

ICMS SYMPOSIUM GETTING A GRIP ON COMPLEX SYSTEMS

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Abstracts

Tom de Greef (TU/e)

Programmable DNA-based Communication in Populations of Synthetic Cells

The development of highly orthogonal molecular communication channels is a crucial step towards engineering artificial cell-scale systems. Here, we present a general and scalable platform entitled 'Biomolecular Implementation of Protocellular Communication' (BIO-PC) to engineer multichannel molecular communication networks between populations of non-lipid microcapsules. Our method leverages the modularity and scalability of enzyme-free DNA strand-displacement circuits to develop protocellular consortia that can sense, process and respond to DNA-based messages. We engineer a rich variety of biochemical communication devices capable of cascaded amplification, bidirectional communication, sender-receiver functions and distributed computational operations. Encapsulation of DNA strand-displacement circuits allows their use in concentrated serum where non-compartmentalized DNA circuits cannot operate. BIO-PC enables reliable execution of distributed DNA-based molecular programs in biologically relevant environments and opens new directions in DNA computing and minimal cell technology.

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Molecular Charge Transport Networks: the good, the bad, and the ugly of multiscale modelling

Electronic transport processes determine the functionality of materials in many electronic devices. From a modeling perspective, the quantum nature of the electrons requires, in principle, considering solutions to the time-dependent Schrödinger Equation with both many electrons and many nuclei – a futile effort at realistic time- and length scales for real-world materials.

For many molecular materials, their inherent disorder provides some way out of this conundrum by allowing to coarse-grain the coupled, continuous electron-nuclear dynamics to sequences of tunneling processes between a few localized states. Such states and the rates for tunneling in between them define a molecular charge transport network or graph.

Explicit multiscale models aim at determining the details of this graph, and with that the resulting transport processes on it, from first-principles, e.g., quantum-mechanical, models at very small scales in a bottom-up fashion that ideally preserves predictiveness. This ambition faces several challenges, if not obstacles. In this talk, I will introduce in more detail the idea behind the coarse-graining (the good), discuss how many choices and therefore uncertainties there are to build the network from first-principles models (the bad), and try to address what such models can *actually* be useful for (the ugly?).

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Matin Jafarian (TU Delft)

Cluster synchronization as the central mechanism of free recall in working memory networks

We study free recall, i.e., the reactivation of stored memory items, namely patterns, in any order, of a model of working memory. Our free recall model is based on a biologically plausible modular neural network composed of H modules, namely hypercolumns, each of which is a bundle of M minicolumns. The coupling weights and constant bias values of the network are determined by a Hebbian plasticity rule. Using techniques from nonlinear stability theory, we show that cluster synchronization is the central mechanism governing free recall of orthogonally encoded patterns. We discuss the role of heterogeneous coupling weights and bias values of minicolumns' dynamics in free recall. Our analysis shows that having non-identical couplings and bias values for different patterns increases the possibility of their free recall.

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