Efficient materials modelling on HPC with Quantum ESPRESSO, Siesta and Yambo

In recent years, computing technologies underlying materials modelling and electronic structure calculation have evolved rapidly. High-performance computing (HPC) is transitioning from petascale to exascale, while individual compute nodes are increasingly based on heterogeneous architectures that every year become more diversified due to different vendor choices. In this environment, electronic structure codes also have to evolve fast in order to adapt to new hardware facilities. Nowadays, state-of-the-art electronic structure codes based on modern density functional theory (DFT) methods allow treating realistic molecular systems with a very high accuracy. However, due to the increased complexity of the codes, some extra skills are required from users in order to fully exploit their potential.

This training material gives a broad overview of important fundamental concepts for molecular and materials modelling on HPC, with a focus on three of the most modern codes for electronic structure calculations (QUANTUM ESPRESSO, SIESTA and Yambo). Theory sections are interleaved with practical demonstrations and hands-on exercises.

QUANTUM ESPRESSO is one of the most popular suites of computer codes for electronic-structure calculations and materials modelling at the nanoscale, based on density-functional theory, plane waves, and pseudopotentials. It is able to predict and give fundamental insights about many properties of materials, molecular systems, micro and nanodevices, biological systems, in many fields, providing a huge amount of data for data-driven science applications.

SIESTA is a pseudopotential-based DFT software whose strength lies in its use of atomic-like strictly-localised basis sets: the use of a “good first approximation” to the full problem decreases the number of basis functions needed to achieve a given accuracy, and the finite support of the orbitals leads to sparsity in the Hamiltonian and overlap matrices, thus enabling the use of reduced-scaling methods. The functionalities of SIESTA include, amongst others, the calculation of energies and forces, molecular-dynamics simulations, band structures, densities of states, spin-orbit couplings, van der Waals functionals, hybrid functionals, DFT+U for correlated systems, real-time TDDFT, and density-functional perturbation theory.

YAMBO is an open-source code implementing first-principles methods based on Green's function (GF) theory to describe excited-state properties of realistic materials. These methods include the GW approximation, the Bethe Salpeter equation, nonequilibrium GF (NEGF) and TDDFT, allowing for the prediction of accurate quasiparticle energies (e.g. ARPES band structures), linear and non-linear optical properties, capturing the physics of excitons, plasmons, and magnons. It is also possible to calculate temperature-dependent electronic and optical properties via electron-phonon coupling and nonequilibrium and non-linear optical properties via NEGF real-time simulations (pump-probe experiments, etc).

MAX (MAterials design at the eXascale) is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current and future High-Performance Computing (HPC), High Throughput Computing (HTC) and data analytics technologies. MaX's challenge lies in bringing the most successful and widely used open-source, community codes in quantum simulations of materials towards exascale and extreme scaling performance and make them available for a large and growing base of researchers in the materials' domain.

⚙ Prerequisites

- Some familiarity with density functional theory (DFT), self-consistent field (SCF) calculations and plane wave basis sets is desirable as the workshop will not cover the fundamental theory of these topics.
- Familiarity with working in a Linux environment and some experience with working on an HPC system is needed to participate in the hands-on exercises.

Who is the course for?

This workshop is aimed towards researchers and engineers who already have some previous experience with materials modelling and electronic structure calculations.

Quick Reference

Instructor's guide

Why we teach this lesson

Intended learning outcomes

Timing

Preparing exercises

e.g. what to do the day before to set up common repositories.

Other practical aspects

Interesting questions you might get

Typical pitfalls

About the course

In this workshop, participants will learn how to launch the most common types of calculations (e.g. scf, phonons, quasi-particle energies, time-dependent properties) using QE, Yambo and BigDFT, how to prepare input files and how to read output files in order to extract the desired properties.

Best practices for efficient exploitation of HPC resources will be discussed, with particular emphasis on how to use the different schemes of data distribution (e.g. plane waves, pools, images) in combination with the different parallelization and acceleration schemes (MPI, OpenMP, GPU-offload) available in QE.

Schedule for 4 half-day workshop

Day 1, QUANTUM ESPRESSO

Time	Section
09:00-09:15	Welcome and introduction to ENCCS
09:15-09:30	Introduction to Max-CoE and MaX flagship codes
09:30-10:00	Overview of the QE suite of codes and main features
10:00-10:25	Coffee break
10:25-13:00	PWSCF for HPC and GPU

Day 2, QUANTUM ESPRESSO

Time	Section
09:00-09:45	Introduction to Density Functional Perturbation Theory
09:45-10:15	Introduction to Time Dependent Density Functional Perturbation Theory
10:15-10:30	Coffee break
10:30-13:00	Phonons and time dependent properties on HPC and GPU

Day 3, Yambo

Time	Section
09:00-09:20	Overview of the Yambo code and its main features and performance

Time	Section
09:00-10:00	Introduction to the GW approximation
10:00-10:20	Coffee break
10:20-13:00	Hands-on tutorial: A guided tour through GW simulations

Day 4, BigDFT

Time	Section
09:00-09:30	Introduction to BigDFT
09:30-10:00	Introduction to PyBigDFT: System Manipulation
10:00-10:30	Remote Runner (Presentation & Walkthrough/Hands-on)
10:30 - 11:00 | Coffee break	
11:00 - 12:00 | Cubic Scaling BigDFT (Hands-on)	
12:00 - 13:00 | Linear Scaling BigDFT (Hands-on)	

See also

- ENCCS: https://enccs.se/
- MAX-CoE: http://www.max-centre.eu/
- Follow ENCCS on LinkedIn, or Twitter
- Follow MAX-CoE on LinkedIn, or Twitter.

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Credits

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Instructional Material

Software