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S E M I N A I R E

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« Integrative Approaches for Current Problems in Structural Biology »

Although the fundamental forces between atoms and molecules are almost fully understood at a theoretical level, and computer simulations have become an integral part of research activities, the application of these methods to large biomolecules still faces important practical difficulties due to the combinatorial explosion of possible interactions involved. Developing efficient structure prediction algorithms thus remains a major scientific challenge in computational biology.
I will give a brief overview of computational methods for structure prediction developed in our team at Inria Grenoble. In particular, I will demonstrate how machine/deep learning can be used in current problems of computational structural biology. Also, I will present SAXS and SANS-assisted flexible fitting of structures into experimental profiles, large-scale deformation of molecular structures using nonlinear normal modes, FFT-accelerated techniques for docking and fitting, and symmetry-assisted modelling methods.

Jeudi 31 janvier 2019
14h00

Salle de conférence