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Seminario prof. K. RUUD

Wednesday May 9, at 14.45 c/o Room A1, III floor
Department of Chemical Sciencies Ed. C11 - via Giorgieri 1, Trieste

Prof. Kenneth Ruud, Department of Chemistry,
University of Tromsoe, Norway

Title: A New Future for Finite-Element methods? Multiresolution Analysis in Chemistry.

Abstract: In the talk, I will present multiwavelet functions as a new set of basis functions in quantum chemical calculations. The multiwavelets have several important mathematical properties that in principle can be beneficial in quantum chemical calculations in comparison to conventional basis functions such as Gaussian basis functions and plane waves. In particular, the use of wavelet functions allows for strict error control in the calculated energies (and properties). In the so-call non-standard representation of functions and operators, the operators can be shown to be sparse, banded matrices, making the approach inherently linearly scaling. A key element in the potential success of the approach is the ability to perform a strict separation of 3-dimensional operators into products of 1-dimensional operators of known accuracy, and this will be demonstrated. The propects for use of the formalism in chemical applications will be outlined.

La Direzione