

AMCOS

Conference and Tutorial on
Analysis and Modelling of Complex Oscillatory Systems

March 19-23, 2018
PRBB, Barcelona



Universitat
Pompeu Fabra
Barcelona



The electronic version of this booklet can be found at:
<https://amcosconference.com/>

The open-source \LaTeX template, AMCOS_booklet, used to generate this booklet is available at https://github.com/maximelucas/AMCOS_booklet

Contents

About	4
AMCOS	4
COSMOS	4
Organizing committee	4
Timetable	5
Tuesday, 20 of March	5
Wednesday, 21 of March	6
Thursday, 22 of March	7
List of Posters	12
Tuesday Session	12
List of Participants	13
Useful Information	14
How to get to the PRBB?	14
Partner Institutions and Sponsors	16
Sponsors	16

About

This is a generic version of the real AMCOS conference booklet for which this L^AT_EX template was generated. All information about the use and distribution of this template, and all related codes, can be found at https://github.com/maximelucas/AMCOS_booklet.

AMCOS

The conference on Analysis and Modeling of Complex Oscillatory Systems (AMCOS) aims to bring together theoretical and experimental researchers working on the state of the art in the field of complex oscillatory systems.

The main topics of the conference comprise both (a) the modeling of complex systems and the emergence of collective behavior, as well as (b) the analysis of complex data sets in order to infer the underlying structure and functionality of networks. Particular focus will be put on oscillatory phenomena in neuroscience.

COSMOS

The AMCOS Conference is organized by the Early Stage Researchers (ESRs) of the Marie Curie Initial Training Network led by Arkady Pikovsky of Potsdam University. COSMOS trains 15 ESRs at the interface between Physics, Applied Mathematics, and Life Sciences, integrating theoretical and data-driven methods, in 7 universities across Europe.

Organizing committee

Gloria Cecchini	Marco Faggian	Aleksandra Pidde
Rok Cestnik	R. Janis Goldschmidt	Bastian Pietras
Pau Clusella	Marc Grau Leguia	Eero Satuvuori
Nicolás Deschle	Maxime Lucas	Çağdaş Topçu
Federico Devalle	Irene Malvestio	Clément Zankoc

Timetable

CT: Contributed Talk, IS: Invited Speaker, KL: Keynote Lecture, IT: Invited Talk.

Tuesday, 20 of March

8:30–9:00	Registration		
9:00–9:10	Welcome remarks		
9:10–10:05	KL	Leon Tremblay Montreal, Canada	Title of a keynote lecture
10:05–10:30	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
10:30–11:00	Coffee		
11:00–11:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
11:40–12:45	CT	Marc Smith Brussels, Belgium	Title of contributed talk with math and paragraphs
12:45–14:00	Lunch		
14:00–14:30	CT	Marc Rodriguez Barcelona, Spain	Title of contributed talk with math and references
14:30–15:05	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
15:05–15:30	Coffee		
15:30–16:00	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
16:00–17:10	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
17:10–19:30	Poster session with Wine & Cheese		

Wednesday, 21 of March

9:00-9:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
9:40-10:10	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
10:10–12:45	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
10:45–11:10	Coffee		
11:10–11:40	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
11:40–12:10	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
12:10–12:45	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
12:45–14:00	Lunch		
14:00–14:30	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
14:30-15:00	CT	Marc Fournier Brussels, Belgium	Title of contributed talk
16:30–18:00	Excursion		
20:00	Conference Dinner		

Thursday, 22 of March

9:00 – 9:40	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
9:40–10:20	IS	Hiroya Sato Tokyo, Japan	Title of invited speaker
10:20–10:45	IT	Franck Schmidt Munich, Germany	A Special Talk about Diversity in Science
10:45–11:10	Coffee		
11:10-11:40	CT	Marc Jansen Amsterdam, The Netherlands	Title of contributed talk and references and a figure
11:40–12:35	KL	Leon Tremblay Montreal, Canada	Title of a keynote lecture
12:35–12:45	Poster Prize & Conclusion		
12:45–14:00	Lunch		

Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface

Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²

¹ Manisa Celal Bayar University Applied Research Center - Manisa, Turkey

² Manisa Celal Bayar University Department of Physics - Manisa, Turkey

³ Manisa Celal Bayar University Technical Sciences Vocational School - Manisa, Turkey

Computational dynamic emission spectroscopy in rigid medium solvents is a highly difficult technique. In recent years, technological improvement makes realistic models capable of experimental observables is possible. In this study, we have improved a successful simulation strategy in excitation and emission energies using hybrid models. The selected high layer target molecules and low and mobile layer water molecules are optimized with together. The hybrid QM/MM level is a powerful tool to efficiently is described the interactions of a molecule with its solvent medium. In this context, we simulate static and dynamic excited and emission spectra using COBRAMM interface protocol at the B3LYP/AMBER for rigid solvent models, TIP3P models are used within the mobile MM layer up to 50 nanometers radius away, for methyl derivatives of indole to a room-temperature. The QM/MM optimization calculations give us reliable structures both ground and excited states. Energy fluctuation of systems involves four states starting on the S0-S3, computations have been carried out by the same level for 150 femtoseconds. These calculated processes in ultrafast time scale have been explained how the evolution of excited and emission spectra when solvent molecules are movable. S0 and S1 geometry optimization of molecule in water droplet consisting of 500 TIP3P water are computed B3LYP/6-311++G(d,p) basis set and all low and mobile layer data was obtained Amber GAFF force field. S1 state geometry is converged approximately within 120 optimization cycles while the S0 optimization cycle takes longer time because of librational movements of water. Because this librational motion causes chaos at the RMS/D value, the number of mobile molecules has been reduced from the optimization steps. The energy difference between the first excited and ground state has a fluctuating character. The distribution of these fluctuations has been analyzed to create Fluctuating Gap Distribution (FGD) which reveals the most appropriate excitation/emission wavelengths.

Keywords

QM/MM md, Absorption and Emission, Lineer Response Theory

Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface

Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²

¹ Manisa Celal Bayar University Applied Research Center - Manisa, Turkey

² Manisa Celal Bayar University Department of Physics - Manisa, Turkey

³ Manisa Celal Bayar University Technical Sciences Vocational School - Manisa, Turkey

Computational dynamic emission spectroscopy in rigid medium solvents is a highly difficult technique. In recent years, technological improvement makes realistic models capable of experimental observables is possible. In this study, we have improved a successful simulation strategy in excitation and emission energies using hybrid models. The selected high layer target molecules and low and mobile layer water molecules are optimized with together. The hybrid QM/MM level is a powerful tool to efficiently is described the interactions of a molecule with its solvent medium. In this context, we simulate static and dynamic excited and emission spectra using COBRAMM interface protocol at the B3LYP/AMBER for rigid solvent models, TIP3P models are used within the mobile MM layer up to 50 nanometers radius away, for methyl derivatives of indole to a room-temperature. The QM/MM optimization calculations give us reliable structures both ground and excited states. Energy fluctuation of systems involves four states starting on the S0-S3, computations have been carried out by the same level for 150 femtoseconds. These calculated processes in ultrafast time scale have been explained how the evolution of excited and emission spectra when solvent molecules are movable. S0 and S1 geometry optimization of molecule in water droplet consisting of 500 TIP3P water are computed B3LYP/6-311++G(d,p) basis set and all low and mobile layer data was obtained Amber GAFF force field. S1 state geometry is converged approximately within 120 optimization cycles while the S0 optimization cycle takes longer time because of librational movements of water. Because this librational motion causes chaos at the RMS/D value, the number of mobile molecules has been reduced from the optimization steps. The energy difference between the first excited and ground state has a fluctuating character. The distribution of these fluctuations has been analyzed to create Fluctuating Gap Distribution (FGD) which reveals the most appropriate excitation/emission wavelengths.

Keywords

QM/MM md, Absorption and Emission, Lineer Response Theory

Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface

Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²

¹ Manisa Celal Bayar University Applied Research Center - Manisa, Turkey

² Manisa Celal Bayar University Department of Physics - Manisa, Turkey

³ Manisa Celal Bayar University Technical Sciences Vocational School - Manisa, Turkey

Computational dynamic emission spectroscopy in rigid medium solvents is a highly difficult technique. In recent years, technological improvement makes realistic models capable of experimental observables is possible. In this study, we have improved a successful simulation strategy in excitation and emission energies using hybrid models. The selected high layer target molecules and low and mobile layer water molecules are optimized with together. The hybrid QM/MM level is a powerful tool to efficiently is described the interactions of a molecule with its solvent medium. In this context, we simulate static and dynamic excited and emission spectra using COBRAMM interface protocol at the B3LYP/AMBER for rigid solvent models, TIP3P models are used within the mobile MM layer up to 50 nanometers radius away, for methyl derivatives of indole to a room-temperature. The QM/MM optimization calculations give us reliable structures both ground and excited states. Energy fluctuation of systems involves four states starting on the S0-S3, computations have been carried out by the same level for 150 femtoseconds. These calculated processes in ultrafast time scale have been explained how the evolution of excited and emission spectra when solvent molecules are movable. S0 and S1 geometry optimization of molecule in water droplet consisting of 500 TIP3P water are computed B3LYP/6-311++G(d,p) basis set and all low and mobile layer data was obtained Amber GAFF force field. S1 state geometry is converged approximately within 120 optimization cycles while the S0 optimization cycle takes longer time because of librational movements of water. Because this librational motion causes chaos at the RMS/D value, the number of mobile molecules has been reduced from the optimization steps. The energy difference between the first excited and ground state has a fluctuating character. The distribution of these fluctuations has been analyzed to create Fluctuating Gap Distribution (FGD) which reveals the most appropriate excitation/emission wavelengths.

Keywords

QM/MM md, Absorption and Emission, Lineer Response Theory

Static and Dynamic Modeling of N-Methyl-Indole (N=1-6) in Water at the B3LYP/AMBER Level Using the COBRAMM Interface

Caglar KARACA¹, Fehmi BARDAK², Etem KOSE³, Ahmet ATAC²

¹ Manisa Celal Bayar University Applied Research Center - Manisa, Turkey

² Manisa Celal Bayar University Department of Physics - Manisa, Turkey

³ Manisa Celal Bayar University Technical Sciences Vocational School - Manisa, Turkey

Computational dynamic emission spectroscopy in rigid medium solvents is a highly difficult technique. In recent years, technological improvement makes realistic models capable of experimental observables is possible. In this study, we have improved a successful simulation strategy in excitation and emission energies using hybrid models. The selected high layer target molecules and low and mobile layer water molecules are optimized with together. The hybrid QM/MM level is a powerful tool to efficiently is described the interactions of a molecule with its solvent medium. In this context, we simulate static and dynamic excited and emission spectra using COBRAMM interface protocol at the B3LYP/AMBER for rigid solvent models, TIP3P models are used within the mobile MM layer up to 50 nanometers radius away, for methyl derivatives of indole to a room-temperature. The QM/MM optimization calculations give us reliable structures both ground and excited states. Energy fluctuation of systems involves four states starting on the S0-S3, computations have been carried out by the same level for 150 femtoseconds. These calculated processes in ultrafast time scale have been explained how the evolution of excited and emission spectra when solvent molecules are movable. S0 and S1 geometry optimization of molecule in water droplet consisting of 500 TIP3P water are computed B3LYP/6-311++G(d,p) basis set and all low and mobile layer data was obtained Amber GAFF force field. S1 state geometry is converged approximately within 120 optimization cycles while the S0 optimization cycle takes longer time because of librational movements of water. Because this librational motion causes chaos at the RMS/D value, the number of mobile molecules has been reduced from the optimization steps. The energy difference between the first excited and ground state has a fluctuating character. The distribution of these fluctuations has been analyzed to create Fluctuating Gap Distribution (FGD) which reveals the most appropriate excitation/emission wavelengths.

Keywords

QM/MM md, Absorption and Emission, Lineer Response Theory

List of Posters

Tuesday Session

List of Participants

John1 Doe1	Barcelona, Spain
John2 Doe2	Barcelona, Spain
John3 Doe3	Barcelona, Spain
John4 Doe4	Barcelona, Spain
John5 Doe5	Barcelona, Spain
John6 Doe6	Barcelona, Spain
John7 Doe7	Barcelona, Spain
John8 Doe8	Barcelona, Spain
John9 Doe9	Barcelona, Spain
John10 Doe10	Barcelona, Spain
John11 Doe11	Barcelona, Spain
John12 Doe12	Barcelona, Spain
John13 Doe13	Barcelona, Spain
John14 Doe14	Barcelona, Spain
John15 Doe15	Barcelona, Spain
John16 Doe16	Barcelona, Spain
John17 Doe17	Barcelona, Spain
John18 Doe18	Barcelona, Spain
John19 Doe19	Barcelona, Spain
John20 Doe20	Barcelona, Spain
John21 Doe21	Barcelona, Spain
John22 Doe22	Barcelona, Spain
John23 Doe23	Barcelona, Spain
John24 Doe24	Barcelona, Spain
John25 Doe25	Barcelona, Spain
John26 Doe26	Barcelona, Spain
John27 Doe27	Barcelona, Spain
John28 Doe28	Barcelona, Spain
John29 Doe29	Barcelona, Spain

Useful Information

Talks will be held at the **Conference Hall-Auditorium** of PRBB. It is situated on the first floor of the central courtyard and has independent access from the rest of the building (through stairs located at the ground floor, main entrance of PRBB).

Coffee breaks and lunches will be offered in the half-covered terrace in front of the main entrance of the conference hall.

The **poster session** will be held on Tuesday and Wednesday night on the **ground floor** of the PRBB.

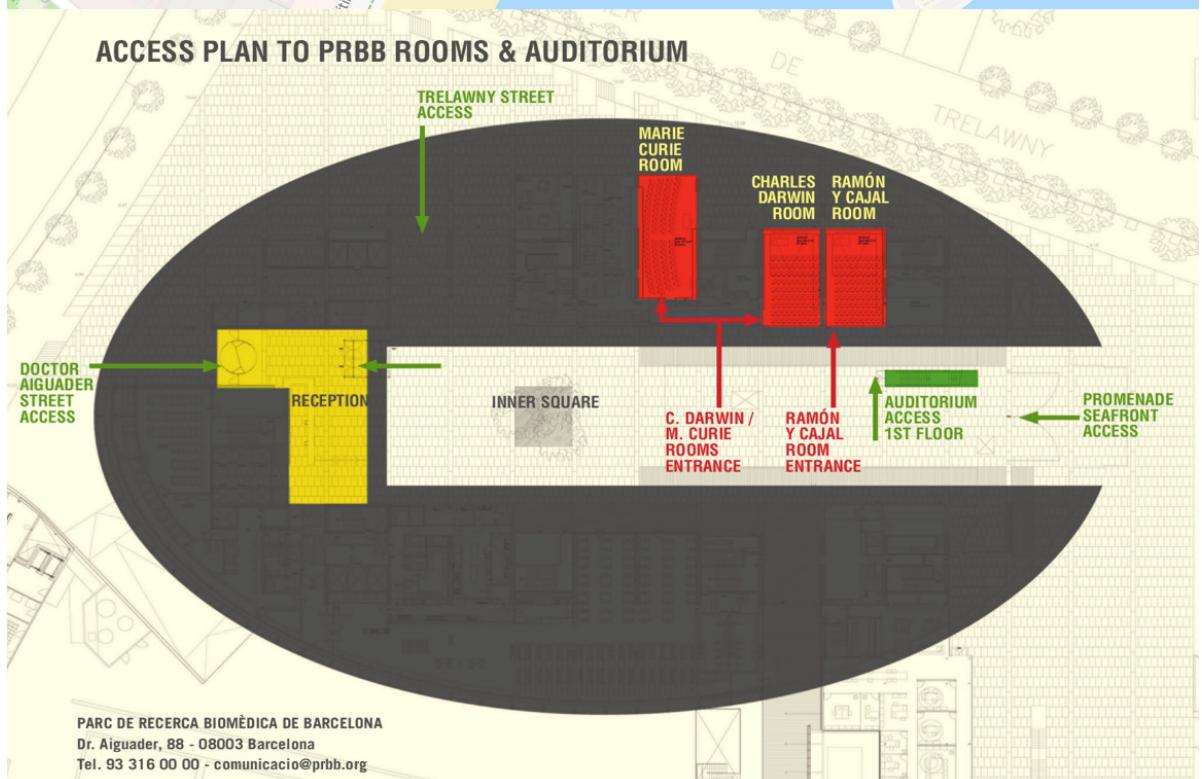
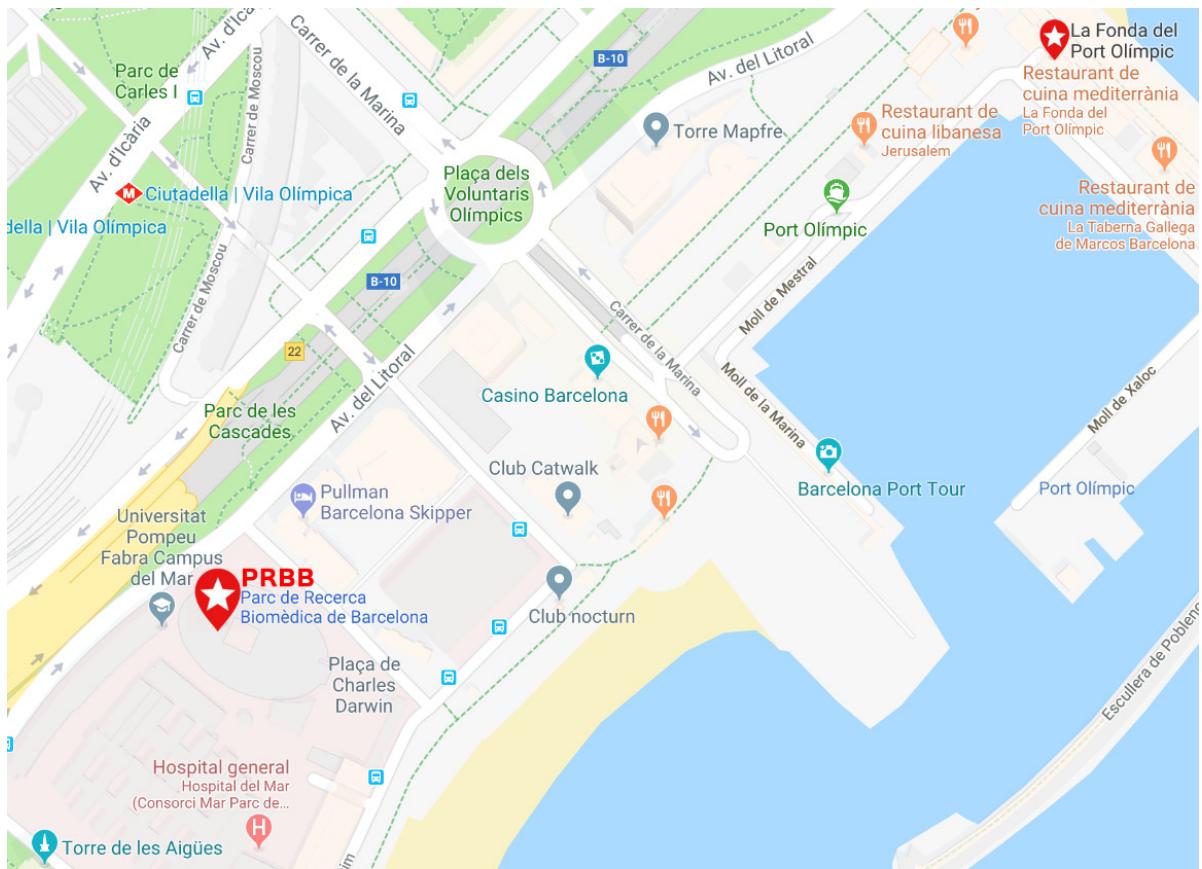
Wi-Fi will be available during the conference. The PRBB also provides access to an eduroam network.

The **conference dinner** will be held at the "The best restaurant", at Some Street, 39, Barcelona.

How to get to the PRBB?

The PRBB building overlooks the Ronda del Litoral and is next to the twin towers of the Olympic Village: Torre Mapfre and Arts Hotel. The address is Carrer del Dr. Aiguader, 88, 08003 Barcelona, Spain. and can be reached by:

- **Subway:** yellow line, L4, station Ciutadella/Vila Olímpica,
- **Bus:** lines V21, 14, 36, 41, 45, 59, 71, 92, D20,
- **Tram:** line 4, stop Vila Olímpica.



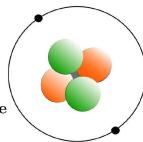
Partner Institutions and Sponsors

The AMCOS conference is part of the COSMOS project, funded by the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 642563.

Sponsors

Lancaster Helium Ltd

Purveyors of Isotopically Purified ${}^4\text{He}$



images/logos/Partnerlogos/springer.pdf

