

Prof. Daniel Kressner

Mathematics Institute of Computational Science and Engineering - MATHICSE

SEMINAR OF NUMERICAL ANALYSIS

➤ **WEDNESDAY 9 NOVEMBER 2011 - ROOM ME B331 - 16.15 pm**

Prof. Paola Boito, (Univeristy of Lille, France) will present a seminar intitled:

"Decay bounds for matrix functions and an application to electronic structure computation"

Abstract:

Functions of banded or otherwise sparse matrices often exhibit properties of off-diagonal decay. Using tools from matrix analysis and polynomial approximation, we study this decay behavior under rather general hypotheses and give a priori asymptotic bounds that do not depend on matrix size.

A motivation for this work comes from computational quantum chemistry and solid state physics. Localization occurs for certain choices of basis functions in many physical systems, thus giving a Hamiltonian that is banded or sparse. The associated density matrix can then be obtained via linear scaling methods, since its elements are expected to exhibit fast off-diagonal decay which allows for a banded approximation. Our goal is to give a rigorous mathematical proof of the validity of this approximation.

Applications of bounds for matrix functions are not limited to computational physics. The talk will present examples of how our approach can be used to estimate matrix functions that describe the connectivity properties of networks.

This is joint work with Michele Benzi and Nader Razouk.

Lausanne, 1st November 2011/AQ/DK/cr