Using HPC in the description of molecular spectra

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Plan of a tutorial with hands-on sessions.

Prerequisites: Access to applications and computing resources needed for attendees: PRACE Tier-1 at WCSS;
Number of attendees: 15;
Time and schedule: Preferred one day tutorial (8h), possible: two days (2x4h) or four days (4x2h);

1) Why use supercomputers in chemistry, or how supercomputers will yield a golden age of chemistry?

Chemists or materials scientist think of new ideas based on intuition and experience; synthesizing and testing those ideas involve a tremendous amount of errors, time and money. It can take months to evaluate a single new material, and most often the outcome is below expectations. As it was found at the Massachusetts Institute of Technology, it takes an average of 15 to 20 years for even a successful material to move from lab testing to commercial application.

However, thanks to the development of high performance supercomputers (HPC) both chemistry and materials science are on the verge of a revolution - nowadays, it is possible to design new materials from the bottom up using supercomputers and first-principle physics. Similar to other areas of science, the development of high performance supercomputers had a profound impact on chemistry:

- Calculations changed the number of experimental investigation which need to be carried out;
- A theoretical investigation often precede an experimental;
- Calculations broadening the understanding of the investigated phenomena;
- In some cases calculations have replaced experiment (e.g. Who would nowadays try to determine equilibrium geometries for small molecules experimentally?).

Computers did not simply automate what had previously been made manually, but make it possible to create an entirely new approach to chemistry, namely computational chemistry.

This tutorial attempts to demonstrate the use of HPC and computational chemistry in the one of the main branches of chemistry: spectroscopy.

2) Computational Chemistry on Supercomputers

- Plan:
  - to demonstrate the success of computational chemistry by illustrating the percentage usage of total CPU time at PRACE systems by chemistry applications.

3) Simulation & model: UV-ViS spectra of molecular systems

- Plan:
  - Elementary discussion of UV-Vis spectroscopy.
  - Cover the fundamentals of computational chemistry method used to describe electronic spectra of molecules: *ab initio* (CIS, TDHF, MCSCF) and TD-DFT.

4) Simulation steps

- Plan:
  - Worked out examples for various computational packages such as: Gaussian, GAMESS, Molpro and Dalton.
  - Presentations of the input files format for different quantum chemistry packages.
  - Important keywords required for reliable calculations.
- Access to applications and computing resources needed for attendees: PRACE Tier-1 at WCSS.

5) Running a simulations

- Plan:
  - Overview of the sample job *s*ubmission scripts for Gaussian, GAMESS, Molpro and Dalton packages.
  - Some notes and tips on job submissions.
- Access to applications and computing resources needed for attendees: PRACE Tier-1 at WCSS.

5) Analysis and visualization

- Plan:
  - Overview and comparison of the output files produced from calculations in different programs.
  - Location of the most important sections of the output files.
  - Comparison of the results obtained at different levels of theory with experimental data.
  - Visualization of the calculated UV-Vis spectra.
- Access to applications and computing resources needed for attendees: PRACE Tier-1 at WCSS.

6) Technical issues

- Plan:
  - Challenges for high accuracy models.
  - Scaling and parallelism in conventional implementations.

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