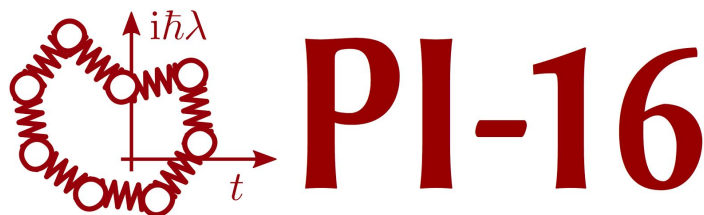# Final report on CECAM/Psi-k School on Path Integral Quantum Mechanics: Theory, Simulation and Application

Organisers: *Mariana Rossi, Michele Ceriotti, Tom Markland, and Mark Tuckerman*
Dates: *13-17 June, 2015*

1. Summary

From June 13 to 17 we convened a School on Path Integral Quantum Mechanics at the CECAM headquarters in Lausanne, Switzerland. The school gathered together 18 speakers (12 invited and 6 contributed) and 40 participants affiliated to 14 different countries, setting a milestone for the theory and practice of Path Integral (PI) techniques for the atomic-scale modelling of the quantum behavior of materials and molecules. We received a total of 82 applications to attend the school and unfortunately could not accept more participants only due to space constraints in the lecture room. This underlines the growth of this field and the importance the community is giving to it.

The interest in path integral (PI) methods has rapidly grown over the past decade due to the development of efficient algorithms that, in many cases, now allow nuclear quantum effects to be included at a cost barely higher than that of performing a simulation with classical nuclei. These developments have been accompanied by increased accessibility of PI methods due to their implementation in a number of open source molecular dynamics and electronic structure codes. These advances have allowed nuclear quantum effects to be included in the treatment of large systems by a
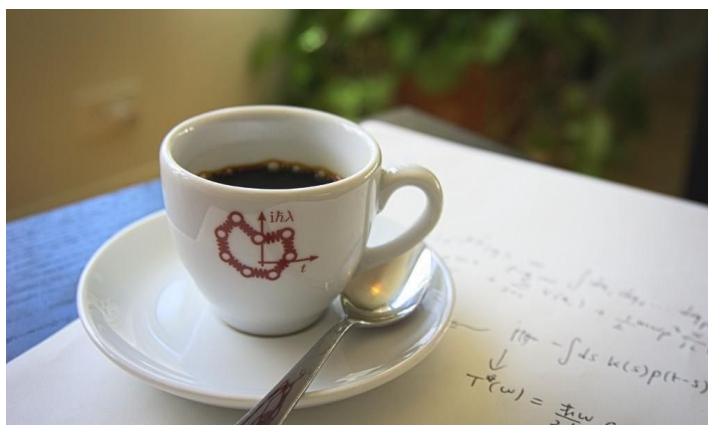
wide range of users, with a low computational cost. Indeed, as electronic structure methods have become more accurate the error introduced by not including the quantum nature of the nuclei is often of the same order of magnitude as the one coming from the electronic structure treatment when treating systems with light atoms.

The school focused on didactic talks aimed at introducing the participants to the methods and simulation techniques to treat imaginary and real time path integrals, for both adiabatic and non-adiabatic dynamics. Invited and contributed speakers were encouraged to give lectures that explained the methods in great detail, so that the students could benefit the most from the school, even if this was their first contact with path integral methods. These lectures were also made available in the CECAM website (https://www.cecam.org/workshop-5-1314.html).

Hands-on sessions were mostly based on the i-PI (http://epfl-cosmo.github.io/gle4md/index.html?page=ipi) program, which is a Python wrapper code that interfaces with other codes (ab initio or not) for the evaluation of the interactions between the atoms. For this session, the participants received personalized USB sticks with the full environment and all software they needed for the exercises.

To encourage interaction between the participants and speakers the school had a poster session and three Q&A sessions. For the poster session all students were highly encouraged to bring posters regardless of whether it was on path integrals since for many this was their first introduction to the area. The poster session had extremely high-quality posters both on path integrals and other subjects and received many compliments from speakers and participants. In order to motivate discussion, we set up "anonymous" Q&A sessions, in which the participants would write questions on a piece of paper after the lectures and the speakers would answer all questions out loud by the end of the day.

We received generous funding from CECAM, Psi-k, and the Journal of Chemical Physics. With this funding we were able to contribute to the participation costs of 12 participants, give multiple poster prizes, and a provide useful conference items: personalized USB sticks (containing the software and exercise files and handouts) and personalized coffee cups that the participants could use to minimize the waste generated during the conference and take home as a memento from the week they spent at this school. More details on our school follow below.

2. Goals and important outcomes from the school

The main goal of this school was to introduce participants to path integral quantum mechanics methods. This is a topic that is often absent from the standard program of physics or chemistry undergraduate and graduate courses, and (as mentioned above) has become more important in the past decades. We devised the school such that even a person who was not at all familiar with path integral techniques would be able to grasp the fundamental concepts and pursue further development in the subject. In order to accomplish these goals we asked all the speakers to give introductory and didactic talks in their subjects, which they all did. We received feedback from the students that they were found the level of the talks very good. We have also provided all the slides of the talks and put together a reading list for each topic we covered in the school. This list was requested by some students, that wanted to further deepen their knowledge in topics they saw for the first time in the school. We hope that this will make more groups use path integral methods, and that the quality of path integral calculations will be increased in the groups where it is already in use.

Some of our participants were already quite knowledgeable in the field, but still could profit from our school's coverage of more advanced path integral techniques. An important aspect of this school was that it focused on both imaginary time and real time path integrals. Among the participants who came in with existing knowledge of path integral methods most were only familiar with one or the other. Thus they could benefit from many of the lectures.

A last important goal we tried to achieve with this school was to make the practical sessions as easy as possible to start, and as easy as possible to keep after the school was over. We gave the participants USB keys with the whole environment and software needed for the exercises pre-installed. They could also run the exercises within this environment, thus automatically saving their data in the USB key. This was overall a success, with the only problem being the speed of the USB data transfer in some computers. We think it is a format that can be tried again with few improvements.

3. Topics covered in the lectures

We had a large range of topics covered in our school, which we detail below. This was, perhaps, the broadest presentation of path integral methods made in a school/course so far. All the slides for the invited and contributed lectures were made public in the conference website, and can be downloaded from:
https://www.cecam.org/workshop-5-1314.html.

Invited lectures:

T. Markland - Introduction to Imaginary-Time Path Integrals
- Derivation of imaginary time path integral expression
- Reinserting the momenta and PIMD - mass matrix etc.
- Evolving the ring polymers - normal modes and staging transformations, a brief recap on developing integrators using Liouville operator splitting and resonance barriers in PIMD
- Thermostatting of PIMD - non ergodicity challenges etc., targeted thermostatting schemes PILE and NHC, GLE as a thermostat for PIMD

O. Marsalek - Path Integral Estimators
- Position-dependent operators
- Kinetic energy - primitive and virial
- Free energy change upon isotope substitution

M. Ceriotti - Accelerated Path Integral Techniques
- A brief introduction to Generalized Langevin Equation thermostatting
- Generalized Langevin Equations for path integrals
- High-order path integrals
- Ring-polymer contraction and multiple time stepping

M. Tuckerman - Advanced Path Integral Molecular Dynamics
- Open-chain path integrals and momentum-dependent observables
- Path integrals in the NPT ensemble
- Adaptive resolution and path integrals in the grand-canonical ensemble

A. Michaelides - Ab Initio Path Integrals
- A brief introduction to Ab initio methods (DFT)
- Challenges in combining DFT and path integrals
- Examples

E. Brown - Indistinguishable Particles
- Path integral exchange (formulation)
- Important examples of exchange in quantum processes
- Equivalence of bosons and fermions in path integrals
- PIMC sampling
- Fermion sign problem

- Possible routes around the sign problem

M. Tuckerman - Time Correlation Functions
- Brief review of linear response theory and derivation of quantum time correlation functions
- Different types of time correlation functions and the connection between them
- Path integral representation of time correlation functions
- Challenges in the calculation of quantum time correlation functions via path integrals

N. Makri - Real Time Path Integrals - Introduction & Exact Methods
- Path integral representation of the real time propagator, semiclassical limit, and the sign problem
- Influence functional and Gaussian response
- Iterative decomposition of the path integral for numerically exact treatment of system-bath dynamics
- The classical and quantum mechanisms of decoherence
- Quantum-classical path integral: rigorous dynamics of a quantum system in an atomistic solvent

N. Ananth - Non-Adiabatic and Semiclassical Dynamics
- Deriving the Van Vleck propagator from the real-time propagator
- Initial Value representation and flavors; HK-IVR, EFB-IVR, FB-IVR
- LSC-IVR
- Mixed quantum-classical IVR
- Brief look at nonadiabatic dynamics in the SC-IVR framework
- Approximate methods for solution: Surface Hopping
- Approximate methods for solution: Ehrenfest Dynamics
- Semiclassical non-adiabatic dynamics: Mapping formalism and linearization

S. Althorpe - Matsubara Dynamics
- Motivation: quantum Boltzmann statistics with classical dynamics underpins CMD, RPMD, TRPMD, etc.
- Recap of linearized semiclassical approx (i.e. classical Wigner) & its failure to satisfy detailed balance
- Sketch of Matsubara dynamics derivation and demonstration that it satisfies db
- Origin of CMD and RPMD.
- Use of Matsubara to generate alternative db-satisfying quantum stat/classical dynamics methods

M. Rossi - RPMD and CMD Approaches to Quantum Dynamics
- Brief recap on correlation functions
- How CMD and RPMD approximate correlation functions
- Caveats with the approximations
- How TRPMD approximates correlation functions
- How a typical calculation works
- Examples of successes and failures of the methods

J. Vanicek - Quantum Rate Theories and Instanton Methods
- Quantum rate constant from the flux-flux correlation function
- Classical and quantum transition state theories
- Semiclassical and quantum instanton approximations
- Kinetic isotope effects

Contributed talks and abstracts:

Igor Poltavskyi - Extending the Applicability of Path-Integrals with Perturbation Theory

The quantum nature of nuclear motions plays an important role in many different properties of molecules and materials. The standard approach to model nuclear quantum fluctuations in chemical and biological systems is to use path integral (PI) molecular dynamics (MD). Unfortunately, conventional PIMD simulations can have an exceedingly large computational cost due to the need to employ an excessive number of coupled classical subsystems (beads) for quantitative accuracy or poor statistical sampling. We propose to synergistically combine perturbation theory [1-3] with the Feynman–Kac imaginary-time path integral approach to quantum mechanics and derive an improved non empirical PI partition function and estimators. The developed perturbed path-integrals (PPI) technique [4] requires the same ingredients as the conventional method, but additionally employs inter-particle forces (which are typically neglected after making a corresponding step in the dynamics) to increase the accuracy of estimators for thermodynamic observables. This allows to improve the efficiency of PIMD simulations by an order of magnitude without any empiricism. The PPI method has the same statistical convergence as the underlying second-order PIMD simulation and can be applied with any kind of thermostat or barostat. Results are presented for the thermodynamics of fundamental model systems, liquid water modeled with a classical potential, ab initio simulations of small molecules, and proton transport through a graphene layer. For all of these examples, the PPI method demonstrates an efficiency

comparable to the best existing approaches [5-6], without requiring any parameterization or code modification, paving the way toward seamless and accurate modeling of nuclear quantum effects in realistic molecules and materials.

[1] L. D. Landau and E. M. Lifshitz, Statistical Physics, Butterworth-Heinemann, Oxford, 1980. [2] E. Wigner, Phys. Rev. 40, 749 (1932). [3] G. E. Uhlenbeck and L. Gropper, Phys. Rev. 41, 79 (1932). [4] I. Poltavsky and A. Tkatchenko, Chem. Sci. 7, 1368 (2016). [5] M. Ceriotti, G. Bussi, and M. Parrinello, Phys. Rev. Lett. 102, 020601 (2009). [6] A. Pérez and M. E. Tuckerman, J. Chem. Phys. 135, 064104 (2011).

Vincent Balleneger - Direct numerical path integral calculation of virial coefficients in the equation of state of Coulomb matter

Coulomb matter, i.e. charged nuclei and electrons interacting solely via the Coulomb potential, is a fundamental model for matter which can be investigated by various many-body techniques. Calculating precisely the equation of state of a proton and electron gas in regimes of full or partial ionization is important in several fields, especially in stellar physics. Since a quantum system at thermal equilibrium is formally equivalent to a classical system of interacting loops (or ring polymers), its grand-canonical partition function can be expanded using Mayer diagrams [1]. These diagrams are built with points, or more precisely loops, which represent quantum particles and bonds that express interactions between them. At low densities, only few Mayer diagrams contribute to the equation of state at a given order. Collecting all diagrams with up to N interacting particles leads the screened cluster equation of state (EOS) at order N [2]. This EOS involves cluster functions defined by imaginary-time path integrals for a small number of charged particles interacting via a screened Coulomb potential. These functions are analogous to virial coefficients; they depend on the temperature and also on the density due to a collective screening effect arising from long-range Coulomb interactions. We calculated numerically the path integrals in the first few-body cluster functions for a hydrogen-helium mixture [3]. These functions account for effects like screened Coulomb interactions between ionized particles, formation and ionization of bound entities (H and He atoms, H2 molecules, He+, H2+,... ions) as well as modifications in the spectra of bound states at finite density. Since a cluster function is not an expectation value, we performed a direct Monte Carlo sampling of the corresponding path integrals with an importance sampling function to capture the contributions of both ionized and bound states at low temperatures [3].
Instead of the standard technique for computing Coulombic path integrals (use of an effective path action with a smoothed out Coulomb singularity), we introduced a new adaptive non- uniform discretization scheme in which the paths are discretized more

finely in regions where the potential is strong. This scheme handles effectively the Coulomb divergence, even in the attractive case, thanks to the number of beads not being fixed. It is slightly more efficient than using a uniform discretization with the effective cumulant potential. After a brief sketch of the derivation of the screened cluster EOS, I will focus on the numerical calculations of two- and three-body cluster functions and show some numerical results.

[1] D.C. Brydges and P.A. Martin, Coulomb systems at low density: A review, J. Stat. Phys. 96, 1163–1330 (1999). [2] D. Wendland, The equation of state of the hydrogen-helium mixture with application to the Sun, Ph.D. thesis, Ecole Normale Supérieure de Lyon (2015). [3] D. Wendland, V. Ballenegger and A. Alastuey, Quantum partition functions of composite particles in a hydrogen- helium plasma via path integral Monte Carlo, J. Chem. Phys. 141, 184109 (2014).

Marco Nava - Path Integral Metadynamics and Beyond

The problem of sampling a probability density can become particularly difficult when there are several metastable states separated by large energy barriers. One of the approaches proposed to tackle this problem involves using quantum effects; zero point energy is in fact expected to reduce the effective height of the potential barriers while tunneling provides one more channel by which the system can reconfigure itself. Path Integral (PI) methods provide an easy and natural way to introduce these effects, in practice, however, this trail has not been thoroughly explored because it was soon observed that tunneling events in PI methods are rarely sampled even in simple 1D systems with modest barriers[1]. In this presentation we show a way to lift this limitation using Metadynamics[2] and present a new enhanced sampling method based on a replica exchange scheme of Hamiltonians with different de Broglie wavelengths[3]. The limits are discussed and a further generalization for classical sampling is also presented.
[1] G. E. Santoro and E. Tosatti, Journal of Physics A: Math. Gen. 2006, 39, R393. [2] R. Quhe, M. Nava, P. Tiwary and M. Parrinello, J. Chem. Theory Comput. 2015, 11, 1383. [3] M. Nava, R. Quhe, F. Palazzesi, P. Tiwary and M. Parrinello, J. Chem. Theory Comput. 2015, 11, 5114.

Sadrach Pierre - Proton-Coupled Electron Transfer Reactions - Path integral based dynamics

Proton-coupled electron transfer (PCET) plays a significant role in many important biological processes such as tyrosine oxidation in photosynthesis and the proton

pumping mechanism of cytochrome c oxidase during respiration [1]. Uncovering the multiple competing pathways for photo-induced PCET remains a significant theoretical challenge. Here, we will discuss a recently developed path-integral (PI) based method, Mapping-Variable Ring Polymer Molecular Dynamics (MV-RPMD), that allows for the simulation of multi-electron non-adiabatic dynamics in the condensed phase [2]. We derive an optimized MV-RPMD expression for real-time correlation functions using the symmetric Trotter approximation, and we demonstrate its superior numerical properties. We apply this method to a model PCET system bath and generate proton and solvent probability distributions. We investigate equilibrium and dynamic properties of model PCET systems using the standard position-space representation of the proton and using an equivalent discrete diabatic proton-electron state representation. Analysis of the trajectory ensemble in both cases yields insights into the mechanism of electron and proton transfer.

[1] J. Kretchmer, T. F. Miller III, J. Chem. Phys. 138 (2013), 134109 [2] N. Ananth. J. Chem. Phys. 139 (2013), 064103

Federica Agostini - Quantum-Classical Approaches to Electronic Non-Adiabatic Processes

The Born-Oppenheimer (BO) approximation is widely employed to account for the coupling between electrons and nuclei when describing dynamical processes in molecular systems. It relies on the assumption that the typical time-scales of electronic and nuclear motion in a molecule are adiabatically separable. This hypothesis allows to write the full electron-nuclear wave function as a single product of an electronic eigenstate, for each fixed nuclear configuration, and a time-dependent nuclear wave function. Such an approximation is fundamental for our understanding of molecular processes. However, it is not suited when non-adiabatic effects due the coupling between the nuclear motion and excited electronic states become important, which are essential to understand phenomena such as vision, photovoltaic processes and Joule heating in molecular junctions. The talk will show how the BO approximation can be made exact [1], by preserving the single product form of the full electron-nuclear wave function and accounting for electronic excitations. This exact factorization approach will be introduced and used as a tool [2] to interpret non-adiabatic processes [3]. Furthermore, algorithms will be derived [4, 5, 6] to describe electronic non-adiabatic processes employing a description of nuclear dynamics in terms of classical trajectories. Applications to model systems [4, 5] and to small molecules [6] will be presented to numerically validate such quantum-classical scheme.

[1] A. Abedi, N. T. Maitra and E. K. U. Gross, Phys. Rev. Lett., 105, 123002 (2010). [2] A. Abedi, F. Agostini, Y. Suzuki and E. K. U. Gross, Phys. Rev. Lett., 110, 263001 (2013). [3] F. Agostini, A. Abedi, Y. Suzuki, S. K. Min, N. T. Maitra and E. K. U. Gross, J. Chem. Phys., 142, 084303 (2015). [4] F. Agostini, A. Abedi and E. K. U. Gross, J. Chem. Phys., 141, 241101 (2014). [5] S. K. Min, F. Agostini and E. K. U. Gross, Phys. Rev. Lett., 115, 073001 (2015). [6] A. Scherrer, F. Agostini, D. Sebastiani, E. K. U. Gross and R. Vuilleumier, J. Chem. Phys., 143, 074106 (2015).

Jeremy Richardson - Instanton rate theory

Instanton theory [1] has been used for over 40 years to predict low-temperature reaction rates and is known to include accurately the quantum effects of tunnelling and zero-point energy. Although instanton theory cannot be applied directly to liquid systems, it can be used to compute the rate of gas-phase reactions and diffusion of atoms and molecules on surfaces very efficiently. It can also be used as a tool to understand how related path-integral rate theories describe tunnelling and has been instrumental in showing the deficiencies of centroid-based transition-state theory and in understanding the success of ring-polymer molecular dynamics [2]. Despite many successful applications, instanton theory has never before been obtained from first principles, relying instead on the "Im F" premise. I will outline a new rigorous derivation [3], based on a semiclassical approximation to path integrals in the classically forbidden region. The same approach can be used to derive a golden-rule instanton approach for nonadiabatic electron-transfer reactions [4, 5], and thus unifies the adiabatic (where the Born-Oppenheimer approximation is valid) and nonadiabatic limits of reaction rates into one theory. Some applications of the methods will be given and the relationship between instanton theory and ring-polymer molecular dynamics highlighted.

[1] William H. Miller. J. Chem. Phys. 62, 1899 (1975). [2] Jeremy O. Richardson and Stuart C. Althorpe. J. Chem. Phys. 131, 214106 (2009). [3] Jeremy O. Richardson. arXiv:1512.04292 [physics.chem-ph]. Under review by J. Chem. Phys. [4] Jeremy O. Richardson, Rainer Bauer, and Michael Thoss. J. Chem. Phys. 143, 134115 (2015); arXiv:1508.04919 [physics.chem-ph]. [5] Jeremy O. Richardson, J. Chem. Phys. 143, 134116 (2015); arXiv:1508.05195 [physics.chem-ph].

Conference program:

	Monday	Tuesday	Wednesday	Thursday	Friday
8:45-9:15	Registration				
9:15-9:30	Welcome				
9:30-10:00	Introduction to Imaginary-Time Path Integrals (Markland)	Accelerated Path Integral Techniques (Ceriotti)	Time Correlation Functions (Tuckerman)	Semiclassical Dynamics (Ananth)	Matsubara Dynamics (Althorpe)
10:00-10:30					
10:30-11:00			Contributed talk IV	Coffee Break	
11:00-11:30	Coffee Break			Non-Adiabatic Semiclassical Dynamics (Ananth)	Quantum Rate Theories and Instanton Methods (Vanicek)
11:30-12:00	Path Integral Estimators (Marsalek)	Advanced Path Integral Molecular Dynamics (Tuckerman)	Real Time Path Integrals - Introduction & Exact Methods (Makri)		
12:00-12:30				RPMD and CMD Approaches (Rossi)	Contributed V
12:30-13:00	Contributed Talk I	Contributed Talk II			Contributed VI
13:00-13:30	Lunch				Closing remarks
13:30-14:00					Lunch
14:00-14:30					
14:30-15:00	Practical I	Path integrals for indistinguishable particles (Brown)	Practical II	Practical III	
15:00-15:30					
15:30-16:00		Contributed Talk III			
16:00-16:30	Coffee Break				
16:30-17:00	Practical I	Ab Initio Path Integrals (Michaelides)	Practical II	Practical III	
17:00-17:30					
17:30-18:30	Q/A & Discussion		Q/A & Discussion	Q/A & Discussion	
Evening		Poster Session	Conference Dinner: Tribeca www.tribeca-lausanne.ch		

4. Set up of hands-on session

For three hands-on sessions that happened during the workshop, we decided to try a new setup in which each participant brought her/his own laptop and we distributed (personalized) USB-keys containing a fully functional VirtualBox Ubuntu/Linux image containing all the software necessary for the exercises. The participants only needed to install VirtualBox in their computers and start the system from the USB. Also, it was easy to take all the material they produced with them after the school was over. Even though the speed of the USB keys was not optimal at times, it was an overall successful experience, which received good feedback from the participants. We are keeping the Ubuntu/Linux image and all material used for the hands-on sessions in these links: https://www.dropbox.com/s/e7cqhpgkgt2rc5k/PI16-VBOX.zip?dl=0   and https://github.com/epfl-cosmo/pimd-tutorial.

The topics covered on the 3 hands-on session were:
1. Introduction to PIMD simulations
2. Advanced PIMD simulations
3. RPMD and CMD simulations

The software used was all open source, based on the interface of the i-PI (http://epfl-cosmo.github.io/gle4md/index.html?page=ipi) program with LAMMPS (http://lammps.sandia.gov/) and CP2K (https://www.cp2k.org/).

5. Q&A sessions at the event

Students were encouraged to interrupt during the lectures to ask questions whenever they occurred. However, to supplement this, we also set up three 1 hour Q&A sessions where the lecturers would answer questions written on pieces of papers anonymously by the students. This approach was found to be highly effective, since even though the students may have felt shy to ask questions and initiate discussions in front of the whole audience, while these submitted questions were being answered, a great deal of discussion was initiated. We also had good feedback from this format of discussion and the students participated in large numbers at all sessions.

6. Poster session and poster prizes

As mentioned above, the poster session was one of the highlights of the conference. The Journal of Chemical Physics provided 1000 USD sponsorship for poster prizes. Since all posters were of very high quality, and it was difficult to choose a single best or second best poster, we awarded a total of 1200 CHF that we split between a 1st prize group, and a 2nd prize group, consisting of 4 people each.

The participants in the group that were awarded the 1st prize (200 CHF each) were:

- Ashleigh BARNES, USA, University Of Tennessee
  "Evaluation of a perturbative treatment of three-body interactions in HCP He-4"
- Giovanni DI LIBERTO, Italy, Università degli Studi di Milano
  "Accurate and efficient prefactors for the semiclassical initial value representation propagator"
- Sinja KLEES, Germany, Ruhr-Universität Bochum
  "Towards Molecular Dynamics Simulations of Aqueous Electrolyte Solutions Employing Neural Network Potentials"
- Joe NAPOLI, USA, Stanford University
  "Nuclear Quantum Effects on the Structure and Dynamics of Concentrated Acid Solutions"

The participants in the group that were awarded the 2nd prize (100 CHF each) were:

- Joseph CENDAGORTA, USA, New York University
  "Competing Quantum Effects in the Rate of Hydrogen Diffusion in Type II Clathrate Hydrates"
- Christoph SCHRAN, Germany, Ruhr-Universität Bochum
  "Nuclear Quantum Effects on Charge Transfer in the Hydrogen Bond of Gas Phase Dimers and Liquid Water"
- Felix UHL, Germany, Ruhr-University Bochum
  "Accelerated Path Integral Methods for Molecular Systems at Ultra-low Temperatures"
- Jelle WIEME, Belgium, Center for Molecular Modeling
  "Investigating the heat capacity of metal-organic frameworks"

There were lively discussions and many participants were happy to stay until 10 p.m. discussing their posters. All posters presented and the corresponding abstracts can be found in the conference website https://www.cecam.org/workshop-3-1314.html.

7. Impressions from the participants

We received enthusiastic feedback from many of the participants, as well as suggestions for further improvements that we have incorporated in the discussion above. Some students also sent us some (unsolicited) e-mails to express their satisfaction, that we quote below.

Wei Fang
I want to thank you and all the organizers for the very successful workshop on path-integral. I had a wonderful time in Lausanne and enjoyed almost all the talks! I've got a lot of input from the extensive talks that covers from the basics and cutting-edge developments on the imaginary time PI, to real time dynamics with SC methods, to calculating reaction rates with PI approaches.

One week is just impossibly short to discuss all topics in the area, if the workshop was longer, I would like to know more about RPMD rate theory and it's applications to molecular systems. In general I wish more applications of the various theories could be discussed as I somehow got the impression that SC dynamics are not very good and non-adiabatic methods are only viable for simple models (which of course some people will disagree :P).

I also liked the exercise section and find it very helpful to me even I have used i-pi before. I think the idea of using a virtual machine worked really well (and free USB sticks? yes please!). And the toolbox you've made is very useful, I wish I had known it earlier.

Tim Wiles

I found the workshops very helpful, especially:

- The virtual machine

- The toolbox of scripts

- The memory sticks

The workshops were very guided but I believe this was the correct thing to do: It allows students to move onto the analysis more quickly.

Perhaps sample *outputs* could be included in the tutorial folder. This means students with slow machines who could not converge the calculations can still run the analysis.

Efram Braun

Thank you very much for putting on the CECAM course. I learned a lot during it, and I was thoroughly satisfied with the lectures and the lab exercises

Halua Pinto de Magalhães

Thank you for the school. I liked particularly the 3 last days, that were more oriented towards applications.

8. Full list of speakers and participants

1. Federica AGOSTINI, Germany, Max Planck Institute of Microst...
2. Chiara Donatella AIETA, Italy, Università degli Studi di Milano
3. Stuart ALTHORPE, United Kingdom, University of Cambridge
4. Nandini ANANTH, USA, Cornell University
5. Daniel J ARISMENDI ARRIETA, Spain, Institute of Fundamental Physics ...
6. Luigi BAGOLINI, Italy, CNR-IOM (Sissa)
7. Vincent BALLENEGGER, France, Université de Franche-Comté
8. Ashleigh BARNES, USA, University Of Tennessee
9. Nicole BELLONZI, USA, Chemistry Department, University of...
10. Raúl BOMBÍN ESCUDERO, Spain, Polytechnic University of Catalon...
11. Ethan BROWN, Switzerland, ETH Zurich
12. SUTIRTHA CHOWDHURYUSA, USA, University of Rochester
13. Matthew CHURCH, USA, Cornell University
14. Giovanni DI LIBERTO, Italy, Università degli Studi di Milano
15. Tahereh GHANE, Germany, Institute of Theoretical Physic...

16. Somayeh KHAZAEI, Germany, Martin Luther University of Hal...
17. Matthew KRZYSTYNIAK, United Kingdom, Rutherford Appleton Labo...
18. Xinyang LI, USA, University of Rochester
19. Lachlan LINDOY, United Kingdom, University of Oxford
20. Nancy MAKRI, USA, University of Illinois
21. Ondrej MARSALEK, USA, Stanford University
22. Franz Michel MARTINEZ RIOS, Canada, University of Alberta
23. Gerard MCCAUL, United Kingdom, King"s College
24. Rodrigo MENCHÓN, Argentina, Instituto de Física Rosario -...
25. Angelos MICHAELIDES, United Kingdom, University College London
26. Tobias MORAWIETZ, Austria, University of Vienna
27. Majid MORTAZAVI, Germany, Fritz Haber Institute of the Ma...
28. Joe NAPOLI, USA, Stanford University
29. Marco NAVA, Switzerland, ETH Zurich
30. Samuel NTIM, Italy, International Centre for Theoreti...
31. Sadrach PIERRE, USA, Cornell University
32. Igor POLTAVSKYI, Luxembourg, University of Luxembourg
33. Sandeep Kumar REDDY, France, student
34. Jeremy RICHARDSON, United Kingdom, Durham University
35. János SARKA, Hungary, Eötvös University
36. Edmund SIMPSON, United Kingdom, King"s college London
37. Karl-Mikael SVENSSON, Sweden, University of Gothenburg
38. Jiri VANICEK, Switzerland, Swiss Federal Institute of ...
39. Hendrik WIEBELER, Germany, Universität Paderborn
40. Jelle WIEME, Belgium, Center for Molecular Modeling, ...
41. Tim WILES, United Kingdom, Bristol University Schoo...
42. Monika WILLIAMS, USA, Stanford University
43. Robert ARBON, United Kingdom, University of Bristol
44. Emanuele BOATTINI, Italy, EPFL
45. Efrem BRAUN, USA, University of California, Berkeley
46. Joseph CENDAGORTA, USA, New York University
47. Bingqing CHENG, Switzerland, EPFL
48. Romain DUPUIS, Spain, Donostia International Physics Ce...
49. Wei FANG, United Kingdom, University College London
50. Leonid KAHLE, Switzerland, Swiss Federal Institute of ...
51. Venkat KAPIL, Switzerland, EPFL
52. Konstantin KARANDASHEV, Switzerland, Swiss Federal Institute of T...
53. Aaron KELLY   , Germany, Max Planck Institute for the St...
54. Sinja KLEES, Germany, Theoretical Chemistry, Universi...

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