

# Curriculum Vitae of Giovanni Ciccotti

Updated 08 June 2020



## Principal Research Activities

The focus of my research activity is on developing algorithms for Molecular Dynamics simulation of complex systems in condensed phases. From the, from now ancient, SHAKE algorithm (a procedure to introduce holonomic constraints in MD) or the Subtraction Technique (a noise reducing approach to compute the response to weak external fields in Nonequilibrium MD) to the introduction of the Blue Moon's ensemble (to simulate in MD rare events) and techniques to simulate Brownian motion to the most recent, and still very active, field of rigorous algorithms to compute nonadiabatic quantum-classical dynamics, the attempt is to widen the domain of computer simulation in condensed matter with a particular emphasis on MD (as distinguished from the very close but different MC - Monte Carlo). Together with that, I have been, and still am, also interested in challenging applications of atomistic MD simulations ranging from surface/interface physics problems in Materials sciences to simulations of biological molecules to find atomistic level explanations of their behavior or functioning mechanisms. More generally, I am interested in considering a variety of developments/applications in the simulation of systems of Statistical Mechanics interest.

## Education

*Laurea in Physics cum laude*, University of Roma “La Sapienza”, 1967.

## Fellowships, Named Lectures and Honors

- Visiting Professor at EPFLausanne, at times January – July 2017
- Researcher Associated to IAC « Mauro Picone », Istituto di Applicazioni del Calcolo, CNR, April 2016 - present
- Guest Scientist at Dept of Mathematics & Computer Science, Free University of Berlin, July 2015 – January 2016

- Emeritus Professor at « La Sapienza » from December 2015
- Emeritus Professor at UCD from December 2013
- European Physical Society Fellow from 2013
- Professor of Physics and PI of SFI, on leave from “La Sapienza” in 2010, School of Physics, University College of Dublin, from September 2009 to August 2013.
- "Professeur Associé" at Université de Paris VI on April 2008.
- MIT Visiting scientist to National University of Singapore, February 2007.
- Academic Professor to Accademia dei Lincei (Professore Linceo), 2005-2008.
- "Professeur Associé" at Université de Paris VI on September 2005.
- "Professeur Associé" at Université de Paris VI on September 2004.
- Fellow of the Institute of Physics (from 2004).
- Visiting researcher associated to CNRS, Vitry, France, from October 2003 to January 2004 and from July to August 2004.
- "Professeur Associé" at Université de Paris VI on September 2002.
- Schlumberger Lecture, University of Cambridge, 2000.
- Schlumberger Professor in Chemistry Department and Visiting Fellow of Corpus Christi College at University of Cambridge, UK, in the academic year 1999-2000.
- Recipient of the Berni J. Alder CECAM Prize in 1999.
- "Professeur Associé" at Université de Paris VI on October 1998.
- Visiting Professor at Dept. of Chemistry, Univ of Colorado at Boulder, from October to November 1987 and from October to December 1988.
- Visiting Professor at Dept. of Chemistry, Univ of Toronto, Canada, from December 1987 to July 1988.
- Visiting Researcher, on leave of absence from Roma, at the "Section de Recherches en Métallurgie Physique" of CEA, Saclay in the academic year 1986-1987.
- "Professeur Associé" at Université de Paris VI from October to December 1984.
- Visiting on leave of absence from Roma the "Section de Recherches en Metallurgie Physique" of CEA, Saclay, in the academic year 1981-1982.
- Visiting CECAM (Centre Européen de Calcul Atomique et Moléculaire), Orsay, from March 1974 to August 1975, and many times to present.
- CNR Fellowship in the High Energy Theoretical Group of Rome 1 Physics Departement from June 1968 to November 1971.

## **Employments**

- Professore ordinario of Structure of Matter, Dept of Physics, University of Roma "La Sapienza", (1990 to 2014 )
- Professore associato of Molecular Physics, Dept of Physics, University of Roma "La Sapienza", (1980 to 1990)
- Professore incaricato of Molecular Physics, Dept of Physics, University of Roma "La Sapienza", (1977 to 1980)
- Professore incaricato of Statistics, Dept of Genetics, University of Roma "La Sapienza", (1974 to 1980)
- Professore incaricato of Mathematical Statistics, Dept of Mathematics, University of Camerino, (1973 to 1978)
- Professore incaricato of History of Physics, Dept of Physics, University of Lecce, (1971 to 1973)

## **Teaching and Departmental/University duties**

- 1971 - 1973 course in History of Physics (University of Lecce, master level)
- 1973 - 1977 course in Mathematical Statistics (University of Camerino, master level)
- 1974 - 1981 course in Statistics for biologists (master level)

- 1977- 1994 course in Molecular Physics (master level)
- 1994 - 2005 course in Structure of Matter (master level)
- 2008 - 2014 course in Quantum Mechanics (undergraduate level)
- 2008 - 2014 course in Atomistic Simulations (master level)
- 2008 -2014 course in Advanced Simulations (PhD Level)
- ✓ 1982 -2014 (with period of absence due to international duties) Deputy Director to the Department Library
- ✓ 1987 - 2007 In charge, by Rector nomination, of the University project to create the computerize library catalogue of the whole University libraries (the Physics catalogue was fully recorded by 2002).
- ✓ 1994 - 1998 Director of CICS Department (Interdepartmental Center for Scientific Computations)
- ✓ 2010 - 2013 Member of the Committee for the Maintenances of the Department

## **Publications**

Over **220** papers in such Journals as: The Journal of Chemical Physics, Physical Review Letters, The Journal of Physical Chemistry, Biophysical Journal, Journal of Computational Physics, Molecular Physics, Journal of Statistical Physics, Physical Review...

Present (08/06/2020) data on Google Scholar: h-index, 57; Sum of times cited, 30940; Highest cited papers, 17026, 1007, 854, 738, 585, 577.

## **Books**

- ◆ “*Computer meets Theoretical Physics: the new frontier of Molecular Simulation*”  
G. Battimennli, G. Ciccotti, and P. Greco  
Springer, Berlin, (2020)
- ◆ “*Molecular Dynamics Simulation*”  
Book from a Special Issue of Entropy,  
G. Ciccotti, M.Ferrario, and C. Schuette, Eds.  
MDPI, Basel, 2014
- ◆ “*Constraints: From physical principles to molecular simulations and beyond*”  
Special Topics issue of the European Physical Journal,  
P.Echenique, and G.Ciccotti, Eds.  
Springer, Berlin, 2011
- ◆ “*Computer Simulations in Condensed Matter: From Materials to Chemical Biology*”  
M.Ferrario, G.Ciccotti, and K.Binder, Eds.  
LNP Voll. 1&2, Springer, Berlin, 2006
- ◆ “*Bridging time scales: Molecular simulations for the next decade*”  
SIMU Conference, Konstanz 2001  
P.Nielaba, M.Mareschal, and G.Ciccotti, Eds.  
Springer, Berlin, 2003
- ◆ “*Simulation of classical and quantum dynamics in condensed phase*”  
Euroconference 1997  
B.J.Berne, G.Ciccotti, and D.F.Coker, Eds.  
World Scientific, Singapore, 1998

- ❖ *“MC and MD of condensed matter systems”*  
Euroconference 1995  
K.Binder, and G.Ciccotti, Eds.  
SIF, Bologna, 1996
- ❖ *“Simulation of Liquids and Solids. Molecular Dynamics and MonteCarlo methods in Statistical Mechanics. A reprint book.”*  
G.Ciccotti, D.Frenkel, and I.R.McDonald, Eds.  
North Holland, Amsterdam, 1987
- ❖ *“Molecular Dynamics Simulation of Statistical Mechanical Systems”*  
“E.Fermi” SFI Summer School 1985  
G.Ciccotti, and W.G.Hoover, Eds.  
North Holland, Amsterdam, 1986

### **International Initiatives**

- ❖ Chairman of the Accademia dei Lincei meeting on the perspectives of a European cyber-infrastructure (June 2005) and, subsequently, co-organizer of the ESF initiative: “European Computational Science: The Lincei Initiative: from computers to scientific excellence”, May 2006 - June 2008.
- ❖ Principal proponent for “La Sapienza” of the Erasmus Mundus ATOSIM project for a Master in Computational Physics (2006 - present)
- ❖ Director with Kurt Binder of the Erice Euroconference “Computer Simulations in Condensed Matter: From Materials to Chemical Biology”, July 2005.
- ❖ Principal proponent with M.Mareschal (coordinator) and Daan Frenkel of the European Science Foundation Programme: “Challenges in molecular simulations: bridging the length and time-scale gap (SIMU)”, (1999 - 2008).
- ❖ Director with D.Coker and B.J.Berne of the Euroconference “Computer Simulation of rare events and the Dynamics of classical and quantum condensed matter systems”, 7-18 July 1997.
- ❖ Director with K.Binder of the Euroconference “Monte Carlo and Molecular Dynamics of Condensed Matter Systems”, 1-28 July 1995.
- ❖ Director of Centre Europeen de Calcul Atomique et Moleculaire (CECAM, Paris and since 1994 Lyon), from October 1990 to September 1994.
- ❖ Principal Investigator of the NATO grant for the project “Molecular Dynamics of ion pair reactions in polar solvent”, from 1987 to 1993.
- ❖ Italian Investigator for the EEC contract ST2J-0094-2-I on “Modelisation sur ordinateur en science des materiaux”, years 1986-1988.
- ❖ Principal Investigator of the NATO grant (n.1865) for the project “Computer Simulation of Condensed Matter by Deterministic and Stochastic Molecular Dynamics” with A.Bellemans (Brussels) and I.R.McDonald (Cambridge). From 1979 to 1986.
- ❖ Director (with W.G.Hoover) of the International School of Physics “E.Fermi” in the summer 1985 (XCVII course) on Molecular Dynamics Simulation of Statistical Mechanical Systems.

## **Professional Societies**

- Fellow of the Institute of Physics, IOP.
- Fellow of the European Society of Physics, EPS.
- Member of Italian & European Physical Society, American Chemical Society, and Institute of Physics.

## **European & International Committees, Editorial Boards and Scientific Boards**

- Member of PRACE Access Committee (2017- )
- Member of CECAM Council, as observer (2005-12); as “La Sapienza” representative (2012 - 2015)
- Member of the Management Committee for Ireland of the COST Action “Fundamental Problems in Quantum Physics” (2011 - 2015)
- Member of the Steering Scientific Committee of the European PRACE project for HPC (2010 - 2014)
- Member of the Scientific Committee of the HPC Irish Center ICHEC (2010 - 2013)
- Principal Investigator of the Science Foundation of Ireland PI grant (2009 - 2014)
- Member of the Visiting Committee of CEA, France, 2008.
- Member of the Steering panel of the ESF (European Science Foundation) Forward Look on European Computational Science Forum: The “Lincei Initiative”: from computers to scientific excellence” 2006 - 2008.
- Steering panel of ESF program SimBioMa, 2006 - 2009; of COST action 13, “Bridging the time and length scale”, 2003 - 2007, and of EU Erasmus Mundus project, 2006 - 2009.
- “Membre étranger” du Conseil de perfectionnement du département de chimie de l’École Normale Supérieure de Paris, 2005 to 2010.
- German DFG referee for various initiative, in particular for the large SFB/Transregional Collaborative Research Centre 6 (2003 - 2015) but also referee for American NSF, Norwegian, Austrian & Spanish NSF’s.
- INFN member and, from 2002 - 2003, Chairman of European Physical Research Organizations (EUPRO), 1998 - 2005.
- INFN (National Institute of Physics of Matter) representative to ESF from 1998 to 2005; Member of the Selection Committee of PESC Chairman in 2001.
- Foreign member of the Collaborative Computational Projects Steering Panel (CCPSP) of EPSRC from 1996 to present.
- Member of the Referee Panel of the EU project on High Performance Computing (and its previous versions) HPC-Europa, 1995 to 2012.
- Member of the Advisory boards of:
  - Sci- MDPI (2014 - )
  - Entropy-MDPI (2014 - )

- European Journal of Physics (2003 - 2010)
- Chemical Physics (1996 - 2002)
- Journal of Computer-aided Material Design (1994 - end)
- Computational Materials Science (1993 - end)

#### **Other studies and activities:**

- Member of the Editorial board of "Fundamenta Scientiae", Strasbourg, publisher Pergamon Press, from 1980 to 1986.
- Two books in Italian: “Il computer incontra la fisica teorica: la nuova frontiera della simulazione molecolare”, (Roma, Carocci, 2020, also in English by Springer), “L'Ape e l'Architetto” (Milano, Feltrinelli, 1976; Slavic transl. 1978; French transl. as “l'Araigné et le Tisserand”, 1979; updated and reprinted in 2012 by Franco Angeli, Milano) and some papers or book chapters in history and philosophy of science, science and society, and popularization.

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