Curriculum Vitæ et Studiorum

Maria Valentini

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Personal data

Maria Valentini was born in Fermo (Italy) the 21 May 1966. She is married, of Italian nationality and her present work address is: CRS4, **C**entro di **R**icerca, **S**viluppo e **S**tudi **S**uperiori in **S**ardegna, Edificio 1, P.S.T. POLARIS, I-09100 Pula (CA) (tel. +39-070-9250-424; fax +39-070-9250-216; e-mail maria@crs4.it)

Qualifications

1998 Ph. D. degree in Physics with the thesis *Analytical and numerical studies of the relativistic dynamics of charged particles in electromagnetic field : applications to cyclic accelerators and P.I.C. code* under the supervision of Prof. J. M. Buzzi, Laboratoire de Physique de Milieux Ionisee (PMI), Ecole Polytechnique, Palaiseu, FRANCE.

1991 University degree (Laurea) in Physics with the thesis *Large scale structures and motions in the Universe* under the supervision of Prof. A. Messina. Università degli Studi di Bologna. Specialization in Cosmology.

Scientific experience and career

Researcher **CRS4**
Cagliari, Italy

October 1999 until today: She is Researcher in the *Fuel Cell* area working at the production of models and software for Polymer Electrolyte Membrane Fuel Cells. Reasearch includes efforts related to the understanding of structure and transport properties of polymer electrolytes by means of Molecular Dynamics.

February 2005: She is currently working in the project "NUME: Nuove Membrane ed Elettrodi per celle a combustibile" funded by MIUR in collaboration with teams from Italian Universities for a duration of 36 months.

May 2005: She has been working in the organizing comitte of the training course on "Fuel Cell Modeling and Optimization",addressed to researchers coming from Eastern European countries, under the UNESCO and the MATT (Ministero dell'Ambiente e della Tutela del Territorio) joint sponsorship. As part of her duty she has been charged of the courses on Fuel Cell Materials "Computational methods for materials characterization" and on Simulations "Molecular Dynamics of Nafion" and "Introduction to Fuel cell simulation software MIC3.0".

December 2002 December 2004: Partecipate to the project "Materiali elettrolitici e sistemi elettrodici per celle a combustibile

polimeriche" funded by MIUR (Ministero dell'Istruzione, dell' Universit e della Ricerca). In the context of the project in collaboration with teams from Italian Universities, she has been developing models and molecular dynamics simulation codes for new proton conducting membranes for Polymer Electrolyte Membrane (PEM) Fuel Cells.

October 1999 – October 2001: She has been working on the industrial project "CRF99:Modellazione di Fuel Cells a Metanolo Diretto" with CRF-Centro Ricerche Fiat developing new mathematical models for the description of mass and charge transport and electrochemical reactions for the simulation of performances of Polymer Electrolyte Membranes Fuel Cells (PEMFC).

Ph. D. Student — **Laboratoire de Physique de Milieux Ionisee (LPMI)**
Ecole Polytechnique, Palaiseu FRANCE

April 1994 – May 1998: Benefits of a Marie Curie Institutional Grant from European Community to work in the area of numerical simulation of plasma for particle accelerators. As the first stage of the building of an Electron Cyclotron Resonance (ECR) plasma source for the production of radiological X-rays she studied the dynamics of relativistic particles in a circularly polarized electric field and a transverse constant magnetic one by means of relativistic Hamiltonian formalism to show the integrability of the system. The results have been applied to the testing and optimization of an ECR source at LPMI. As part of her research she has performed also analytical and numerical studies of Maxwell equations in order to test initial and border conditions for relativistic Particle in Cell (PIC) type codes for plasma simulations.

Junior Researcher — **CRS4**
Cagliari, Italy

April 1992 – April 1994: Researcher in the *Parallel Computing Group* (Dr P.Rossi, Leader) developing parallel algorithms in N-body problems. She has studied systems of small polyatomic molecules (dipoles, water molecules)by means of MD and mixtures of colloidal particles mainly using Brownian Dynamics simulation. For those simulations numerical alghoritms have been developed on parallel computers (CM-200, SP1, CM-5) both in data–parallel and message passing style.

Computer Experience

Programming Languages: FORTRAN90, HPF and basic knowledge of C and C++.

Languages

Her mother-tongue is Italian. She is fluent both in English and in French.

Publication List

Journals papers

J.1. A. Bourdier, M. Valentini and J.Valat: "Hamiltonian structure of motion and dynamics of a particle in a constant homogeneous magnetic field and a transverse electric field" , *Physics Letters A*, **215**, 219–228, June 1996.

J.2. A. Bourdier, M. Valentini and J.Valat "Dynamics of a relativistic charged particle in a constant homogeneous magnetic field and a transverse homogeneous rotating electric field" , *Phys. Rew. E*, **5**4 , 5, 5681–5691, November 1996.

J.3. C. Geronimi, F. Bouchut, M.R. Feix, H. Ghalila, M. Valentini and J.M. Buzzi , "Transient electromagnetic Field", *Eur. J. Phys.* ,**1**5, 102–107 (1997).

J.4. G. Murgia, L. Pisani, Maria Valentini and B. D'Aguanno, " Modelling of electrochemistry and mass transport in Polymer Electrolyte Membrane Fuel Cells, PEMFC", *J. Electrochem. Soc.*, **1**49, A31 (2002).

J.5. L. Pisani, G. Murgia, Maria Valentini, and B. D'Aguanno, " A new semi-empirical approach to performance curves of Polymer Electrolyte Fuel Cells", *J. Power. Sources*, **1**08,192 (2002).

J.6. L. Pisani, G. Murgia, Maria Valentini, and B. D'Aguanno, "A working model of Polymer Electrolyte Fuel Cells: comparison between theory and experiments.", *J. Electrochem. Soc.*, **1**49, A898 (2002).

J.7. L. Pisani, Maria Valentini and G. Murgia " Analytical Pore Scale Modeling of the Reactive Regions of Polymer Electrolyte Fuel Cells", *J.Electrochem.Soc.*,**1**50, A1549-A1559 (2003).

International Conference Proceedings

P.1. Carlo Nardone, Pietro Rossi and Maria Valentini, "Parallel Implementation of the 'Multiple Time Scales' Algorithm for Molecular Dynamics Applied to Flexible Water Models" ,in *"Science on the Connection Machine System", J.M. Alimi A. Serna and H. Scholl Eds., p.325* Proc. 2nd. European Connection Machine users meeting (Paris, Oct. 1993).

P.2. A. Bourdier, M. Valentini and J. Valat "Study of the Dynamics of a particle in a constant homogeneous magnetic field and a transverse homogeneous rotating electric field in the development of an X-ray source", in proc. EPAC'96, Sitges (Barcelona), Spain, June 1996.

P.3. L.Pisani, M. Valentini, G. Murgia, B. D'Aguanno *"Effects of the catalyst layer pourous structure on the performances of PEM Fuel Cells"*, New Materials for Electrochemical Systems, Montreal, Canada, July 6-11 2003

P.4. B. D'Aguanno and M.Valentini *"A Molecular Dynamics study of hydrated Nafion: monomer vs. polymers models"* , ICCP-4, Como, Italy, February 18-20 2004.

P.5. M.Valentini, L. Pisani, G. Murgia, M.Pieroni and B. D'Aguanno *"Effects of the Geometrical Designon the Performances of PEM Fuel Cells"*, Fuel Cells Science and Technology, Munich, Germany, October 6-7 2004.

P.6. L. Pisani, G. Murgia, M. Valentini *"SOFC operating on methane: a model analysis"* Fuel Cells Science and Technology, Munich, Germany, October 6-7 2004.

P.7. M. Valentini *"Molecular Dynamics Study of hydrated Nafion"* in proc. Julich Soft Matter Days 2004, Congresscentrum Rolduc, Kerkrade, Netherlands, November 16-19 2004

P.8. M. Valentini and B. D'Aguanno *"Structure and Transport Properties of Nafion Membranes at different levels of Hydration: a Molecular Dynamics Study."* International Conference on "New Proton Conducting Membranes and Electrodes for PEM FCs", Assisi, Italy, October 23-26, 2005

P.9. M. Valentini and B. D'Aguanno *"Molecular Dynamics analysis of hydrated Nafion membranes"* oral presentation at the 6th International Symposium on "New Materials for Electrochemical Systems ", Montreal, Canada, July 9-12, 2006

P.10. A simple analytical model for the conductivity of polymeric sulfonated membranes L. Pisani*, D. W. M. Hofmann, M. Valentini, B. DAguanno CRS4, Italy *"Molecular Dynamics analysis of hydrated Nafion membranes"* 6th International Symposium on "New Materials for Electrochemical Systems ", Montreal, Canada, July 9-12, 2006

Ph.D Thesis

PhT.1. Ph. D. Thesis (These de troisieme cycle) "Analytical and Numerical Studies of the relativistic dynamics of charged particles in electromagnetic field: applications to cyclic accelerators and P.I.C. codes", Ecole Doctorale of the Ecole Polytechnique, Palaiseau, FRANCE, May 1998.

Technical Reports

TR.1. Giuditta Lecca, Ralph Santos and Maria Valentini, *" CMFortran: Connection Machine Fortran"* , CRS4 internal report, Cagliari, 1993.

TR.2. H.Ghalila, M. Valentini and E. Shternbach "Validation of a new algorithm for the charge conserving equation in a P.I.C. electromagnetic and relativistic code" LPMI, Ecole Polytechnique, internal report 3345, 1997.

TR.3. Bruno D'Aguanno, Giovanni Murgia, and Maria Valentini." *MODELLAZIONE DI FUEL CELLS A METANOLO DIRETTO*. " Technical Report CRS4 TR 00/33. CRS4, Center for Advanced Studies, Research, and Development in Sardinia. Cagliari, Italy, 2000.

TR.4. Giovanni Murgia, Lorenzo Pisani, Maria Valentini, and Bruno D'Aguanno. *" Modelling of electrochemistry and mass transport in Polymer Electrolyte Membrane Fuel Cells, PEMFC."* Technical Report CRS4 TR 01/36. CRS4, Center for Advanced Studies, Research, and Development in Sardinia. Cagliari, Italy, 2001.

TR.5. Giovanni Murgia, Bruno D'Aguanno, Lorenzo Pisani, and Maria Valentini. *"SVILUPPO DI UN CODICE PER LA PREVISIONE DELLE PROPRIETA DI FOULING E SLAGGING DI CARBONI: PARTE PRIMA."* Technical Report CRS4 TR 02/50. CRS4, Center for Advanced Studies, Research, and Development in Sardinia. Cagliari, Italy, 2002.

TR.6. G. Murgia, B. D'Aguanno, L. Pisani, and M. Valentini. *" SVILUPPO DI UN CODICE PER LA PREVISIONE DELLE PROPRIETA' DI FOULING E SLAGGING DI CARBONI: PARTE TERZA."* CRS4 Technical Report 04/24. CRS4, Center for Advanced Studies, Research and Development in Sardinia. Pula, Italy, 2004.

TR.7. G. Murgia, B. D'Aguanno, L. Pisani, and M. Valentini. *" SVILUPPO DI UN CODICE PER LA PREVISIONE DELLE PROPRIETA' DI FOULING E SLAGGING DI CARBONI: PARTE SECONDA."* CRS4 Technical Report 04/23. CRS4, Center for Advanced Studies, Research and Development in Sardinia. Cagliari, Italy, 2004.

TR.8. G. Murgia, L. Pisani, M. Valentini, and B. D Aguanno.*A New Semi-empirical Approach to Performances Curves of Polymer Electrolyte Fuel Cells.* Technical Report 04/30. CRS4, Center for Advanced Studies, Research and Development in Sardinia. Cagliari, Italy, 2004.

TR.9. M. Valentini and B. D'Aguanno. *Materiali Elettrolitici e Sistemi Elettrodici Innovativi per Celle a Combustibile Polimeriche.Rapporto per il II Anno di Attivitá* Technical Report 05/04. CRS4, Center for Advanced Studies, Research and Development in Sardinia. Cagliari, Italy, 2005.

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