutectic solvent can be used to copy a gene-length region (over 300 nucleotides) of a mixed sequence template.

Dezso Horváth

University of Szeged, Hungary

Diffusive fingering in a precipitation reaction driven by autocatalysis

The autocatalytic chlorite-tetrathionate reaction is investigated in a gelled medium containing barium ions, resulting in the formation of barium sulfate precipitate in the wake of the reaction front. When the reaction is run at temperatures around the sol-gel transition of the matrix, precipitate patterns resembling those of viscous fingering are observed. The main driving force behind the pattern formation is the selective binding of the autocatalyst that leads to diffusive instability, the presence of the precipitate reaction however modifies the long time behavior of the system.

Atsushi Kamimura

University of Tokyo, Japan

Reproduction of protocells: interplay of different timescale in a catalytic reaction network

Understanding how cellular components can be intergrated into a reproducing cell is essential to unveil the origin of life and to experimentally synthesize protocells. A catalytic reaction newtork provides a basic theoretical model in which different molecular species mutually catalyze the replication of each other. In this talk, I will show relevance of interplay of different timescale of reactions to reproduction, growth-division process and diversity of protocells.

Ramanarayanan Krishnamurthy

Scripps Research Institute, USA

Heterogeneity to Homogeneity: The Emergence of RNA

RNA is viewed as an emergent system where all components of RNA may have been decided at the level of a functioning oligomer/polymer. The critical interdependence of RNA's components – ribofuranose, phosphodiester backbone and purine-pyrimidine base-pairing – for the functioning of RNA seems to be evident, and manifests itself only at the level of the oligomer/polymer. The possibility of selections at the oligomer/polymer level, coupled with the reality of the prebiotic mixtures at the monomer level, leads to a scenario wherein the combinatorial interactions of diverse prebiotic (systems) chemistry leads first to heterogeneous ("pre-RNA") systems from which a homogeneous system (RNA), capable of further evolution, can emerge.

Christoph Kuhn

University Hospital Bern, Switzerland

Weigh the anchor and rock on the wave of lego and perfringo: How the offspring of the first replicating oligomer sustain the RNA-world and open the world of protein synthesis.

This paper presents a sequence of hypothetical processes that leads to an apparatus with the basic structure of the genetic apparatus of biosystems, but strongly simplified. The appearance of an entity in an environment that allows for Darwinian behavior is instantaneous and linked to the creation of matter, which carries information (i.e. weighing the anchor). This information takes meaning with that instant, the appearance of the first entity, which evolves by multiplication, variation, selection (i.e. rocking on the wave of lego and perfringo), and keeps that meaning during the entire evolution of the living - information carrying - state of matter. The semantics of this process is demonstrated by computer simulations. This leaves the challenging task of synthetizing such a replicating oligomer to the experimentalists.

Tom Lenaerts

Université Libre de Bruxelles, Belgium

The bits and bytes of protein domain communication

It has been shown that cells can be considered as behavioural automata that adapt through the interpretation of environmental signals, which are received at (membrane) receptors and relayed to the nucleus where they result in the adjustment of gene regulation. Signal transduction investigates how the cascades of proteins involved in cellular communication convert the initial signal until it reaches its final destination. Our work aims to understand how proteins within such pathways integrate, amplify and filter biological information with the ambition to capture the natural mechanisms of molecular computation. We have taken a bottom-up approach to achieve this goal: Starting from protein domains, i.e. reusable modular independently folding components that can be found in almost all proteins we have in our cells, we have used Shannon's information theory to identify the information that is exchanged between residues in protein domain as a direct result of their conformational coupling. Using different protein domain examples I will show how these predictions are made, that they correlate nicely with experimental results and that we can use it to understand how the activity of Src-like kinases may be regulated.

Charles Liotta

Georgia Tech, USA

The Mechanistic Origin of the 'pH Dichotomy' in the Reaction of Dihydroxyfumarate with Glyoxylate

In the search for chemistries relevant to the origins of life, glyoxylate and its formal dimer dihydroxyfumarate (DHF) have been proposed as potentially important prebiotic building blocks. It has been demonstrated that, in the presence of cyanide ion and at pH13, glyoxylate undergoes a dimerization reaction to form DHF which subsequently reacts with an additional glyoxyate to cleanly produce meso- and d,l-tartrate, and oxalate. This result is in sharp contrast to the reaction of DHF and glyoxylate at pH8 where the products of reaction are dihydroxyacetone (DHA), pentulosonic acid and carbonate. In order to gain a mechanistic understanding of this pH dichotomy, the kinetics associated with the reactions at pH8 and pH13 were measured at several temperatures along with the theoretical calculations (AM1 and DFT) of the activation energies associated with each of the pertinent steps in the proposed reaction pathways. The results of these investigations will be discussed.

Jerzy Maselko

University of Alaska Anchorage, USA

The First Life

In presented chemical systems the self-organizing processes, structures and systems will be presented. In our experiments with continuously pumped chemicals, we move the chemical systems father and father from thermodynamic equilibrium, forcing them to continuously construct more and more complex structures and organizations that have the following properties:

1. Spontaneously formation of chemical cells with a semi-permeable membrane through which chemicals can diffuse in, react with chemicals inside the cell, form structures that can perform tasks, and later the products diffuse out.
2. Formation of different complex chemical structures that are formed by controllable networks of chemical and physical processes.
3. Chemical cells that form multicellular structures that behave as a whole.
4. Spontaneous formation of hierarchical chemical structures with 8 levels of complexity.
5. Cells that can perform different types of movement.

Agnieszka Mensfelt

Poznan University of Technology, Poland

Evolution of morphologies - modeling Foraminifera in Framsticks

This presentation will demonstrate how morphologies can be modeled, simulated and evolved in the Framsticks environment. We will present a simple mathematical model of Foraminifera embryogeny that is based on principal morphological characteristics of these organisms. The concept of the genotype-phenotype mapping will be introduced, and similarity measures will be used to reveal the relationships between a simple Foraminiferal genetic space and a more complex morphological space. As a summary, an evolutionary experiment will be presented in computer simulation.

Jim Pantaleone

University of Alaska Anchorage, USA

Growing a chemical garden at the surface

When moving fluids undergo chemical or physical changes to become solid, they can produce beautiful and intricate structures. Notable natural examples include speleothems, lava tubes, and limestone terraces. In chemistry labs, a popular experiment involves reacting metal salt solutions with silicate solutions. The resulting precipitation structures are biomimetic in appearance and behavior; hence, they are often dubbed "chemical gardens." Their possible technological applications, and the potential role of chemical gardens in the origins of terrestrial life, have revitalized research on this system. The presented experiments explore a novel, quasi-two-dimensional experimental configuration that allows the metal salt solution to spread over the surface of the silicate solution. The observed structures are complex, composed of spiraling channels, transverse periodicity, and branching – all occurring sequentially in one structure. These structures are primarily shaped by buoyancy and interfacial forces. The magnitude of the interfacial tension between the solutions and the precipitation membrane is estimated from initial investigations.

Punit Parmananda

Indian Institute of Technology, India

Collective dynamics of chemo-mechanical oscillators

The dynamics of a chemo-mechanical Mercury Beating Heart (MBH) system is analyzed experimentally. It is observed that different shapes of the mercury drop could be obtained. The redox potential timeseries for this MBH system, corresponding to these different shapes were also recorded. Subsequently, two such oscillators were coupled and the resultant synchronization phenomena studied. Finally, the collective dynamics for an ensemble of MBH oscillators were investigated.

Robert Pascal

Université de Montpellier, France

The Conditions for Self-Organization in Chemical Systems

Thermodynamic stability is not sufficient to understand the development of life through the evolutionary process, which, on the contrary, requires considering another kind of stability of kinetic rather than thermodynamic nature. This approach allows the identification of the conditions needed for dynamic kinetic stability to drive the evolution of chemical systems. One of them was defined as the cost of kinetic irreversibility, which must be covered in order that the system can be driven by this kind of stability and evolve toward an increase in complexity (or organization).

Sandra Pizzarello and M. Bose

Arizona State University, USA

The cosmic trail of reduced Nitrogen towards Earth

We will report on the finding that 15N-enrichments of hotspots in several meteoritic IOMs are reduced by hydrothermal conditions and that the extent of those reductions correlates with the 15N values of the ammonia released by the treatment. Because the presence of reduced nitrogen on the early Earth is a required element in origins of life theories, the data aid significantly towards understanding the prebiotic molecular inventory of our nascent planet as well as inform estimates of the possible habitability of other planetary systems.

Andrew Pohorille

NASA, USA

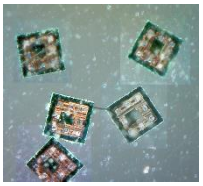
Emergence of Protein Function

Although great strides have been made towards understanding protein evolution, a meaningful extrapolation from contemporary proteins to their earliest ancestors is virtually impossible. In an alternative approach, a number of fundamental questions about the origins of proteins have been probed through a combination of in vitro evolution and computer simulations. Can functional proteins emerge from random sequences of amino acids? How did the initial repertoire of proteins diversify to facilitate new functions? Could other collections of proteins start different evolutionary pathways? Were the structures of ancestral proteins similar to those of modern ones? Although we do not have definitive answers to these questions, important clues have been uncovered. These clues will be discussed in the examples of two distinct classes of proteins – water-soluble enzymes and transmembrane ion channels.

Steen Rasmussen

University of Southern Denmark, Denmark

Novel chemical protocells generated and controlled by solvated electronic microchips



Silicon microchips of size 100μm x 100μm with active electronic sensing and actuation reacting in a chemical environment are shown to form collective macroscopic patterns. Such chips may be fabricated in standard 180nm silicon technology and equipped with custom developed super-capacitors allowing them to react autonomously in fluids. Figure to the right shows micrograph picture of such microchips. The microchips are designed to catalyze reactions with inbuilt electrodes and utilize electro-osmotic flow to propel along in the fluidic system. The chips can also interact with the chemical environment through sensors and actuators controlled by an onboard finite state-machine [1]. We demonstrate that swarms of such chips can generate new types of dynamically stable physical structures, which can move, grow, divide and fuse, controlled by their onboard finite state-machine. These swarm structures define new types of chemical rectors without walls as well as novel hybrid electronic-chemical protocells.

Figure above shows successive divisions of protocellular structures composed of 400 swarming microchips at simulation times 1,000, 24,000 and 58,300.

References [1] J. McCaskill, G. v. Kiedrowski, J. Oehm, P. Mayr, L. Cronin, I. Willner, A. Herrmann, S. Rasmussen, F. Stepanek, N. Packard & P. Wills, Microscale Chemically Reactive Electronic Agents, IJUC 8, 289 (2012).

Kepa Ruiz Mirazo

University of the Basque Country, Spain

Noise and evolution in the RNA World

Artificial compartments and lipid vesicles have been used as model systems to understand the origins and requirements for early cells, as well as to design encapsulated reactors for biotechnology. One prominent feature of vesicles is the semi-permeable nature of their membranes, able to support passive diffusion of individual solute

species into/out of the compartment, in addition to an osmotic water flow in the opposite direction to the net solute concentration gradient. Crucially, this water flow affects the internal aqueous volume of the vesicle in response to osmotic imbalances, in particular those created by ongoing reactions within the system. In this theoretical study, we pay attention to this often overlooked aspect and show, via the use of a simple semi-spatial vesicle reactor model, that a changing solvent volume introduces interesting non-linearities into an encapsulated chemistry. Focusing on bistability, we demonstrate how a changing volume compartment can degenerate existing bistable reactions, but also promote emergent bistability from very simple reactions, which are not bistable in bulk conditions. One particularly remarkable effect is that two or more chemically-independent reactions, with mutually exclusive reaction kinetics, are able to couple their dynamics through the variation of solvent volume inside the vesicle. Our results suggest that other chemical innovations should be expected when more realistic and active properties of compartments are taken into account.

Ricard Solé

ICREA-Complex Systems Lab UPF-IBE, Spain

Terraforming ecosystems with synthetic biological designs

Our planet is experiencing an accelerated process of change associated to a variety of anthropogenic phenomena. The future of this transformation is uncertain, but there is general agreement about its negative unfolding that might threaten our own survival. Furthermore, the pace of the expected changes is likely to be abrupt: catastrophic shifts might be the most likely outcome of this ongoing, apparently slow process. Although different strategies for geo-engineering the planet have been advanced, none seem likely to safely revert the large-scale problems associated to carbon dioxide accumulation or ecosystem degradation. An alternative possibility considered here is inspired in the rapidly growing potential for engineering living systems. It would involve designing synthetic organisms capable of reproducing and expanding to large geographic scales with the goal of achieving a long-term or a transient restoration of ecosystem-level homeostasis. Such a regional or even planetary-scale engineering would have to deal with the complexity of our biosphere. It will require not only a proper design of organisms but also understanding their place within ecological networks and their evolvability. This is a likely future scenario that will require integration of ideas coming from currently weakly connected domains, including synthetic biology, ecological and genome engineering, evolutionary theory, climate science, biogeography and invasion ecology, among others.

Peter Strazewski

Université Claude Bernard Lyon 1, France

How to feed an inanimate evolvable chemical system, supplied with synthetic macromolecules of predictable proper-ties, so as to let it self-evolve into increased complexity and life-like behavior

We are beginning to explore a fully synthetic chemical micro-compartmented and evolvable macromolecular system being ‘fed’ with ‘monomers’ and small-molecular-weight-high-energy compounds, to keep the system permanently out of thermodynamic equilibrium, and thus let it self-evolve into increasingly higher complexity. The initial compounds are giant vesicles composed of different lipidic amphiphiles, synthetic nucleic acids (predominantly synthetic RNA and DNA), synthetic peptides (predominantly made up from added amino acids) and synthetic carbohydrates (often chemically linked to lipids or peptides). While being furnished with more lipid amphiphiles, those giant vesicles that bear the most useful evolved features are expected to gain in population size through serial grow-and-divide self-selection cycles.

Andrew Surman

University of Glasgow, UK

Automated fluidic platforms for prebiotic evolution

Since Stanley Miller's famous experiment, many of the steps towards 'bottom up' creation of living systems have been demonstrated in isolation. To make further substantial advances, rather than demonstrate potential, it is becoming clear that we must link these processes in more complex systems. To achieve this, we face challenges in terms of efficiency (yield) and complexity (analysis, combinatorial explosion). To overcome these, we must automate both synthesis and analysis, exploring otherwise intractably huge parameter spaces and product data. Here I present an overview of our group's efforts in this direction, and some of our first results.

Kazuhito Tabata

The University of Tokyo, Japan

Hybrid Cell - Single Cell Bacterium Fused Microdevice

One major goal of synthetic biology is the design of an artificial cell. Prokaryotes make the easiest model, because they have a simple structure that contains only a cell wall, cell membrane and cytosol. However, these components are not enough, as mixing them into a liposome does not result in a cell regeneration. One reason is because the buffer we use to disrupt the cell and acquire its cytosolic content significantly decreases the concentration one or two magnitudes. A second reason is the function of the bilayer membrane used to enclose this content is insufficient. To overcome these problems, we have developed a lipid bilayer covered femto-Liter chamber. To test our system, we introduced GFP-labeled E. coli protoplasts were introduced into the chamber, Fusion between the chamber and bacteria protoplast resulted in increased fluorescence and caused the cytoplasmic components of the bacteria to disperse throughout the chamber, and the membrane components bonded with the lipid bilayer, as described above. In other words, a hybrid cell was achieved. GFP fluorescent intensity of an each hybrid cell was changed with time. The average slope of the fluorescence intensity from the hybrid cells was slightly negative, a result likely due to protein degradation. However, if 5 mM ATP was added to the chamber in advance, the average slope was slightly positive. This result was attributed to protein synthesis caused by the ATP. We are currently conducting viability assessments of the hybrid system. We will present this reactor in detail and its application to 0the hybrid cell.

Ágota Tóth

University of Szeged, Hungary

Morphology control by flow-driven precipitation

We show that flow-driven precipitation can result in the selective production of a crystalline structure for calcium carbonate. The experimental results reveal that the local mixing, maintained by the concentration and density gradients, favours the nucleation and growth of high-purity calcite microcrystals identified with Raman microscopy. Under appropriate chemical composition, tubular membrane-like structures develop in the copper-phosphate system. Scanning electron microscopy of the solid structures reveals that microflowers and nanorods appear in the inner wall of the tubes on increasing flow.

Renate Wackerbauer and Jacopo Lafranceschina

University of Alaska Fairbanks, USA

Chaotic transients in a network of Morris-Lecar neurons

Spatiotemporal chaos collapses to either a rest state or a propagating pulse solution in a ring network of diffusively coupled, excitable Morris-Lecar neurons. The addition of weak excitatory synapses can increase the Lyapunov exponent, expedite the collapse, and promote the collapse to the rest state rather than the pulse state. A pulse solution may no longer be asymptotic for certain network topologies and (weak) synapses.

Stephan Weiss

University of Michigan, USA

Coupled Belousov-Zhabotinsky reactors

Using numerical and experimental tools, we study the coupling of two spatially extended Belousov-Zhabotinsky (BZ) reactors. We find various kinds of synchronisations as a function of the coupling strength, the chemical concentrations, and the initial spiral patterns. While for large coupling strength the patterns in both reactors become identical, for small coupling strength the initially steady spiral cores become mobile and follow synchronised trajectories For example, when a single spiral exists in each of the reactors, then the spiral cores follow circular trajectories if both spirals have the same sense of rotation and straight parallel trajectories if both spirals have opposite senses of rotation.

Lidia Yamamota

Memorial University of Newfoundland, Canada

Emergence in Artificial Chemistries

Artificial Chemistries (ACs) are man-made virtual or physical systems where objects are transformed in interactions, like molecules in chemical reactions. The field of Artificial Chemistries started as spin-off of Artificial Life, motivated by a desire to pinpoint and understand the emergent phenomena driving the transition from nonliving to living matter, and to create new forms of synthetic life from the bottom up, in vitro or in silico. The applications of ACs range from chemistry and biology to nuclear physics, economics, and computing.

This talk will give an overview of emergent phenomena in ACs, and will demonstrate some using a new software package called PyCellChemistry, written in Python. The package will be released this summer to allow everyone interested in Artificial Chemistries to program their own ACs.

Victor V. Yashin

University of Pittsburgh, USA

Achieving synchronization with active hybrid materials: Coupling self-oscillating gels and piezoelectric films

Our goal is to develop materials that compute by using non-linear oscillating chemical reactions to perform spatio-temporal recognition tasks. The material of choice is a polymer gel undergoing the oscillatory Belousov-Zhabotinsky reaction. The novelty of our approach is in employing hybrid gel-piezoelectric micro-electro-mechanical systems (MEMS) to couple local chemo-mechanical oscillations over long distances by electrical connection. Our modeling revealed that (1) interaction between the MEMS units is sufficiently strong for synchronization; (2) the mode of synchronization depends on the number of units, type of circuit connection (serial of parallel), and polarity of the units; (3) each mode has a distinctive pattern in phase of oscillations and generated

voltage. The results indicate feasibility of using the hybrid gel-piezoelectric MEMS for oscillator based unconventional computing.

Sheng-sheng Yu

Georgia Tech, USA

Ester-Mediated Amide Bond Formation and the Prebiotic Origin of Peptides

The results of the Miller-Urey experiments and meteorite investigations have demonstrated that amino acids, the building blocks of peptides, might have existed in the prebiotic world. However, a prebiotically plausible process for the polymerization of amino acids is still unclear. The polycondensation of amino acids is unfavorable in aqueous solution and high temperature is necessary. Here, we found a simple system composed of α-hydroxy acids and amino acids is capable of forming peptide bonds under a relatively mild condition. Hydroxy acids form metastable oligoesters in the oscillating (hot dry/cool wet) system and transit into mixed esteramide oligomers via the ester-amide exchange reaction. By using ion mobility-mass spectrometry and ion mobility-tandem mass spectrometry, we observe the enrichment of amino acids in the oligomers, and the formation of a peptide backbone during the repeated dryingrehydration cycles. The presence of peptide bonds is further confirmed by infrared spectroscopy and two-dimensional nuclear magnetic resonance analysis. Quantitative nuclear magnetic resonance analysis suggests a 40% yield of peptide bonds can be achieved. A kinetic model was developed to validate the proposed mechanism and to predict the system behavior under new conditions. These results demonstrate a simple system exhibiting key features for the emergence of peptides.

Nicolle Zellner

Albion College, USA

Rethinking Solar System Bombardment: New Views on the Timing and Delivery of Lunar Impactors

As our closest planetary neighbor, the Moon provides the most clear and complete history of impact events in the inner Solar System since its formation ~4.5 billion years (Ga) ago. With samples from the Apollo missions and recent orbital data, the Moon continues to provide scientific answers to questions about its impact flux; however, the timing of this flux is not well understood.
Recent interpretations of lunar orbital data and improved sample analyses have called into question the long-standing view of the lunar cataclysm, the supposed "spike" in impacts ~3.9 Ga. In this talk, I will present new views on this impact flux, resulting from evidence in both orbital and sample data. I will also describe how the Moon's impact record, if properly interpreted, can be used to gain insights into how the Earth has been influenced by impacting events over billions of years.