Developmental robotics in a chemistry lab

Curious robotic assistants as tools for the exploration of complex physicochemical systems in the real world

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***Abstract* — The study of complex systems in the real world (e.g. reaction-diffusion systems, self-propelled droplets) is mostly guided by phenomenological observations made by curious scientists. But should we wait until luck, time or serendipity produce such phenomena before our eyes? Or can we actively design tools whose aim is to discover interesting phenomenon for us to later analyze? We believe principles from developmental robotics can help when designing curious robotic assistants for lab environments. Such robots would be able to perform physical or chemical experiments with the aim to explore the states a complex system can exhibit, a challenge alike sensory-motor exploration in humans and robots. In this tutorial, we will introduce this innovative application field and showcase examples from robotic assistants at work in our chemistry lab and how they help us characterize our chemical systems more effectively. Our aim is to highlight the potential benefits of interdisciplinary work at the interface of physics, chemistry, robotics and AI.**

***Index Terms* — sensory-motor exploration, curiosity-driven learning, complex chemical systems, real world exploration**

I. Target Audience

The tutorial will be of special interest for researchers interested in sensory-motor exploration and its application outside of robotics and developmental sciences. We will review the problems of the exploration of forward and inverse models in robotics as well as algorithmic principles such as goal-babbling and curiosity-driven learning. We will then showcase examples from robotic assistants at work in our chemistry lab and how they help us characterize our chemical systems more effectively – illustrating the potentially fertile alignment between DevRob principles and the exploration of real world systems encountered in physics and chemistry labs. Overall this tutorial should be of interest to any researchers curious about possible applications and implications of their research outside the usual fields covered by the ICDL-EPIROB conference.

II. Concept

Complex physicochemical systems represent a burgeoning area for chemical research [1]. For example, a few groups from across the fields of chemistry and physics are investigating the chemical and physical driving forces behind the behaviors exhibited by oil-in-water droplets such as movement, chemotaxis, division and fusion [2]. To study and model such systems accurately, one must be able to discover and reproduce interesting phenomena – a difficult challenge due to the non-linear relationship between the chemical composition and the behaviors of such systems. For example, in oil-in-water droplet systems most of the possible experiments will lead to stationary droplets while, in other parts of the chemical space, small changes in composition or temperature can drastically affect the observed behaviors [3].

But how do we come to find those interesting regions of the chemical space without any prior knowledge of the system? Specifically, for droplets, how can we efficiently get to know the range of possible behaviors (speed, division, vibration) that can be achieved as a function of the droplets' chemical composition? This problem should be familiar to researchers interested in sensory-motor exploration in robots and humans. Finding what behaviors a droplet system can exhibit is much alike to finding what positions the end effector of a robotic arm can reach with respect to the positions of its joints. Or learning to explore what our own body can do according to the electrical impulses sent to our muscles.

The field of developmental robotics has explored various mechanisms for self-exploration by taking inspiration from the learning processes occurring in humans [4]. Algorithmic principles have been derived around the concept of motor or goal babbling [5] as well as intrinsic motivation such as curiosity driven exploration [6]. These methods have been shown to structure the exploration of an unknown system and enables the collection of more rewarding and useful observations of the system. In this tutorial, we will present evidence from our lab that such algorithmic tools are beneficial for the exploration of physical and chemical systems.

More specifically, we will make the case that physicochemical systems encompass most issues and challenges studied in the field of developmental robotics, yet in a real-world setup simple enough to be sampled and analyzed using automated platforms and online algorithms – making the full complexity of the real-world accessible to algorithmically driven search. In such systems there is redundancy and there are non-reachable areas, whilst the mapping between input and output is often non-linear. Simultaneously, their complex dynamics are often too hard to model accurately or not computationally tractable in decent time [7]. This is due to the different time and space scales at work: molecular scale interactions; chemical transformations, phase transitions (evaporation, dissolution) and fluid mechanics considerations. The only choice is to explore the system in the real world which comes with a substantial time and financial cost – a topic directly aligned with sensory-motor exploration in a life-time from a limited number of trials.

We propose the following schedule for a half day tutorial (3.5 hours):

Time	Topics	Speaker
14.00 – 14.10	Presentation of tutorial schedule, speakers and the Cronin Group	J. Grizou
14.10 – 14.25	Connecting the digital world to the chemical world. Why? How? What challenges? Relevance to the field of DevRob.	J. Grizou
14.25 – 14.45	Oil-in-water droplets. What are they? How do they behave? Why are they interesting?	L. Points
14.45 – 15.05	Introduction to goal oriented learning: from motor to goal babbling and curiosity-driven learning	J. Grizou
15.05 – 15.30	Robotically assisted exploration of oil-in-water droplets	J. Grizou
15.30 – 16.00	Coffee Break: live demonstration of oil-in-water droplets and discussion around posters	L. Points
16.00 – 16.25	Using data from robotic assistants to better understand chemical systems: theory and examples	L. Points
16.25 – 17.00	Beyond oil-in-water droplets, more examples from the lab	J. Grizou
17.00 – 17.25	Open discussion. Other fields of applications? What limitations, challenges & opportunities? How would you take part in this?	L. Points
17.25 – 17-30	Concluding remarks and take home messages	J. Grizou

As a first step towards smart robotic assistants for labs, we recently demonstrated the robotically assisted optimization of oil-in-water droplet systems [3]. We developed an automated platform able to control droplet composition and volume and record their motion. Subsequently, computer vision analysis - able to extract behavioral metrics from droplets' videos - and a genetic algorithm – able to make autonomous decisions about which experiments to perform next, were used to explore this system. We have since expanded in many directions and explored (1) how the chemical and physical environment biases the systems behaviors - using the environment as an experimental variable, (2) how humans compare with active learning algorithms in probing the crystallization envelop of some compounds, and (3) how goal babbling and curiosity-driven learning algorithms enable the quick characterization of what can be done with our droplet systems.

We believe this tutorial is relevant to the ICDL-EPIROB community, not only as it showcases an innovative application of the field, but more fundamentally because the exploration of real world problems encountered in chemistry are aligned with the foundation of the DevRob field itself. The potential of this interdisciplinary research expands beyond the simple application of well-established methods across fields. Convergent challenges emerge: how can we efficiently explore a chemical system whose properties are unknown in advance? How can robots and algorithms discover and be curious? Could chemical systems become useful problems for testing new algorithms?

III. Speakers

Jonathan Grizou obtained a PhD in the Flowers lab under the supervision of Manuel Lopes and Pierre-Yves Oudeyer, for which he received the 'Prix Le Monde de La Recherche 2015'. He then joined the Cronin Group to apply DevRob principles to real world systems. He is leading the Chemobot team composed of 8 scientists (PostDocs and PhDs) dedicated to the development of curious robotic assistants as tools to explore physicochemical systems.

Laurie Points obtained his MChem in Chemistry from the University of York, including a year in industry at Infineum, for which he was awarded the Salters' Graduate Award 2014. Now in the 3rd year of his PhD studies, Laurie works within the Chemobot team utilising smart robotic assistants to investigate oil-in-water droplets, both developing the chemistry used and analysing the underlying physicochemical driving forces behind droplet behaviour.

References

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