ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

SS 2007-2008, No. KUMAR-SWIS-MP12	Start:	19.02.2008
	Finish:	25.08.2008

Title of the project

Hybrid Reaction Modeling of the Extended Self-Assembly Problem

Author **Loïc Matthey**

Project description

We propose a new modeling framework inspired by chemical reaction processes. Our approach consists in defining the processes and the interactions within the system in term of reactions. Such a definition can be applied to many systems, ranging from biochemical systems to swarm robotics. In particular, we aim at exploiting the toolbox developed in the context of hybrid system modeling and simulation.

The concept of extended self-assembly is the following: given a set of passive building blocks A, B, C, and D, how to obtain, with a maximal yield, the products X, Y, and Z using a set of N active transporters? What is the smallest set of reactions leading to these products? More importantly, how shall we design the building blocks and their transporters in order to fit this set of reactions? The reaction set may also involve intermediate products and be influenced by external factors. We draw inspiration from the DNA translation, and more specifically the tRNA transport molecules, which bring protein building blocks to the ribosomes. Our research may have impact on the understanding of such biological processes occuring at the nanoscale.

We envision a modeling framework that is sufficiently general to accommodate with the extended self-assembly problem, as well as the classical self-assembly problem. The validation of our models will be achieved using realistic simulation (Webots), or numerical simulations (Matlab) of various robotics systems. First, we will implement a simple example of assembly using robots as active transporters.

Tasks

- Do a literature review of actual reaction rate modeling and hybrid system simulations.
- Formalize the augmented self-assembly problem.
- Propose a modeling framework for the augmented self-assembly problem.
- Solve the smallest reaction set problem and the transporter behavior problem.
- Choose a test case study and model it using the framework.
- Simulate the test case using Matlab and/or Webots.
- Compare the results of the model and the simulation.
- Depending on the results, modify and propose improvements to better fit the data. Iterate on the last steps.

Oral presentations	The date and time of the intermediate and final presentations will be specified mutually by the student, supervisor, and professor. Presentations and accompanying slides must be in English and in MS Powerpoint format. Rehearsal presentations with the project supervisor before the official talk are strongly encouraged.
Final report	All of the student's work shall be submitted on a CD (report, presentation, source code, documentation, media, etc.) as well as a hard copy of the report (English, double-sided, unbound). One copy will be required for the SWIS library (delivered to Corinne Farquharson, administrative assistant of SWIS, BC232), and additional copies may be requested by the project supervisor for his/her records. The final report must use the standard cover page and include a copy of this extended proposal just after the cover page. The report must be submitted in PDF format, and the source files (Latex recommended, MS Word accepted) should be contained in the CD-ROM, as well as the final presentation. A complete draft of the report must be submitted to the responsible supervisor at least *two weeks* before the final deadline. Revisions and comments will be returned in a timely fashion and will need to be incorporated into the final version of the report.
Web visibility	The student's name will be listed on the SWIS web site (under people/undergraduate) and hyperlinked to an appropriate home page if possible (either personal, or a brief page on people.epfl.ch). At the end of the project, with the help of the supervisor, a 1-page summary, a definitive project abstract, and one picture of the project will be posted (see http://swis.epfl.ch/teaching/student_projects/ for examples). It should be finalized and approved by the supervisor. Additional movies and pictures can be posted according to SWIS guidelines and after supervisor approval. This page will remain on the SWIS site under the section "past student projects" and the student's name will be moved to the "alumni" section. The project will not be considered concluded until the dedicated web page is available on-line.
Supervision	Spring Berman (UPenn), Vijay Kumar (UPenn), Grégory Mermoud
Place of work	University of Pennsylvania, USA
Recommended literature	DT Gillespie. Stochastic simulation of chemical kinetics. Annual Review of Physical Chemistry, 58:35–55, 2007 Eric Klavins. Programmable self-assembly. IEEE Control Systems Mag., 27:43–56, 2007 GM Whitesides and B Grzybowski. Self-assembly at all scales. Science, 295(5564):2418–2421, 2002
Signature of the Professor	
	Prof. Alcherio Martinoli, Swarm-Intelligent Systems Group