Séminaire LIONS

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Adaptive algorithms for modeling and simulating nanosystems

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This talk will present our current work on designing a unified theoretical framework for Adaptive Molecular Dynamics (AMD). Unlike previous "a priori" simplification approaches, adaptive molecular dynamics can predict the set of active degrees of freedom at each time step, based on the current state of the molecular system (atom positions and velocities), the internal forces (van der Waals, electrostatic, dihedral), the applied external forces (e.g., the force applied by the user through a haptic device), and the precision threshold specified by the user (i.e. maximum number of active joints, or total acceleration threshold). This allows the user to efficiently model complex molecular systems on cheap laptop or desktop computers.

We will introduce some underlying algorithms and present interactive demonstrations of SAMSON (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems), our molecular modeler, on biological and chemical examples. In particular, we will show how the adaptive framework may be used to model flexibility and determine the electronic structure of complex chains and molecular systems, carbon nanotubes, etc.