Deciphering time in nanoscale confinements

Developing an analysis tool to calculate residence time in nanoscale confinements.

"Each time was a new time"

Ernest Hemingway?, of course yes. A timeless quote to frame a central problem: how much time does a body spend in a given space. For macroscopic bodies, the more massive the body, the slower it moves. But what happens when the body is just a tiny ion or a single water molecule? Surface effects, thermal fluctuations, and the discrete nature of matter start to dominate at the nanometer scale, producing residence times that cannot be predicted by macroscopic approaches. The goal of this project is to implement a computational tool to calculate the residence time of atoms and molecules within nano-scale confinements. This tool will be used to quantify the residence time of molecules in nanochannels, such as synthetic nanopores and carbon nanotubes.

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PREREQUISITES
Familiarity with Python/TclTk
Interest in learning molecular dynamics software (LAMMPS/NAMD)
Ability to work independently

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In the CSE Lab we combine computational methods, computer science tools and domain specific knowledge to solve scientific and engineering problems in areas such as Fluid Mechanics, Nanotechnology and Life Sciences. The core computational competences of our group are in particle methods and in stochastic optimization techniques. Motivated by challenges in application fields, we focus on identifying the common elements among computational techniques and on formulating common methodological, algorithmic and software structures that facilitate their further development.