0.1 Report on 2nd CP2K Tutorial: Enabling the Power of Imagination in MD Simulations

ETH Zürich, Hönggerberg

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Sponsored by psi-k and CECAM

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http://www.cecam.org/workshop-529.html

Report

The goal of the CP2K tutorial was to provide researchers and students in the field of molecular simulations a survey of the most relevant computational tools implemented within the CP2K program package (http://cp2k.berlios.de/), and to encourage modular, flexible, and problem oriented thinking while using them. We designed the lectures and practical sessions to let the researchers acquire the knowledge to be able to teach less experienced people in their home institutes. Furthermore, the tutorial provided good networking opportunities: by letting other people working in the molecular simulation field know each other, by meeting distinguished researchers, and by establishing contacts that may lead to research collaborations in the future.

We specifically covered the use of different levels of theory: ab-initio DFT, classical Hamiltonians, semi-empirical NDDO and hybrid QM/MM simulations. Particular attention was paid in presenting these methodologies like they are implemented in CP2K. In a second step, we demonstrated how to apply these levels of theory to several methods - provided by CP2K - for exploring potential and free energy surfaces, to characterise molecular reactions or physical phenomena, in particular: molecular dynamics, band methods, ionic relaxation methods, vibrational analysis, and metadynamics. At the same time we covered the calculation of properties (NMR, XAS) as well as several other features of the DFT-part of the code, such as hybrid exchange-correlation functionals and DFT dispersion corrections, and more in general the usage of multiple `force_evals` (section specifying the type of theory used to obtain the forces on the ions) which is the core of the flexibility behind the usage of CP2K. Lectures on real-

case applications were also proposed, to give a flavour of results that can be obtained by exploiting the features and flexibility of CP2K.

Although brief introductions were provided, both at the different levels of theory and on the explorative tools, the emphasis was placed on their practical usage and the relevant implementation details in CP2K. Therefore, this second tutorial, similarly to the first one, deliberately targeted researchers with experience in fields where the presented techniques are well established, and who already possessed a (strong) background in computational chemistry or physics.

Key lectures

The five days were divided into two parts: morning sessions with lectures and afternoon sessions held on terminals where the participants could practice with prepared exercises, or alternatively with their own research projects.

The lectures of the first days concentrated on general algorithms and methods. In the subsequent days the lectures concentrated more on specific and detailed methodologies. On the last day short presentations delivered by some of the participants gave an overview of scientific topics in which CP2K has either already been applied to or that could potentially be used for.

The first day focused on the characteristics and the parallel efficiency in the density functional theory (DFT-)module QuickStep in CP2K (M. Iannuzzi), and a general lecture on error analysis of molecular dynamics algorithms (J. Hutter).

In the terminal session of the afternoon we first introduced the input structure of CP2K. Subsequently we provided 30 molecular structures that could be used by the participants to practice energy and force calculations, and geometry optimisations. Due to the limited computational power available, we encouraged the participants to use semi-empirical Hamiltonians, classical force fields (provided for some of the molecular structures), and in few cases DFT. The high flexibility of the code allows a deep understanding of its methodologies even without the need of using a DFT Hamiltonian.

The lectures of the second day focused on the semi-empirical methods implemented in CP2K (T. Laino), the X-ray absorption and nuclear magnetic resonance spectroscopy spectroscopies (M. Iannuzzi), and the van der Waals/dispersion force schemes (A.P. Seitsonen) currently implemented in CP2K/QuickStep. The afternoon session continued with general examples aimed at familiarising with different methodological modules: `GEO_OPT` (the geometry optimisation module), MD (the molecular dynamics module). All the examples were executed, similarly to the first day, employing several kinds of Hamiltonians.

This way, during the first two days we built the infrastructure in order to focus in the subsequent days on more elaborate topics, namely either different Hamiltonians or various MD methodologies.

The main topics of the lectures on the third day were ensembles and thermostats in the molecular dynamics simulations (G. Bussi), Monte Carlo simulation of liquid/vapour interfaces (W. Kuo because Matthew McGrath was not able to come), classical Force Fields (W. Kuo), and QM/MM methods (T. Laino). The afternoon sessions were organised in a different way compared to

the first two days: Instead of working on simple molecular systems, we provided real-case scenarios where the different methodologies presented during the whole week were extensively used. We provided all needed files to set up the problem, input files as well as output files. These examples being real case studies, most of the exercises would have required computational resources beyond the ones available for the tutorial. Nonetheless, we found that these examples, on which participants worked for the rest of the week, were extremely instructive: Participants had the opportunity to see input files prepared by expert users, check the generated output, and have examples on post-processing. Each participant was free to work on the favourite topics, and pose related questions to the experts present. Many of the participants, starting from the given examples, could initialise the CP2K-setup for research problems they want to investigate. At the end of the week, the participants had an overview on how CP2K features can be exploited in a fruitful way.

In the fourth and fifth day we covered potential energy (T. Laino) and free energy (M. Iannuzzi) exploration tools by presenting nudged-elastic band methods and the metadynamics. We further demonstrated state-of-the-art applications of CP2K at surfaces and interfaces: on self-assembly (C. Pignedoli) and adsorption of molecules on metallic surfaces (G. Santarossa), dye-sensitised solar cells (F. Schiffmann) on oxide surfaces, and graphene (A.P. Seitsonen) on a semiconducting substrate. The short talks by nine participants on their research topics concluded the lecture sessions.

Feedback

All the students gave a very good evaluation of the tutorial, shown either during the hands-on part of the tutorial or during their presentation time. We note that this is a remarkable result, since more than 40 % of the attendees were researchers or lecturers with considerable teaching experience. The idea of giving the participants the opportunity to show their research problems was also extremely useful to us to understand what people find most useful in the code and what they miss. Several presenters had already a clear idea on how to employ the CP2K package once back at home to solve their problems, and a few people showed also interest in implementing features currently missing in CP2K that would become useful in their research activity.

A general remark was made about the computational power available for the tutorial. Although the general part of the hands-on exercises were tuned in order to run on commodity desktops, most of the attendees would have been pleased by a larger computational power. In fact, while the need for computational resources was not an issue for the first two afternoon sessions, it it would have been highly required (although we provided output files) for the last 3 afternoons.

Overall the tutorial can be considered to be very successful. We could attract expert researchers as we received an overwhelming number of applications from all over the world. Individual feedbacks collected by one-to-one questions indicate that the program was of high value, very interesting and useful for the

participants. Several students remarked the particular value of the hands-on part.

Our major concern was being forced to reject more than two times the number of accepted participants. The interest in CP2K is clearly growing year by year and we strongly stress the need for such tutorials that do not focus entirely on one specific topic or methodology but rather on the full capability of a simulation package. We believe that a series of tutorials on different computational packages (including CP2K itself) would be extremely useful for the scientific community. Our wish is that both the satisfaction of the participants and the interest shown for the code (more than 85 applications) will be convincing arguments for having the 3rd CP2K tutorial in 2013.

Programme

Day 1 - February 7th

- Welcome
  - 08:30 to 08:45
- Methods for DFT electronic structure calculations
  - 08:45 to 09:35 - Marcella Iannuzzi: GPW and GAPW electronic structure calculations
- High performance computing
  - 09:45 to 10:30 - Urban Borštnik: High performance computing with CP2K
- Advanced DFT methods: hybrid functionals
  - 11:00 to 11:50 - Joost VandeVondele: Hybrid functionals
- Ab initio molecular dynamics: BO vs CP
  - 12:00 to 12:50 - Jürg Hutter: Methods for ab initio molecular dynamics
- Hands-on: starting up, using GPW with different functionals, `GEO_OPT` and AIMD
  - 14:00 to 18:30 - Exercises

Day 2 - February 8th

- Semiempirical Hamiltonian
  - 08:30 to 09:20 - I-Feng William Kuo: Force fields and molecular mechanics
  - 09:30 to 10:30 - Teodoro Laino: NDDO
- Properties

  - 11:00 to 12:00 - Marcella Iannuzzi: Core level Spectroscopy and NMR
  - 12:00 to 12:50 - Ari Paavo Seitsonen: van der Waals corrections in approximative DFT-KS functionals
- Hands-on: FF, DFT properties, vdW, semiempirical methods
  - 14:00 to 18:30 - Exercises

Day 3 - February 9th

- Sampling
  - 08:30 to 09:20 - Giovanni Bussi: MD ensembles and thermostats
  - 09:30 to 10:20 - Matthew McGrath: MC simulations of liquid/vapour interfaces
- QM/MM
  - 11:00 to 12:00 - Teodoro Laino: QM/MM methods
  - 12:00 to 13:00 - I-Feng William Kuo: MM and QM/MM for bio applications
- Hands-on: real systems simulations
  - 14:00 to 18:30 - Exercises
- 20:00 to 23:00 - Conference dinner

Day 4 - February 10th

- Rare events: bands methods
  - 08:30 to 09:30 - Marcella Iannuzzi: Free energy calculations by MD
  - 09:30 to 10:30 - Gianluca Santarossa: Structural rearrangement and catalytic processes
- Applications
  - 11:00 to 12:00 - Marcella Iannuzzi: Metallic interfaces and nanomesh
  - 12:00 to 13:00 - Teodoro Laino: Band methods
- Hands-on: real systems simulations
  - 14:00 to 18:00 - Exercises

Day 5 - February 11th

- Large systems multiscale applications
  - 08:30 to 09:30 - Carlo Antonio Pignedoli: Nanostructures and adsorption on metallic surfaces
  - 09:30 to 10:30 - Florian Schiffmann: Dye sensitised solar cells

- Future challenges
  - 11:00 to 11:30 - Ari Paavo Seitsonen: Graphene and more
  - 11:30 to 11:40 - Alexander Kulesza: Optical properties of metal cluster-biomolecule hybrid systems
  - 11:40 to 11:50 - Giorgio Lanzani: The acquatic chemistry of aluminium: kinetics and dynamics
  - 11:50 to 12:00 - Ling Ge: Solute-solvent and solvent solvent interactions in molecular liquids
  - 12:00 to 12:10 - Volker Haigis: Trace element partitioning between silicate melts
  - 12:10 to 12:20 - An Ghysels: Understanding MOFs framework flexibility by Monte Carlo simulation
  - 12:20 to 12:30 - Jose Gomes: Simulation of the early stages of the synthesis of nanoporous materials
  - 12:30 to 12:40 - John Kattirtzi: Calculating acidity constants of the β-$MnO_2(110)$ surface from density functional theory based molecular dynamics
  - 12:40 to 12:50 - Jennifer Guerard: Using CP2K to estimate reorganisation energies and redox potentials of environmental organic contaminants in aquatic systems
  - 12:50 to 13:00 - Jeffrey McMahon: Finite-temperature and quantum-proton effects in atomic metallic hydrogen
- Hands-on: real systems simulations
  - 14:00 to 18:00 - Exercises

Lectures

Most of the lectures are available at the internet site of the tutorial.

List of participants

- Belgium
  - An Ghysels (Center for Molecular Modeling)
- Colombia
  - Ramiro Cardona (Universidad Nacional de Colombia)
- Finland
  - Giorgio Lanzani (Cewic - Centre of Expertise in the Water Industry Cluster - Thule Institute, University of Oulu)

- France
  - Romain Jonchiere (UPMC)
  - Sébastien Le Roux (Institut de Physique et Chimie des Matriaux de Strasbourg)
- Germany
  - Volker Haigis (Helmholtz-Zentrum Potsdam Deutsches Geoforschungszentrum)
  - Emiliano Ippoliti (German Research School for Simulation Sciences GmbH)
  - Barbara Kirchner (University of Leipzig, Wilhelm-Ostwald Institute of Physical and Theoretical Chemistry)
  - Alexander Kulesza (Freie Universität Berlin, Fachbereich Physik)
  - Maria Eugenia Tucceri (Max Planck Institute for Chemistry)
- Hungary
  - Janos Daru (Chemical Research Center Budapest)
- Ireland
  - Alin Marin Elena (University College Dublin)
  - Mahdi Shirazi (Tyndall National Institute)
- Italy
  - Giovanni Bussi (The International School for Advanced Studies, Trieste)
  - Alessandro Motta (consorzio INSTM)
  - Jacopo Sgrignani (CNR-IOM-DEMOCRITOS)
- The Netherlands
  - Omar Valsson (University of Twente)
- Poland
  - Andrzej Bil (Faculty of Chemistry, University of Wroclaw)
- Portugal
  - Jose Gomes (CICECO, University of Aveiro)
- Spain
  - Jaime Gómez-Díaz (ICIQ, Tarragona)
- Sweden

  - Ida Josefsson (Fysikum, Stockholm University)

- Switzerland
  - Urban Borštnik (Physical Chemistry Institute, University of Zurich)
  - Beat Büsser (ETH Zürich)
  - Julian Garrec (Ecole Polytechnique Federale de Lausanne)
  - Jennifer Guerard (EPFL)
  - Jürg Hutter (University of Zurich)
  - Jaap Kroes (Swiss Federal Institute of Technology Lausanne - EPFL)
  - Hans Peter Lüthi (ETH Zurich)
  - Luis Pegado (PSI - Paul Scherrer Institut)
  - Carlo Antonio Pignedoli (Swiss Federal Laboratories for Materials Testing and Research - EMPA)
  - Gianluca Santarossa (ETH Zurich)
  - Andrea Scaramucci (ETH Zurich)
  - Joost VandeVondele (University of Zurich)

- United Kingdom
  - Ling Ge (Imperial College London)
  - John Kattirtzi (University of Cambridge)
  - Florian Schiffmann (University College London)

- USA
  - I-Feng William Kuo (Lawrence Livermore National Laboratory)
  - Jeffrey McMahon (University of Illinois at Urbana–Champaign)
  - Jim Pfaendtner (University of Washington)