

# CECAM (Centre Européen de Calcul Atomique et Moléculaire) Activities' Report - Year 2017

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## 1. Introduction

CECAM (European Center for Calculating Atomics and Molecules, <http://www.cecaml.org/>) is a European organization that promotes frontier research in the computational sciences. The focus of CECAM are atomistic and molecular simulations applied to the physics and chemistry of condensed matter, to materials science and to biological and medical chemistry. CECAM is organized in a district headquarters (EPFL) in Lausanne, Switzerland, and has 18 nodes across the various participating countries. Below is a list of nodes with the countries of affiliation:

- [CECAM-AT](#)
- [CECAM-FI](#)
- [CECAM-FR-MOSER](#)
- [CECAM-FR-RA](#)
- [CECAM-FR-GSO](#)
- [CECAM-DE-MM1P](#)
- [CECAM-DE-JUELICH](#)
- [CECAM-DE-MMS](#)
- [CECAM-DE-SMSM](#)
- [CECAM-IRL](#)
- [CECAM-ISR](#)
- [CECAM-IT-SIDE](#)
- [CECAM-IT-SMART](#)
- [CECAM-IT-SIMUL](#)
- [CECAM-NL](#)
- [CECAM-ES](#)
- [CECAM-UK-HARTREE](#)
- [CECAM-UK-JCMAXWELL](#)

The italian nodes are: SIMUL - Istituto Italiano di Tecnologia (IIT), SMART - Scuola Normale Superiore (SNS) and SIDE - Scuola Internazionale Superiore di Studi Avanzati (SISSA).

## 2. Main activities carried on by CECAM during 2017 relevant for Italy and for CNR

Italy participates in the CECAM Council with four Institutions, CNR and the three node-related Institutions IIT, SNS and SISSA. Italy is in fact the country with the largest number of Institutions in the CECAM Council. During the year 2017 a fifth Italian Institution, the University of Bologna and CINECA, has joined CECAM.

The activities of CECAM are carried out through the scientific actions of the nodes and through the organization of international workshops, schools and conferences. CECAM provides an average support of €12,000 per event, as well as logistical and organizational support (secretarial, Web pages, contact management, hotel booking, etc.).

In 2017 50 workshops were organized, 6 of these events were organized by CNR researchers on a total of 9 events organized by Italian Institutions (see Appendix A).

For the year 2017, out of the many organized workshops, 3 have been organized by CNR staff. There are also numerous CNR researchers among the invited speakers and participants in CECAM initiatives.

In 2017, 3 Schools were organized by CNR researchers and 1 Conference, Appendix A.

### **3. Activities carried out within the Union during 2017 and impact on the Italian scientific community**

During 2017 I have attended as CNR representative the general CECAM Council Meetings, held at the headquarters in Lausanne in November, 2017.

In the meeting we discussed the financial lines for 2018-2019 and the activities carried out in 2017 were evaluated. From 2017 onwards CNR pays a 30,000 Euros fee, homogenizing the fee to that of the other institutions, with considerable savings for the CNR. This reduction has no impact on CNR's activities and presence.

The call for workshop proposals for the year 2019 is currently open, <http://www.cecama.org/submitting.html>. To encourage the widest possible participation by CNR staff, several messages have been sent to the scientific community, providing information and supporting the proposals.

### **4. Evaluation of the participation in terms of benefits and membership cost**

The CNR presence in CECAM is important to maintaining and strengthening Italy's weight in the European computational community, which in fact is largely identified in CECAM as its main organization and representative body. From a cost/benefit point of view, the amount of funds raised for workshop, conference and school organization substantially exceeds the annual paid fee. It is therefore obvious that the economic benefits from access to funds are clearly in favor of CNR and of Italian researchers. By supporting CECAM, CNR has the opportunity to further strengthen its weight in scientific calculations and simulations, launching initiatives in areas of interest between physics, materials science and chemistry as well as biological and medical chemistry. These activities are widely recognized at the European level and many call for proposals in the H2020 program are inherent to computational science, modeling and simulation. Recently CECAM coordinated the presentation of European initiatives that attracted considerable funding, such as the E-CAM project. This project, funded by H2020, aims to create an electronic infrastructure (e-infrastructure) dedicated to software development, training and consulting in modeling and simulation. CNR's participation at CECAM can also be an opportunity to access to European funding otherwise difficult to access to the single researcher operating in modeling and simulation.

### **5. Evaluation of Italians' attendance and how to improve interest and involvement**

I personally consider very important to highlight the opportunity of workshop organization by linking the call for proposals in the CNR Departments websites and in the Institutional website. In 2017 there have been 7 events organized by CNR staff and a significant attendance of Italian researchers, see Appendix A.

### **6. Italian experts with important roles within the Union or within related Commissions and Programs (if known)**

The deputy director of CECAM is Dr. Sara Bonella, Università di Roma La Sapienza.

The president of CECAM is Prof. Alessandro Laio, SISSA and CNR-DEMOCRITOS.

The past president of CECAM is Prof. Christophe Dellago, University of Vienna, Austria.

### **7. If Union with CNR Commission, short summary about the 2017 CNR Commission activities**

N/A

### **8. Notes (if any)**

N/A

## 9. Conclusions

CECAM is set up as European reference in modeling and computational simulation activities, recognized in major H2020 calls as a center for scientific and technological development. The CNR's participation to CECAM is strategic as it allows our staff to be represented at the decision-making venue and to have access to funding for organizing workshops. With the entry of a new Italian partner, Italy is the country with the largest number of member institutions, thus being able to pursue a positive synergy for the Italian research system. I fully supports the continuation of CNR's participation in CECAM.

Signature

A handwritten signature in blue ink, appearing to be 'G. U. J.', written in a cursive style.

Perugia, 15/05/2018

## Appendix A

### Participation of Italian researchers to CECAM activities in 2017 (highlighted are those activities organized by CNR staff)

#### Conferences 2017

##### 1) Ab initio Spin-orbitronics

Location : The conference will take place at Hotel Promenade in Montesilvano, Pescara (Italy)  
*September 25, 2017 - September 29, 2017*

- Silvia Picozzi  
Consiglio Nazionale delle Ricerche CNR-SPIN, Chieti, Italy
- Stefan Blügel  
Forschungszentrum Jülich, Germany
- Ingrid Mertig  
Martin Luther University Halle, Germany

#### Workshops 2017

##### 1) Recent Advances on the Glass and Jamming Transitions

Location : CECAM-HQ-EPFL, Lausanne, Switzerland  
*January 9, 2017 - January 11, 2017*

- Patrick Charbonneau  
Department of Chemistry, Duke University , USA
- Ludovic Berthier  
Laboratoire Charles Coulomb UMR 5221 CNRS - Université de Montpellier, France
- Francesco Zamponi  
LPT, ENS Paris, France

##### 2) 2nd NOMAD (Novel Materials Discovery) Industry Workshop

Location : Hamburg  
*February 6, 2017 - February 7, 2017*

- Alessandro De Vita  
King's College London and University of Trieste, United Kingdom
- Matthias Scheffler  
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany
- Angel Rubio  
Max Planck Institute for the Structure and Dynamics of Matter, Germany

##### 3) Challenges across Large-Scale Biomolecular and Polymer Simulations

Location : CECAM-AT  
*February 21, 2017 - February 24, 2017*

- Ivan Coluzza  
Center for Cooperative Research in Biomaterials, Spain
- Samuela Pasquali  
Paris Descartes University, France
- Barbara Capone  
Università degli Studi Roma Tre, Italy
- Christoph Dellago  
University of Vienna, Austria
- Tamar Schlick  
New York University, USA

##### 4) Ion Transport from Physics to Physiology: the Missing Rungs in the Ladder

Location : CECAM-HQ-EPFL, Lausanne, Switzerland  
*April 3, 2017 - April 5, 2017*

- Lucie Delemotte  
KTH Science for Life Laboratory, Sweden
- Vincenzo Carnevale  
Temple University - Philadelphia, USA
- Rebecca Howard  
Stockholm University, Sweden
- Ute Hellmich  
Johannes Gutenberg-Universität Mainz , Germany
- Brad Rothberg  
Temple University School of Medicine, USA

### **5) Recent advances in numerical methods for micro and macro models in fluid dynamics**

Location : CECAM-IT-SIMUL

*April 5, 2017 - April 7, 2017*

- Maurizio Falcone  
Università di Roma "La Sapienza", Italy
- Giovanni Ciccotti  
University of Rome La Sapienza, Italy
- Simona Perotto  
Politecnico di Milano, Italy
- Gianluigi Rozza  
SISSA, Trieste, Italy

### **6) Cell and tissue motility**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*May 3, 2017 - May 5, 2017*

- Luca Giomi  
Lorentz Institute, Netherlands, The Netherlands
- Julia Yeomans  
Oxford University, United Kingdom
- Benoit Ladoux  
CNRS and Paris Diderot University, France

### **7) Theoretical Chemistry for Extended Systems: systematically improvable electronic structure methods**

Location : CECAM-FR-GSO

*May 22, 2017 - May 24, 2017*

- Arjan Berger  
University Paul Sabatier, France
- Michel Caffarel  
University Paul Sabatier, Toulouse, France
- Thierry Leininger  
Laboratoire de Chimie et Physique Quantiques UMR5626 CNRS Université Toulouse 3, France
- Dirk Andrae  
Physikalische und Theoretische Chemie - Institut für Chemie und Biochemie - Freie Universität Berlin, Germany
- Stefano Evangelisti  
Universite Paul Sabatier, France

### **8) Green's function methods: the next generation III**

Location : CECAM-FR-GSO

*June 6, 2017 - June 9, 2017*

- Pina Romaniello  
University Paul Sabatier, France
- Arjan Berger  
University Paul Sabatier, France
- Francesco Sottile  
Ecole Polytechnique, Palaiseau, France

### **9) The future of biomembrane simulations: hidden pitfalls and future challenges**

Location : CECAM-FR-RA

*June 6, 2017 - June 9, 2017*

- Markus Deserno  
Carnegie Mellon University, Pittsburgh, PA, USA
- Claire Loison  
Institut Lumière Matière, France
- Luca Monticelli  
CNRS, University of Lyon, France
- Stefano Vanni  
University of Fribourg, Switzerland

### **10) Seeking synergy between dynamics and statistics for non-equilibrium quantum processes**

Location : ENS Paris

*June 6, 2017 - June 9, 2017*

- Federica Agostini  
Université Paris-Sud, Laboratoire de Chimie Physique, France
- David Coker  
Boston University, USA
- David Lauvergnat  
Université Paris-Sud, Laboratoire de Chimie Physique, France
- Aaron Kelly  
Dalhousie University, Canada

### **11) Bridging the worlds of electromagnetic and quantum simulations**

Location : CECAM-ISR

*June 20, 2017 - June 23, 2017*

- Amir Boag  
Tel Aviv University, Israel
- Vitaliy Lomakin  
University of California, San Diego, USA
- Stefano Maci  
University of Siena, Italy
- Shanker Balasubramaniam  
Michigan State University, USA
- Oded Hod  
Tel Aviv University, Israel
- Amir Natan  
Tel Aviv University, Israel

### **12) Rheology of gel networks: combining experimental, computational and theoretical insights**

Location : CECAM-FR-RA, CBP in Lyon, France

*June 21, 2017 - June 23, 2017*

- Kirsten Martens  
LIPhy, University Grenoble Alpes & CNRS, France
- Emanuela Del Gado  
Georgetown University, USA
- Sebastien Manneville  
ENS Lyon, France
- Veronique Trappe  
University of Fribourg, Switzerland
- Beatrice Ruta  
University Lyon 1 & CNRS, France

### **13) Challenges in reaction dynamics of gas-surface interactions and methodological advances in dissipative and non-adiabatic processes**

Location : CECAM-FR-GSO  
*June 26, 2017 - June 29, 2017*

- Fernand SPIEGELMAN  
LCPQ/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France
- Didier LEMOINE  
LCAR/IRSAMC, CNRS and Université Toulouse III Paul Sabatier, France
- Bret JACKSON  
Department of Chemistry, University of Massachusetts, Amherst, USA
- Rocco MARTINAZZO  
Department of Chemistry, University of Milan, Italy

#### **14) Electronic Structure Library coding workshop: drivers**

Location : CECAM-IT-SIDE  
*July 10, 2017 - July 21, 2017*

- Stefano de Gironcoli  
International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy
- Ivan Girotto  
International Center for theoretical Physics, Italy
- Fabiano Corsetti  
Synopsys QuantumWise, Denmark

#### **15) ESDW6: Classical MD**

Location : CECAM-NL  
*August 14, 2017 - August 25, 2017*

- Peter Bolhuis  
University of Amsterdam, The Netherlands
- Christoph Dellago  
University of Vienna, Austria
- David Swenson  
Universiteit van Amsterdam, The Netherlands

#### **16) Synergy between quantum computing and high-performance computing**

Location : CECAM-ETHZ, Zurich, Switzerland  
*August 22, 2017 - August 24, 2017*

- Rosa Di Felice  
CNR Institute of Nanoscience, Modena, Italy
- Elisa Molinari  
University of Modena and Reggio Emilia & CNR-NANO, Modena, Italy
- Sara Bonella  
CECAM@EPFL, Switzerland
- Ivano Tavernelli  
IBM-Zurich Research, Switzerland
- Daniel Lidar  
USC, USA
- Seth Lloyd  
Massachusetts Institute of Technology, USA
- Matthias Troyer  
Swiss Federal Institute of Technology Zurich (ETHZ), Switzerland

#### **17) Addressing metastability in interfacial phenomena across multiple time and length scales**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland  
*August 29, 2017 - September 1, 2017*

- Simone Meloni  
Sapienza University of Rome, Italy
- Alberto Giacomello  
Sapienza University of Rome, Italy

- Halim Kusumaatmaja  
Durham University, United Kingdom

### 18) Big-Data driven Materials Science

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

*September 11, 2017 - September 13, 2017*

- Luca M. Ghiringhelli  
Fritz Haber Institute of the Max Planck Society (FHI), Berlin , Germany
- Matthias Scheffler  
Fritz Haber Institute of the Max Planck Society (FHI), Berlin, Germany

### 19) Multiscale modelling of organic semiconductors: from elementary processes to devices

Location : IMAG building, University Grenoble Alpes (see <https://batiment.imag.fr/en/contact-addresses-access>)

*September 12, 2017 - September 15, 2017*

- Thierry Deutsch  
French Alternative Energies and Atomic Energy Commission (CEA), Grenoble, France
- Denis Andrienko  
Max Planck Institute for Polymer Research, Germany
- Xavier Blase  
Institut Néel, CNRS, Grenoble, France
- Alison B. Walker  
University of Bath, United Kingdom
- Francesco Mercuri  
CNR-ISMN, Italy
- Peter Bobbert  
TU Eindhoven, The Netherlands, The Netherlands
- Wolfgang Wenzel  
Karlsruhe Institute of Technology (Germany), Germany

### 20) ESDW8: Meso- and Multiscale Modelling

Location : CECAM-DE-MMS

*September 18, 2017 - September 29, 2017*

- Carsten Hartmann  
BTU Cottbus-Senftenberg, Germany
- Luigi Delle Site  
Institute for Mathematics, FU Berlin, Germany
- Christian Krekeler  
Freie Universität Berlin, Germany

### 21) Disordered protein segments: revisiting the structure-function paradigm

Location : CECAM-FR-MOSER, Institut Henri Poincaré, Paris, France.

*October 3, 2017 - October 6, 2017*

- Sophie Sacquin-Mora  
Laboratoire de Biochimie Théorique, CNRS-UPR9080, France
- Birthe Kragelund  
University of Copenhagen, Denmark
- Ben Schuler  
University of Zurich, Switzerland
- Elena Papaleo  
Danish Cancer Research Center, Denmark
- Chantal Prevost  
Laboratoire de Biochimie Théorique LBT - CNRS UPR 9080, France
- Tâp Ha-Duong  
BioCIS - Faculté de Pharmacie - Université Paris Sud, France

### 22) Insights into skin permeation: from theory to practice



Location : CECAM-HQ-EPFL, Lausanne, Switzerland  
*October 16, 2017 - October 18, 2017*

- Chinmay Das  
University of Leeds, United Kingdom
- Massimo Noro  
Unilever, United Kingdom
- Anna Akinshina  
University of Salford, United Kingdom

### **23) Computational approaches to investigating allostery**

Location : CECAM-HQ-EPFL, Lausanne, Switzerland  
*October 30, 2017 - November 1, 2017*

- Emanuele Paci  
University of Leeds, United Kingdom
- Shoshana Wodak  
VIB, Brussels and University of Toronto, Belgium
- Nikolay Dokholyan  
University of North Carolina, Chapel Hill, USA

### **24) Superconductivity in atomically thin materials and heterostructures**

Location : CECAM-Lugano, Lugano, Switzerland  
*November 20, 2017 - November 23, 2017*

- Milorad Milosevic  
Universiteit Antwerpen, Belgium
- Dimitri Roditchev  
Institut des Nanosciences de Paris, Université Paris, France
- Andrea Perali  
University of Camerino, Italy

### **25) Physics and Chemistry at Fluid/Fluid Interfaces**

Location : CECAM-AT  
*December 11, 2017 - December 13, 2017*

- Marcello Sega  
University of Vienna, Austria
- Pal Jedlovsky  
Eszterházy Károly University, Eger, Hungary, Hungary

## **Schools 2017**

### **1) Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO**

Location : The Abdus Salam, International Centre for Theoretical Physics (ICTP)  
*January 16, 2017 - January 28, 2017*

- Stefano Baroni  
International School for Advanced Studies (SISSA), Trieste, Italy
- Nicola Marzari  
Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland
- Paolo Giannozzi  
University of Udine, Italy
- Andrea Ferretti  
CNR-Institute of Nanoscience, Modena, Italy
- Stefano de Gironcoli  
International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy
- Ivan Girotto  
International Center for theoretical Physics, Italy
- Matteo Cococcioni

Swiss Federal Institute of Technology Lausanne, Switzerland

## 2) Basic techniques and tools for development and maintenance of atomic-scale software

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

March 27, 2017 - March 31, 2017

- Francesco Sottile  
Ecole Polytechnique, Palaiseau, France
- Micael Oliveira  
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Yann Pouillon  
Materials Evolution, Spain
- Damien Caliste  
Alternative Energies and Atomic Energy Commission (CEA), France
- Matthieu Verstraete  
University of Liege, Belgium

## 3) Advanced computing of excited state properties in solids and nanostructures with Yambo

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

April 24, 2017 - April 28, 2017

- Myrta Gruning  
Queen's University Belfast, United Kingdom
- Conor Hogan  
CNR-ISM, Rome and University of Rome Tor Vergata, Italy
- Andrea Marini  
CNR-ISM, Italy
- Alejandro Molina-Sánchez  
University of Valencia, Spain
- Daniele Varsano  
S3, CNR Istituto di Nanoscienze, Italy

## 4) Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond

Location : CECAM-HQ-EPFL, Lausanne, Switzerland

May 15, 2017 - May 19, 2017

- Carme Rovira  
University of Barcelona, Spain
- Mauro Boero  
University of Strasbourg and CNRS - IPCMS, France
- Ari Paavo Seitsonen  
Ecole Normale Supérieure, France
- Ursula Roethlisberger  
Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland

## 5) Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics

Location : CECAM-IT-SIDE

June 14, 2017 - June 30, 2017

- Stefano de Gironcoli  
International School for Advanced Studies (SISSA) and CNR-DEMOCRITOS IOM, Trieste, Italy
- Andrea Dal Corso  
International School for Scientific Studies (SISSA) and CNR-IOM-DEMOCRITOS, Trieste, Italy
- Alessandra Magistrato  
CNR-IOM@SISSA, Italy

## 6) Liquid Crystal Modelling and Simulation: A Comprehensive Introduction

Location : Ettore Majorana Centre, Erice (TP)

July 14, 2017 - July 18, 2017

- Antonio DiCarlo  
CECAM-IT-SIMUL Node, Italy
- Claudio Zannoni  
Universita' di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Italy
- Paolo Biscari  
Politecnico di Milano, Italy
- Paolo Pasini  
INFN - Istituto Nazionale di Fisica Nucleare, Italy

## **7) Hands-on Tutorial on CFD using Code\_Saturne**

Location : CECAM-DE-JUELICH

*October 4, 2017 - October 6, 2017*

- Charles Moulinec  
STFC Daresbury Laboratory, United Kingdom
- Juan Uribe  
EDF R&D UK Research Centre, United Kingdom
- Stefano Rolfo  
STFC Daresbury Laboratory, United Kingdom