ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

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SEMINAR OF NUMERICAL ANALYSIS

- **WEDNESDAY 10 FEBRUARY 2016 - ROOM MA A3 31 - 16h15**

Prof. Michele CERIOTTI (Laboratory of Computational Science and Modelling, EPFL) will present a seminar entitled:

"From atomic environments to meso-scale structures. Mapping complexity in materials"

Abstract:

Atomistic computer simulations give access to increasingly accurate and predictive modelling of materials, chemical and biochemical compounds. As more complex systems become amenable to computation, the sheer amount of data produced by a simulation, as well as its intrinsic structural complexity, make it harder to extract physical insight from modelling. Here I will discuss two different approaches to use a computer to assist in the analysis of a simulation: using machine-learning techniques to recognize recurring structural patterns in a material, and non-linear dimensionality reduction methods to automatically coarse-grain a high-dimensional description of structural landscapes. These techniques simplify and streamline the analysis of atomistic simulations, and provide effective structural descriptors that can be used to accelerate the exploration of free-energy landscapes, making phenomena that happen on longer time scales accessible to simulation. I will also briefly discuss how to build a robust, effective metric to compare molecules and condensed-phase structures, and how this can be used to represent large databases of compounds, and to machine-learn their physical-chemical properties.

Lausanne, 4 February 2016/DK/cr
