TRAN-F-501 INTERNSHIP MIDTERM REPORT

This document should be filled by the student, signed by the student and the host company responsible and returned to the CS Internship Coordinator (Pr. M. Jansen) before the 7th week from the beginning of the internship.

STUDENT'S COORDINATES

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ACADEMIC SUPERVISOR'S COORDINATES

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HOST COMPANY'S COORDINATES

Company name	VUB Artificial Intelligence Lab
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Supervisor	Nowé Ann
Role in the company	Director
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DESCRIPTION OF THE ACTIVITIES DONE IN THE FIRST 6 WEEKS

TITLE OF THE INTERNSHIP:

Creating a computational model for studying aggregation dynamics

DESCRIPTION OF THE INTERNSHIP, OBJECTIVES AND THE PEDAGOGICAL CONTENT (Half page). An explicit statement should be made about the nature of the objectives with respect to the initial ones mentioned in the INTERNSHIP DESCRIPTION Document.

The goal of this internship is to develop a stochastic simulation system for protein aggregation, allowing for easy parameterization and experimentation and to provide scripts for visualization and analysis of the results produced by the simulation. And to study and understand the kinetics behind the amyloid fibril formation and self-assembly phenomenon. Diseases like Alzheimer and Parkinson disease are the result of proteins aggregating into large fractal structures that hinder the cell function or even destroy them. Understanding how aggregates are formed and change over time is important to understand when they become harmful and how maybe treatments affect aggregate formation.

This work is performed in collaboration with the Switch lab in the KU Leuven, who have an extensive expertise in studying aggregation and related diseases. Baseline knowledge will be obtained from them as well as recent literature (e.g. Meisl, G., Kirkegaard, J. B., Arosio, P., Michaels, T. C., Vendruscolo, M., Dobson, C. M., ... & Knowles, T. P. (2016). Molecular mechanisms of protein aggregation from global fitting of kinetic models. Nature protocols, 11(2), 252.).

The goal is to make a minimal system that sufficiently mimics what is known from experiments, finding thus ways to fit the known fluorescence's data. The difficulty here is to find the actual kinetic rates from that fit. It should provide a steppingstone for further research and project applications in that context.

The internship student will be trained in developing this type of software and to think and report about this medically relevant problem. She will also have the opportunity to interact and learn from other members in IB2.

DESCRIPTION OF THE TASKS OR FUNCTIONS ASSIGNED TO THE STUDENT DURING THE FIRST 6 WEEKS (1 page)

Develop a stochastic simulation system for protein aggregation
Allow for easy parameterization and experimentation
Provide scripts for visualization and analysis of the results produced by the simulation.
Look for ways to identify the kinetic rates
Provide models that can explain the observed experimental kinetics

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Demonstrate the results to the collaborating team in Leuven.

DETAILED ACTIVITIES CALENDARS OF THE FIRST 6 WEEKS
(set of items of the form DD/MM/YY: Activity name. What? Where?)

12/08/19 : First day of the internship, Meeting with the supervisor, briefing about the project goals.

13/08/19 : Meeting with the team mates, office set and paper work for office access, getting to know the routines

14/08/19 → 23/08/19 : State of the art

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26/08/19 → 31/08/19 : Doing a more refined research and focusing on specific papers focusing on the problem

02/09/19 → 06/09/19 : Implementation of a simple prototype of an exact numerical simulation method to simulate trajectories of discrete stochastic systems. (Gillespie's Direct Method)

09/09/19 → 20/09/19 : Implementation of Gillespie's Next reaction method in order to be able to consider larger systems

10/09/19 : Skype call with Collaborators of the KU leuven → Re-calibrate the goal. In addition to the simulations models, to understand the kinetics behind amyloid formation especially the lag phase.

13/09/19 → 27/09/19 : In parallel with the Gillespie's Next reaction method simulation, I started doing a state of the art around the ThT kinetics and created methods to plot the different data sent by th collaborators in order to have a better visual.

PLANNING OF THE ACTIVITIES OF THE NEXT 6 WEEKS (1 page)

30/09/19 → 04/10/19 : Research on the lag phase in the amyloid fibril formation and understanding the self assembly phenomenon.

07/10/19 → 11/10/19 : Pose hypothesis and possible solutions to speed up the lag phase and understand the influence of rate constants.

14/10/19 → 25/10/19 : Implementation of the solutions found to speed up the lag phase.

28/10/19 → 31/10/19 : Optimization of all the codes produced during the internship and provide documentation on the codes and use.

REMARKS (if any)

DATE : 25/09/19

Signature of the student

supervisor

Signature of the host company