COMPUTING COLLOQUIUM

INQ: Reinventing the Electronic-Structure Code

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Electronic-structure codes are a fundamental tool for the computational study of matter in the ground and the excited states. They are complex pieces of software that need to be accurate, reliable, and implement a wide array of functionalities and features. On top of that, they need to be computationally efficient and take advantage of modern high-performance computing (HPC) platforms.

In this talk I will present and discuss the development of INQ: a new software package for the simulation of electrons in matter. I will present how on INQ's development we have used new ideas to the problem of making scientific software. These new approaches have allowed us to make a code that is very compact, simple to develop and maintain, computationally efficient, and easy to use for researchers.

INQ was designed from the scratch to run in parallel on multiple GPUs. In TDDFT simulations on GPU-based supercomputers INQ achieves excellent performance. It can handle hundreds and thousands of atoms and scale to thousands of GPUs. The code is open source and it is freely accessible at http://gitlab.com/npneq/inq

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Xavier Andrade is a research scientist with the Quantum Simulation Group at Lawrence Livermore National Laboratory, California. He obtained a Ph.D. in physics from the University of the Basque Country, Spain, and worked as a postdoc at the Department of Chemistry at Harvard University.

He is a world-class expert in the computational simulation of electrons in matter. His research is focused on developing new theoretical models and algorithms for the computational simulation of electrons in materials, as well as how to implement these algorithms in massively parallel computing architectures, in particular graphics processing units (GPUs). He is also interested in the usability aspect of scientific computing, by researching how to make simulation software that is easy to learn and use for scientists.

He has developed computer codes used by institutions and researchers around the globe to simulate materials at the atomic scale. He is currently the lead developer of INQ, a DOE-funded software package for the simulation of electrons under non-equilibrium conditions.

In his free time Xavier enjoys the outdoors and volunteering to build new trails in regional parks to make nature more accessible for everybody. He also plays electric and upright bass in a rock band.

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In-person

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