ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

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SEMINAR OF NUMERICAL ANALYSIS

- **WEDNESDAY 11 DECEMBER 2013 - 16 h 15, ROOM GR A3 30**

Dr. Virginie ERLACHER *(CERMICS, Paris, France)* will present a seminar entitled:

"Greedy algorithms for electronic structure calculations in quantum chemistry"

Abstract:

Abstract: In this talk, a greedy algorithm will be presented in order to compute the lowest eigenvalue and an associated eigenstate for high-dimensional problems, and their numerical behaviour will be illustrated for the computation of the ground-state electronic wavefunction of a molecule, solution of the many-body Schrödinger equation. Usually, these algorithms are implemented in practice using the Alternating Least-Square algorithm, which leads to some computational difficulties in this particular situation due to the antisymmetry of the ground state wavefunction. A computational strategy to overcome this difficulty will be presented and illustrated on several molecules.
(Joint work with Eric Cancès, Tony Lelièvre, Majdi Hochlaf)

Lausanne, 6 November 2013/DK/cr
