

12th Seminar on Modeling

1 April 2014



MAISON DE LA SIMULATION

Electronic Structure Calculation based on Daubechies Wavelets: BigDFT

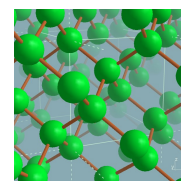


Thierry Deutsch

Head of the atomistic simulation laboratory at CEA-Grenoble

In this talk we will describe in detail a Density Functional Theory method based on a Daubechies wavelets basis set, named BigDFT. We will see that, thanks to wavelet properties, this code shows high systematic convergence properties, very good performances and an excellent efficiency for parallel calculations.

BigDFT code operation are also well-suited for GPU acceleration. We will discuss how the problematic of fruitfully benefit of this new technology can be match with the needs of robustness and flexibility of a complex code like BigDFT.



Interactive Molecular Graphics: seeing and touching molecules in motion

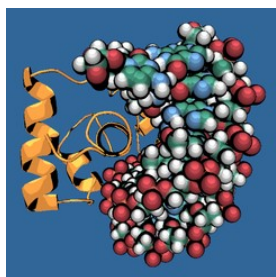
Mars Baaden

Research director at Laboratoire de Biochimie Théorique (CNRS)

Computational biology greatly benefits from approaches such as molecular dynamics simulations to study complex molecular assemblies. In this context, interactive visualization, manipulation and analysis aids hypothesis generation and exploration of large datasets. Integration of experimental data (SAXS, CryoEM, ..) in this modeling process is challenging. I will illustrate these issues through a) work on a complete dystrophin filament

model [1] using our BioSpring simulation engine and b) interactive simulations and analysis of membrane proteins [2].

To tackle the corresponding visualization challenges, my group recently developed the UnityMol framework [3], based on the Unity3D game engine. A particular focus lies on interactive exploration and manipulation using tools such as haptic devices or very recently the LeapMotion controller. Possible display platforms are mobile devices, desktop workstations, display walls and virtual reality setups (CAVE, workbench,..).



Tuesday, April 1st 9:30 AM (coffee offered, talks at 10 AM)
Maison de la Simulation, Digiteo building (565), room 33

Contact: sophie.felix@cea.fr - ☎: 01 69 08 59 67

Mailing list: <https://groupes.renater.fr/sympa/info/mdls-seminar>

<http://www.maisondelasimulation.fr/seminar/>

