Motion Planning with constraints for Nanoscale Simulation

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Place and team: Minatec Campus, Grenoble, France. NANO-D research group at INRIA (http://nano-d.inrialpes.fr)

About the NANO-D research group at INRIA

During the twentieth century, the development of macroscopic engineering has been largely stimulated by progress in numerical design and prototyping: cars, planes, boats, and many other manufactured objects are nowadays designed and tested on computers. Digital prototypes have progressively replaced actual ones, and effective computer-aided engineering tools have helped cut costs and reduce production cycles of these macroscopic systems.

The twenty-first century is most likely to see a similar development at the atomic scale. Indeed, the recent years have seen tremendous progress in nanotechnology - in particular in the ability to control matter at the atomic scale. Similar to what has happened with macroscopic engineering, powerful and generic computational tools will be employed to engineer complex nanosystems, through modeling and simulation.

The NANO-D group, led by Stephane Redon at INRIA, develops novel multiscale, adaptive modeling and simulation methods, which automatically focus computational resources on the most relevant parts of the nanosystems under study. All algorithms developed by the group are gathered into SAMSON, an open-architecture software platform designed by NANO-D (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems).

Objectives

Nowadays, it remains challenging to reproduce accurately with existing simulation tools the phenomena taking place at atomic-scale. One approach to characterize the change that may occur between known states is to provide the minimum-energy path (MEP) [1] which describes the rearrangements and relative positions of the atoms involved in this change from their initial position to their final position. Recently, we have proposed a new approach [2] based on sampling-based motion planning techniques [3] to search the MEP associated to a given change of conformation.

The goal of the internship will be to enhance the motion planning based simulation methods developed in the team in order to allow the specification of given constraints. These constraints will have various possible forms. They will concern either the goal state to be reached, regions of the space to be avoided or criterions regarding the conformations generated along the simulation.

The stage will involve in particular: 1) the formalization of the set of constraints to be allowed, 2) the incorporation of these constraints within the existing algorithmic framework used to perform simulations at nanoscale, 3) the design of a new SAMSON module with an interface allowing a user-friendly specification of the constraints.

[1] D. Sheppard et al, Journal of Chemical Physics, 128:13, 2008.
[2] L. Jaillet, et al., *Sampling-based Path Planning on Configuration-Space Costmaps*. IEEE Trans. of Robotics, Vol 26, 2010.
[3] S.M. LaValle, Planning Algorithms, Part II: Motion Planning, Cambridge University Press, 2006.

Duration

4-8 months, continuation for PhD is possible.

Requirements

- **Strong** computer science and mathematics background (knowledge in motion planning is a plus)
- **Strong** oral, written and interpersonal communication skills (working language: English – knowing French is a plus)
- Good knowledge of C++
- Ability to work independently and with a team