

L'équipe projet Inria Beagle propose un stage de M2.

### Scientific objective

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The research topics of the Beagle Team are centered on the modelisation and simulation of cellular processes. More specifically, we focus on two specific processes that govern cell dynamics and behavior: Evolution and Biophysics. This leads to two main topics: computational cell biology and models for genome evolution.

Beagle contributes computational models and simulations to the study of cell signaling in prokaryotic and eukaryotic cells, with a special focus on the dynamics of cell signaling both in time and in space. Importantly, our objective here is not so much to produce innovative computer methodologies, but rather to improve our knowledge of the field of cell biology by means of computer methodologies.

A population of organisms adapting to a new environment is a dynamic system changing over time at many levels (molecules, networks, individuals, ecosystems). A large amount of empirical and theoretical evidence indicates that in real populations all these levels interact, making the dynamics of adaptation a highly complex phenomenon. In order to understand bacterial evolution, we need large-scale integrative models in which all relevant levels from the molecule to the ecology are simulated.

The Aevol/R-Aevol simulator

(<http://www.aevol.fr>) has been developed by the Beagle team to address such questions. Aevol integrates the molecular and cellular levels to address the evolution of genomic complexity. R-Aevol adds the network level to investigate the evolution of network complexity.

We use multiple modeling methods to study these topics. One of methods is ordinary differential equations (ODE). We have recurrent issues with classical ODE solvers in term of precision and performance.

### Challenging issues

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We are using library for solving ODE but also custom codes. For both, we never have strongly evaluate their precision and their performance. Furthermore, we use default parameter and classical solving methods (explicit euler and runge kutta 45) because they simply work not because it is the best for our case. We need to investigate the available solving methods but also time stepping approach (adaptive or not). To the best of our knowledge, no such work has been done for ODE solver and especially applied to computational biology.

Due to increasingly larger ODE systems but also the increase of their numbers, performance are now critical. Nevertheless, there is no parallel solver that can leverage modern parallel architecture (many-core, GPU, etc.) and thus efficient parallel algorithms need to be proposed. But efficient use of computing resources is only a part toward better performance, finding the best parameters for the solver (and the resolution methods) is critical for having the best performance while keeping good precision. As these parameters (for solving methods and parallelization algorithms) are specific for each problem, using the same one for every problem is counter productive. Nevertheless, it is too much time consuming to find the good parameters' value by hand. Accordingly, we would need an auto-tuning method (deep learning, reinforcement learning, heuristic, ...) to configure ODE solver.

### Internship subject

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The first goal of this internship is to study the state of the art of ODE solver library (and the different solving methods they implement) for the specific problem that interest the Beagle team. By doing so, an in-depth evaluation of both precision and performance of these solvers would be done. Depending of the results of this first goal, the next step would be to propose :

- to adapt state of the art solving methods that are currently missing
- a novel ODE solver library for computational biology
- new parallel algorithms for solving ODE for modern computing resources
- auto-tuning methods for the configuration of ODE solvers

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