

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

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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.

References

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

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References

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 |
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| 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.

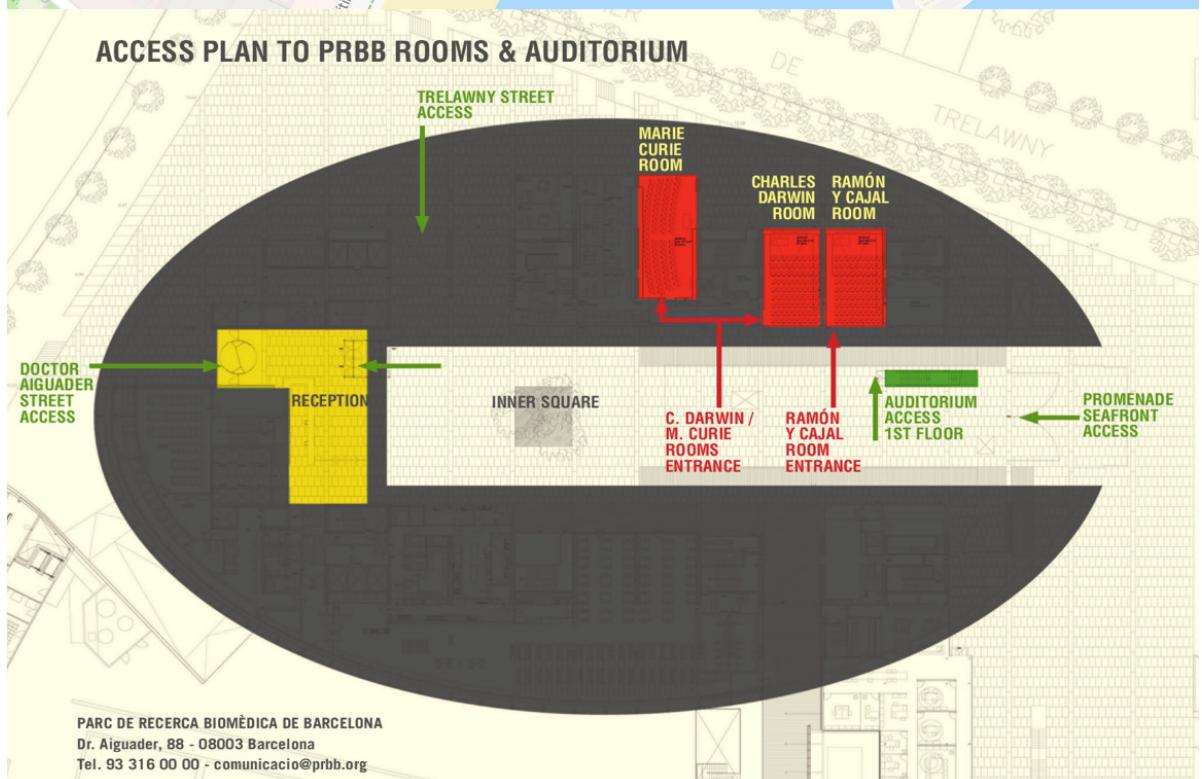
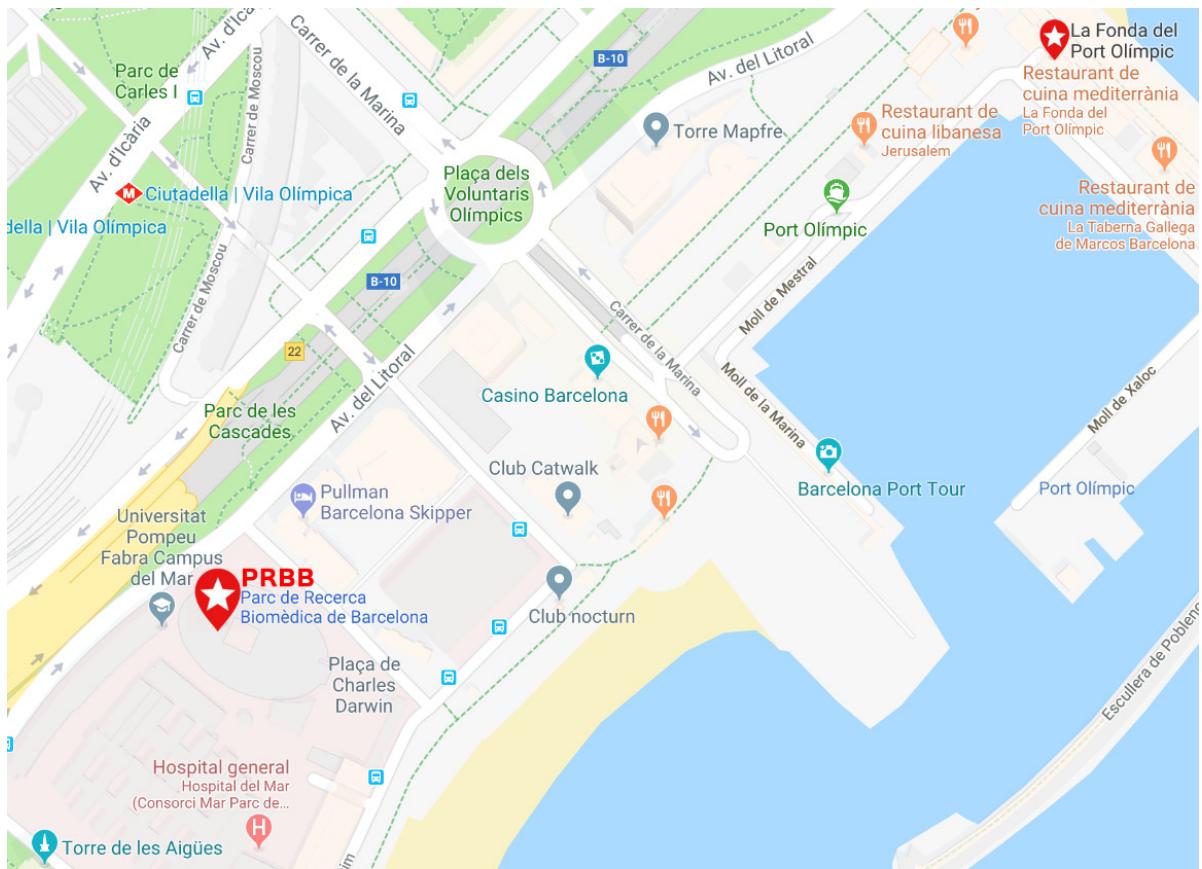
Wi-Fi will be available during the conference. The PRBB also provides access to an eduroam network.

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.



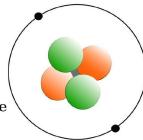
Partner Institutions and Sponsors

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.

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