Multi-scale Quantum Transport Simulations in thousands of cores

The field of nanotechnology continues blossoming with the improvement of nanofabrications and atomic scale manipulation. The capability of producing on-demand material properties is now a reality, which came after years of a combined theoretical and experimental effort to understand the quantum nature of matter. However, in the industry and experiments, it is difficult to fabricate devices within the ideal conditions propose theoretically, the effect of structural disorder, interface quality, and contamination is its a general unknown that can completely change the expected material properties. We used linear scaling quantum transport methods that allow simulating systems containing millions of orbitals, which will enable us to simulate some systems with realistic micrometer size including all quantum effects within the non-interacting approximation. Our approach has been tested in different massively parallelized environments, such as the MareNostrum4 supercomputer, showing a linear scaling behavior with the number of cores up to 1000 cores. Using these resources, we performed state-of-the-art calculations of the transport properties of graphene-based heterostructures, and we determined that they could be potentially useful for low power electronics, and high-speed non-volatile memories. Our results aimed in the first clear observation of the spin Hall effect in graphene/transition metal dichalcogenide heterostructures, and is currently being used to estimate the potential of this heterostructure for spin-orbit torque memories, a candidate to replace standard RAMs. In this talk, I'll briefly introduce our methods and explain how are we able to fully exploit massive parallel environments, also showing why this is of extreme relevance for achieving quantitative predictability that can be related to experimental measurements.