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ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

SEMINAR OF APPLIED MATHEMATICS

MONDAY 09 March 2015 at 09h00, lecture hall BI A0 448 (CIB)

Prof. ***Benjamin STAMM*** *(UPMC-Paris VI - CNRS)*
will present a seminar entitled:

"Numerical methods in electronic structure calculation"

Abstract:

After a general introduction to electronic structure calculation which has become an essential tool in computational chemistry, condensed matter physics, molecular biology, materials science, and nanosciences, we will illustrate in two examples on how mathematicians can intervene and will present some recent progress made in the numerical analysis of such models. The first example focusses on Density Functional Theory Kohn-Sham models, which is to date one of the most widely used approaches in electronic structure calculation, and present some post-processing in order to increase the accuracy of plane-wave approximations. This technique is based on arguments of the perturbation-method where we interpret the exact solution as a perturbation of the numerical solution of the problem which allows to obtain better convergence rates with very little computational overhead.

The second part deals with multi-scale models where different models with different accuracies are coupled in view of simulating larger systems of chemical and biological interest. In particular, continuum solvation models take solvent effects into account, possibly in the framework of a QM/MM/Continuum coupling-strategy. In the past, such continuum solvation models have been the computational bottleneck for applications to large molecules. A new efficient algorithm (ddCOSMO) of linear computational complexity and memory storage with respect to the number of atoms which outperforms the state-of-the-art method developed by York and Karplus by two orders of magnitude and that will soon be distributed in major codes in computational chemistry is presented. We discuss the mathematical aspects of ddCOSMO and illustrate how this new method opens the door to many interesting couplings. Numerical tests underline the theoretical developments in both cases.

Lausanne, March 4, 2015 / mg