Tuesday, April 12, 2022

9h45 – 10h45
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Zoom link: https://epfl.zoom.us/j/67402994561

Error estimation for electronic structure calculations in materials

Mathematical models used to compute electronic structures of materials often involve nonlinear eigenvalue problems. These problems being computationally very costly, several approximations are in use when computing numerical solutions. These approximation include the chosen model, the discretization basis, iterative algorithms stopped after a finite number of iterations. The ability to control the errors linked to these approximations is key to guarantee the accuracy of the computed solutions, as well as to optimise the parameters of the simulations to achieve good compromise between accuracy and computational cost.

In this presentation I will first give an overview of the different approximations used to simulate materials systems in practice. I will then present ways to obtain accuracy guarantees on the solutions of these problems, together with perspectives offered by such error bounds towards efficient simulations and guaranteed codes for materials simulations.