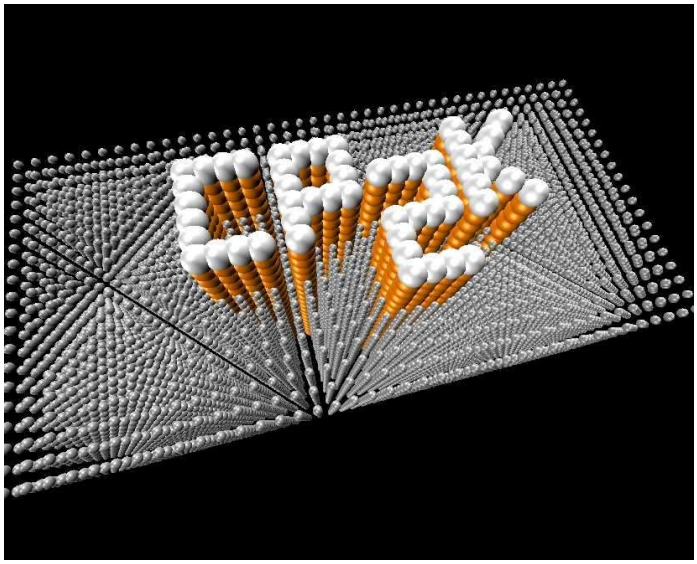
Report

1st CP2K Tutorial: Enabling the Power of Imagination in MD Simulations.



Date:

Feb 09, 2009 - Feb 13, 2009

Location:

ETH Zurich, Zurich, Switzerland

Teodoro Laino
IBM Research, Zurich Research Laboratory

Juerg Hutter
University of Zurich

Marcella Iannuzzi
University of Zurich

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1 Introduction

CP2K [1,2] is a suite of modules, comprising a variety of molecular simulation methods at different levels of accuracy, ranging from *ab-initio* DFT through semi-empirical NDDO approximation to classical Hamiltonians. It is used routinely for predicting energies, molecular structures, vibrational frequencies of molecular systems, reaction mechanisms, and ideally suited for performing molecular dynamics studies. All these methodologies are currently receiving significant attention by researchers, potential users and by people both in academics and industry. Unfortunately, the lack of a manual and of a proper tutorial material connected with a steep learning curve made the access to the code's functionality a quite difficult task for the majority of potential users.

The goal of the CP2K tutorial was to provide to researchers in the field of molecular simulations a survey of the most relevant computational tools implemented within the CP2K program package, and to encourage modular, flexible, and problem oriented thinking while using them. Ideally, the participating researchers had to acquire the proper knowledge to teach less experienced people in their respective groups. Furthermore, the tutorial provided a good opportunity to get to know other people working in the field, to meet distinguished researchers, and to establish contacts that may lead to research collaborations in the future.

The audience consisted of 27 post-graduate students, PhD students, professors, young researchers from universities and laboratories from 14 countries world-wide that were selected from 63 applicants.
Selection was performed on the basis of the personal curriculum. A working knowledge of UNIX/Linux systems was mandatory as well as a basic background in the field of molecular simulations.

In the remainder of this document we provide detailed information about the tutorial objectives, venue, the lecturers, the participants, the tutorial program, the financial aspects and the participants' feedback.

2 Objectives

We specifically covered the use of different levels of theory: *ab-initio* DFT, classical Hamiltonians, semi-empirical NDDO and hybrid QM/MM simulations. 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 characterize molecular reactions or physical phenomena. In particular: molecular dynamics, band methods, ionic relaxation methods, vibrational analysis, metadynamics, and alchemical free energy calculations.

Although brief introductions were provided, both for the different levels of theory and for the explorative tools, emphasis was placed on their practical usage and the relevant implementation details in CP2K. Therefore, this first tutorial 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.

3 Location

The 1st CP2K tutorial took place in the inspiring atmosphere of the ETH Zurich campus Hoenggerberg, Switzerland. The whole group was hosted by the Theoretical Physics Group in the HIT building. We succeeded in having two lecture rooms available (one for the basic lectures during the first two days and one exclusively used for the Hands-on part of the tutorial during the last three days). Both room were fully equipped with top facilities.

ETH Zurich campus Hoenggerberg provides as well extensive computer facilities, a Wi-Fi internet connection and a unique setting for inspiring discussions, informal exchanges and socializing.

All participants were accommodated in two central hotels in the city of Zurich: Leoneck and Bristol Hotel. Although the ETH Zurich campus Hoenggerberg is located quite far from the city center, the transport network of the city of Zurich made an easy task going from the hotels to the campus and vice-versa.

4 Lecturers

In preparation of the tutorial, it was decided to provide a broad view on the available methodologies in CP2K for performing molecular simulations, by covering a whole spectrum of topics ranging from ab-initio DFT to semi-empirical NDDO, from MD to Free Energy techniques. This broad set of topics had to be reflected by the competence of the lecturers. Nonetheless, major efforts were focused on the Hands-on session of the tutorial. For this specific purpose we believe that expert users are the best possible training assistants. Hence, in addition to 7 members of the CP2K developers team, we invited 2 additional expert users from the USA and Germany. In the table below, the two non-members of the CP2K developer team are marked with an asterisk.

Lecturer	*Affiliation*	*Topics*
Rachel Glaves *	Ruhr University – Bochum	Hands-on
Manuel Guidon	University of Zurich	XC and compiling notes
Minghsun Ho *	University of Pennsylvania	CP2K Input structure
Juerg Hutter	University of Zurich	*ab-initio* MD and DFT
Marcella Iannuzzi	University of Zurich	Free Energy methodologies
Teodoro Laino	IBM Zurich Research Laboratories	QMMM, NDDO, MEP
Matthias Krack	Paul Scherrer Institut	QS and Basis Sets + Pseudo
I-Feng William Kuo	Lawrence Livermore National Lab	Classical FF, QMMM
Fawzi Roberto Mohamed	Humboldt University Berlin	Structure of CP2K

5 Participants

In response to the call for participation, we received 63 applications before the deadline (and 5 additional requests after the deadline). Every applicant had to submit a description of his/her background, focus of research or field of interest, expectation about the tutorial (motivation letter), current status and affiliation.
Based on these data we selected 27 participants based on their general qualifications, background, research interests and, less important, by the geographical distribution. The following table summarizes the amount of received applications and accepted participants for each country. In Appendix **A** we provide the whole list of accepted participants.

Country/Category	*Applications*	*Accepted Applications*
Austria	1	0
Belgium	2	1
Bulgaria	2	1
Canada	1	0
China	1	0
Denmark	1	0
France	4	3
Germany	7	3
Japan	4	0
India	1	0
Italy	7	1
Poland	1	1
Russian Federation	1	0
Slovakia	1	0
Spain	4	1
Sweden	1	1
Switzerland	10	8
The Netherlands	4	2
Turkey	5	2
Ukraine	1	1
United Kingdom	1	1
USA	3	1
Women	15	10

The geographical distribution is quite proportional for almost every country with the exception of Switzerland. In fact, the large number of Swiss participants is due to the acceptance of all 5 participation requests from research groups located in the Zurich area. Since attendees living in the Zurich area did not need accommodation, the only expense coming from their participation was the daily allowance. This gave us the possibility to reserve the remaining 20 places for

people not living in the Zurich area. Last but not least, due to the large number of participation requests and after a careful analysis of the budget and of the infrastructure logistics, we decided to increase by 10% the amount of accepted participants not resident in the Zurich area, bringing the final number of available seats for non-resident in Zurich from 20 to 22. The total number of participants is therefore 27: 22 (non-resident) + 5 (resident).

6 Program

The 1st CP2K tutorial program consisted of general lectures during the first two days of the week (February the 9th and 10th) aimed at refreshing some basic concepts in the field of Density Functional Theory (DFT), NDDO semi-empirical approximations, Hybrid QM/MM schemes, Molecular Dynamics and Free Energy methodologies.
On the subsequent two days (February the 11th and 12th), the program was organized to have morning sessions with lectures fully related to CP2K and afternoon ones for running computer exercises in which the morning lessons were applied. The last day (February the 13th) was organized solely into computational exercises arranged according to their thematic group and representing more realistic research problems.

Day 1 - February, 9th 2009

14:00 to 14:30 – **Teodoro Laino** Welcome

14:30 to 15:15 – **Juerg Hutter** "*ab-initio* MD and Density Functional Theory"

16:00 to 16:30 – Coffee Break

15:15 to 16:00 – **Manuel Guidon** "Exchange-Correlation Functionals"

16:30 to 17:30 – **Juerg Hutter** "Self-Interaction Energy and Dispersion"

17:30 to 18:30 – **Fawzi Roberto Mohamed** "Basis Sets and Pseudo-Potentials"

Day 2 - February, 10th 2009

08:30 to 09:15 – **I-Feng William Kuo** "Classical Force Fields"

09:15 to 10:00 – **Teodoro Laino** "QM/MM Electrostatic Couplings"

10:00 to 10:30 – Coffee Break

10:30 to 11:30 – **I-Feng William Kuo** "QM/MM Advanced Topics"

11:30 to 12:30 – **Teodoro Laino "**Semi-empirical NDDO"

12:30 to 14:00 – Lunch Break

14:00 to 15:00 – **Fawzi Roberto Mohamed "**Molecular Dynamics"

15:00 to 16:00 – **Marcella Iannuzzi "**Free Energy Calculations by MD"

16:00 to 16:30 – Coffee Break

16:30 to 17:30 – **Marcella Iannuzzi "**Free Energy Calculations by MD"

17:30 to 18:30 – **Teodoro Laino "**Minimum Energy and Free Energy paths"

Day 3 - February, 11th 2009

08:30 to 10:00 – **Fawzi Roberto Mohamed "**CP2K structure"

10:00 to 10:30 – Coffee Break

10:30 to 12:00 – **Matthias Krack "**Introduction to the DFT module QUICKSTEP"

12:00 to 12:30 – **Minghsun Ho "**Introduction to the CP2K input file syntax 1"

12:30 to 14:00 – Lunch Break

14:00 to 18:30 – **Rachel Glaves "**Hands On - 1"

Day 4 - February, 12th 2009

08:30 to 09:30 – **Minghsun Ho "**Efficiency: OT vs Diagonalization, Preconditioners, Outer SCF and Extrapolation"

09:30 to 10:30 – **Matthias Krack "**Accuracy and Efficiency"

10:30 to 11:00 – Coffee Break

11:00 to 12:00 – **Minghsun Ho "**Introduction to the CP2K input file syntax 2"

12:00 to 12:30 – **Manuel Guidon "**Notes on installing CP2K"

12:30 to 14:00 – Lunch Break

14:00 to 18:30 – **Rachel Glaves "**Hands On - 2"

Day 5 - February, 13th 2009

08:30 to 10:30 – **Rachel Glaves "**Woodward-Hoffmann rules"

10:30 to 11:00 – Coffee Break

11:00 to 13:00 – **Marcella Iannuzzi** "Metadynamics Exercises"

13:00 to 14:00 – Lunch Break

14:00 to 16:00 – **I-Feng William Kuo "**QM/MM Exercises"

16:00 to 16:30 – Coffee Break

16:30 to 18:30 – **Teodoro Laino** "Multiple Force-Eval Exercises"

All presentation slides have been made available on-line [3] at the tutorial website hosted in the CECAM portal as a resource for the preparation of future tutorials and other teaching activities. No hard-copies of slides or other material was distributed to participants in advance.
In Appendix B there's a summary of all lectures. The same material is available on-line [3] with links to titles and slides of the individual activities.

7 Financial

The 1st CP2K tutorial received the following sponsorships: CECAM 15000 EUR, SIMBIOMA (ESF) 4000 EUR and PSI-K 4000 EUR. The total budget was therefore of 23000 EUR which converted in CHF amounts to roughly 34000 CHF. No participation fee was planned.

Each participant, including lecturers, had a daily allowance of 50 CHF per day for 5 days in order to cover meals and transport expenses. Participants and lecturers have been accommodated in double rooms. A few single rooms were provided for women attendees older than 40 y.o. All the accommodations provided were in 3 star hotels with an average price of 185 CHF per double room and 140 CHF per single room.
Travel expenses have been reimbursed to only 4 lecturers (2 from USA and 2 from Germany).
9 Coffee breaks have been arranged for the whole week at the cafeteria of the HIT building in the ETHZ Hoenggerberg campus and a tutorial dinner was organized the night of February the 11th in a local restaurant in Zurich (Neumarkt restaurant). The price per person for the dinner has been kept below 80 CHF (including wines and beverages).

Detailed Financial Report:

Daily allowance (250 CHF x 36)	9000
Hotel accommodation (24 pax // 5 nights)	13533
Coffee Breaks (9 for 36 pax)	2028
Tutorial Dinner (34 pax)	2510
Travel expenses (4 lecturers)	2253
Total (CHF)	29324

The prices reported above may be subject to minor modifications since those reflect the planned expenses. A final report can be asked to Mrs. Emilie Bernard (emilie.bernard@cecam.org) who took care of the administrative tasks of the tutorial.

8 Social Activities

A tutorial dinner was organized in a Zunfthaus (typical Zurich restaurant) for the evening of February the 11th. Apart from this event, the schedule included some leisure time (2 slots of 30 minutes for coffee breaks and 1h:30 minutes for lunch break) for socializing. A discussion forum has been created [4] to facilitate the exchange of information between participants before, during and after the tutorial.

9 Feedback

A student questionnaire was distributed upon the completion of the tutorial. This feedback form is aimed to measure how attendees judged several choices made by the organizers and to gather their opinion on how to improve or to organize more effectively things that did not work properly.
A copy of the questionnaire is attached in Appendix **C**.
We collected 25 out of 27 distributed forms and all of them are available in Appendix **D**[1].

All the students gave a very good evaluation of the tutorial. We note that this is a remarkable result, since more than 60% of the attendees are researchers or lecturers with considerable teaching experience.

There was a general remark about the computational power made available for the tutorial. Although 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. This goal could easily be achieved in the future by involving the Swiss National Supercomputing Center in Manno (CSCS) for the next edition of the tutorial. One possibility would be to reserve some slots on a parallel machine exclusively for the 3 afternoons of the tutorial.

1 The Appendix (**D**) is available only as a password encrypted attachment due to the confidentiality of the information contained in the filled feedback questionnaire.

Another interesting suggestion was made on the organization of the Hands-on session of the tutorial. Specifically one attendee suggested to build-up a branch of 3 different classes of problems: one biological, one chemistry and one solid-state physics. Each attendee may then decide at the starting of the tutorial which class of problem to tackle during the week. All the methodologies explained during the morning sessions may then be applied always to the same system.
Although, there could be some hurdles to overcome, the idea deserves in general a deeper analysis and possibly could be something on which to develop the next-class of exercises for future tutorials.

10 Conclusions

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 feedback (see Appendix **D** available as a password encrypted attachment) from 25 out of 27 participants indicates that the program was of high value, very interesting and useful. Several students remarked the particular value of the hands-on part.
As indicated by the large number of applications, there is a clear need for such tutorial events. Hence we are currently planning a similar event due in 2 years time.

We would like to acknowledge CECAM[5], PSI-K[6] and SIMBIOMA (ESF)[7] for their contribution as main sponsors. Finally, we would like to acknowledge the help of few people for supporting the organization of the tutorial: Wanda Andreoni (CECAM director), Emilie Bernard (CECAM administrative secretary) and Denise Pin (ETH Zurich secretary). We are grateful to Prof. Matthias Troyer for hosting the 1st CP2K tutorial in the theoretical physics department of ETH Zurich, Hoenggerberg campus.

11 References

1. http://cp2k.berlios.de
2. http://groups.google.com/group/cp2k
3. http://www.cecam.org/workshop-273.html
4. http://groups.google.com/group/cp2k_tutorial
5. http://www.cecam.org
6. http://www.psi-k.org
7. http://www.simbioma.cecam.fr/

Appendix A

Whole List of Participants in alphabetical order

Organizers

1. **Hutter Juerg** (hutter@pci.uzh.ch) University of Zurich
2. **Iannuzzi Marcella** (marcella@pci.uzh.ch) University of Zurich
3. **Laino Teodoro** (teodoro.laino@gmail.com) IBM Research, Zurich Research Laboratory

4. **Alfonso-Prieto Mercedes** (malfonso@pcb.ub.es) Research Centre in Theoretical Chemistry - Barcelona Science Park, Spain
5. **Andreussi Oliviero** (oliviero@mit.edu) Massachusetts Institute of Technology, USA
6. **Atamas Nataliya** (tasunia@yahoo.com) Kiev National Taras Shevchenko University, Ukraine
7. **Aviyente Viktorya** (aviye@boun.edu.tr) Chemistry Department Bogazici University 34342 Bebek Istanbul, Turkey
8. **Aytemiz Nevin** (nevin@sdu.edu.tr) Associate Prof. Dr., Turkey
9. **Campomanes Pablo** (pablo.campomanes@epfl .ch) EPF Lausanne, Switzerland
10. **Faraldo-Gomez Jose** (jose.faraldo@mpibp-frankfurt.mpg.de) Max Planck Institute of Biophysics, Germany
11. **Fleurat-Lessard Paul** (Paul.Fleurat-Lessard@ens-lyon.fr) Laboratoire de Chimie, ENS Lyon, France
12. **Gao Ning** (ning.gao@psi.ch) PSI, Switzerland
13. **Gaspari Roberto** (roberto.gaspari@empa.ch) Empa Dübendorf Ueberlandstrasse 129, 8600, Switzerland
14. **Gerra Guido** (guido.gerra@epfl .ch) CECAM, Switzerland
15. **Glaves Rachel** (rachel.glaves@theochem.rub.de) Department of theoretical chemistry, Ruhr-University Bochum, Germany
16. **Grisolia Maricarmen** (grisolia@cemes.fr) Centre d'Elaboration de Matériaux et d'Etudes Structurales (CEMES) Centre d''Elaboration de Matériaux et d''Etudes Structurales (CEMES), France

17. **Guidon Manuel** (mguidon@pci.uzh.ch) University Zuerich, Switzerland

18. **Hesske Holger** (holger.hesske@chem.ethz.ch) ETH Zurich, Switzerland

19. **Ho Minghsun** (minghsun@sas.upenn.edu) University of Pennsylvania, USA

20. **Kaczor Agnieszka** (agnieszka.kaczor@am.lublin.pl) Medical University of Lublin, Poland

21. **KILIÇ Murat** (murat_ch@yahoo.com) University of Amsterdam, The Netherlands

22. **Kosa Monica** (monica.kosa@phys.chem.ethz.ch) Department of Chemistry and Applied Biosciences c/o Professor Michele Parrinello ETH Zurich, USI Campus Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

23. **Krack Matthias** (matthias.krack@psi.ch) Paul Scherrer Institut, Switzerland

24. **Kuo I-Feng William** (kuo2@llnl.gov) Lawrence Livermore National Laboratory, USA

25. **Masia Marco** (marco.masia@uniss.it) Dipartimento di Chimica, Italy

26. **Milet Anne** (Anne.Milet@ujf-grenoble.fr) Université J. Fourier Grenoble, France

27. **Mohamed Fawzi Roberto** (fawzi@gmx.ch) Humboldt University Berlin, Germany

28. **Nguyen Manh-Thuong** (Manh-Thuong.Nguyen@empa.ch) EMPA, Switzerland

29. **Pauwels Ewald** (ewald.pauwels@UGent.be) Center for Molecular Modeling, Ghent University, Belgium

30. **Petkov Peicho** (peicho@phys.uni-sofi a.bg) University of Sofia, Bulgaria

31. **Saßmannshausen Jörg** (jorg.sassmannshausen@strath.ac.uk) University of Strathclyde, UK

32. **Santarossa Gianluca** (gianluca.santarossa@chem.ethz.ch) ETH Zurich, Switzerland

33. **Vilciauskas Linas** (l.vilciauskas@fkf.mpg.de) Max-Planck-Institut für Festkörperforschung, Germany

34. **Violanda Marites** (m.violanda@uu.nl) Nanophotonics, Debye Institute for Nanomaterials Science, Faculty of Science, Utrecht University, The Netherlands

35. **Walewski Lukasz** (Lukasz.Walewski@ruhr-uni-bochum.de) Ruhr University Bochum, Germany

36. **Yun Younsuk** (younsuk.yun@fysik.uu.se) Department of Physics and Materials Science, Uppsala University, Sweden

Appendix B

Whole list of lectures according the program order.

Ab initio Molecular Dynamics and Density Functional Theory
Juerg Hutter, University of Zurich

Exchange-Correlation Functionals
Manuel Guidon, University Zuerich

Self-Interaction Energy and Dispersion
Juerg Hutter, University of Zurich

Molecular Dynamics
Fawzi Roberto Mohamed, Humboldt University Berlin

Classical Force Fields
I-Feng William Kuo, Lawrence Livermore National Laboratory

QM/MM Electrostatic Couplings
Teodoro Laino, IBM Research, Zurich Research Laboratory

QM/MM Advanced Topics
I-Feng William Kuo, Lawrence Livermore National Laboratory

Semi-empirical NDDO
Teodoro Laino, IBM Research, Zurich Research Laboratory

Basis Sets and Pseudo-Potentials
Fawzi Roberto Mohamed, Humboldt University Berlin

Free Energy Calculations by MD: some notes and examples
Marcella Iannuzzi, University of Zurich

Minimum Energy and Free Energy paths
Teodoro Laino, IBM Research, Zurich Research Laboratory

CP2K structure
Fawzi Roberto Mohamed, Humboldt University Berlin

Introduction to the CP2K DFT module QUICKSTEP
Matthias Krack, Paul Scherrer Institut

Introduction to the CP2K input fi le syntax 1
Minghsun Ho, University of Pennsylvania

Hands On - 1
Rachel Glaves, Department of theoretical chemistry, Ruhr-University Bochum

Efficiency: OT vs Diagonalization, Preconditioners, Outer SCF and Extrapolation
Minghsun Ho, University of Pennsylvania

Accuracy and Efficiency
Matthias Krack, Paul Scherrer Institut

Introduction to the CP2K input fi le syntax 2
Minghsun Ho, University of Pennsylvania

Notes on installing CP2K
Manuel Guidon, University Zuerich

Hands On - 2
Rachel Glaves, Department of theoretical chemistry, Ruhr-University Bochum

Woodward-Hoffmann rules
Rachel Glaves, Department of theoretical chemistry, Ruhr-University Bochum

QM/MM Exercises
I-Feng William Kuo, Lawrence Livermore National Laboratory

Appendix C

Feedback Form

1st CP2K Tutorial: Enabling the power of imagination in MD simulations

General Questions:

	Strongly Agree	Agree	Disagree	Strongly Disagree	No Opinion
Was the tutorial clear?					
Was the tutorial useful?					
Was the tutorial of high quality?					
Was the tutorial well organized?					

Logistics:

	Very Good	Good	Fair	Bad	Very Bad
Accomodation/Hotel					
Lecture Room					
Tutorial Room/PC Facilities					
Mensa (Lunch services)					
Coffee Breaks					
Tutorial location (Campus/City)					
Social Dinner					

Lectures: (Please note that the following topics may have been covered by one or more people. In case the topic was covered in more than one lecture and likely by two different people, please, provide an average feedback)

	Very Good	Good	Fair	Bad	Very Bad
Density Functional Theory					
XC Functionals					
Basis Sets and Pseudopotentials					
Molecular Dynamics					
QM/MM					
Free Energy methodologies					
Minimum energy path					
Semiempirical NDDO					
Classical ForceFields					
Input structure of CP2K					
Functionalities of CP2K					
Exercises' explanation					

Exercises/Tutorial examples:

	Very Good	Good	Fair	Bad	Very Bad
Interesting examples					
Coverage of cp2k functionalities					
Complexity of tutorial exercises					
General feedback on exercises					

Do you have any idea on how to improve the tutorial's exercises (making them more appealing, more didactic, more interesting)? Please write below your suggestions..

Comments/Suggestions for improving future CP2K tutorials (your suggestions will be of high value to us)

Thank you for your time!

Appendix D

Feedback Forms collected (25 out of 27)

Important Note

Due to the confidentiality of the information contained in the filled feedback questionnaire this material is made accessible only as a password encrypted attachment.

The filled forms have to be considered nondisclosable and should only be used for the evaluation of the tutorial by referees. For no reason the filled forms (or part of them) should be disclosed without prior authorization of the organizers.