Elias Polak
Elias.Polak@unige.ch
Department of Mathematics and Department of Physical Chemistry
University of Geneva
Switzerland

12th Workshop on Analysis and Advanced Numerical Methods
for Partial Differential Equations (**AANMPDE**),
July 1st-5th, 2019 in Strobl, Austria.

Geneva, July 3, 2019.

Title: A Generalized *Aufbau principle* for Linear Partial Differential Operators

Abstract:
In the early 1920s' Niels Bohr formulated the so–called *Aufbau principle*[1] (German: "building up") as a principle for the characterization of the electron configuration of chemical elements based on quantum mechanical knowledge and on experimental radiation results. This model gave a reasonable physical description of the ground state of an atomic system by ordering the stationary states upwards in the energy level. Soon linear partial differential operators provided eigenfunctions with eigenvalues corresponding to those stationary states at specific energy levels. Now the *Aufbau principle* suggests one should use the eigenstates, that minimize a lower dimensional eigenvalue problem in order to achieve the best approximation to the exact ground state, i.e. the minimum of the expectation value of the operator describing the quantum system. We are going to interpret this idea in a far more general way for linear (unbounded) operators acting on subdomains of Hilbert spaces. We will also explain theoretical difficulties in applications to real chemical problems, where electronic structure theory is working with computation models.[2] However numerical methods for partial differential equations of high dimensional order can profit from this approach as we will see in some computational examples.

[1] N. Bohr, *Über den Bau der Atome*, talk at the nobel prize ceremony in Stockholm 1922, transl. by W. Pauli jr.

[2] A. Szabo and N.S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, Dover Publications, 2015.