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MaX training on SIESTA, an innovative tool for HPC applications in materials science

The SIESTA School, organised by the Centre of Excellence (CoE) MaX, took place from 23 May to 26 May at the Barcelona Supercomputing Center (BSC) in Barcelona. The training aimed to teach both the theory and practical usage of the density functional theory (DFT) code SIESTA.

Stephan Mohr, organiser of the SIESTA School, comments: “The SIESTA School was organised to offer a detailed, dedicated training for researchers interested in using this code for their work. The morning session offered a range of lectures explaining the theory behind SIESTA, given by SIESTA developers. During the afternoon session, participants were able to put this knowledge into practice by actually running the code and interpreting the results, again supervised by a team of experienced SIESTA users and developers. Participation levels were good and, in light of the positive feedback we received, we are planning to repeat this event in the future.”

BSC’s development work on SIESTA, as part of the European CoE project MaX, focuses on further enhancing the performance of this code. Within MaX, SIESTA is used to **perform simulations in the field of materials science**, with the goal of designing new materials with specific properties. However, SIESTA is also widely used outside of materials science, as illustrated by the various fields represented by participants at the SIESTA School.

Rubén Cañadas, internship student at the Protein Modelling group lead by Victor Guallar at BSC, explains

why he attended the course and how he will apply what he has learnt: “In our group we work on protein modelling. Since proteins are complex molecules formed by thousands of atoms, modelling is usually separated between the active core, which is calculated by quantum mechanics, and the rest of the protein, modelled by classical mechanics. The emerging capabilities of codes such as SIESTA make it possible to model entire proteins. Another important feature of the code is that it is open source, which is really useful because usually each lab works with a particular (and often commercial) piece of software and when you move from one lab to another you have to convert your work and spend a huge amount of time learning and adapting yourself to the new software.”

About SIESTA

SIESTA is a code to perform efficient electronic structure calculations and *ab initio* molecular dynamics simulations of molecules and solids. SIESTA's efficiency stems from the use of strictly localised basis sets and from the implementation of linear-scaling algorithms, which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave and all-electron methods.

SIESTA is open source and is gaining more and more popularity. Apart from its most obvious applications in the field of materials physics and chemistry, it is increasingly used by researchers in geosciences, biology, and engineering. Currently there are several thousand users all over the world.

About MaX CoE

MaX is a user-focused, problem-oriented European Centre of Excellence (H2020 e-infrastructure) which aims to foster EU leadership in materials modelling, simulations, discovery and design. It works at the frontiers of current and future High Performance Computing (HPC) technologies, in order to enable the best use and evolution of HPC for materials research and innovation. MaX is creating an ecosystem of capabilities, ambitious applications, data workflows and analysis, and user-oriented services. The MaX strategy is focused at enabling the exascale transition in the domain of materials science, by developing advanced programming models, novel algorithms, domain-specific libraries, in-memory data management, software/hardware co-design and technology-transfer actions.

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