Loriano Storchi, PhD

Education

Università degli Studi di Perugia (Italy)
Ph.D. In Chemistry (Computational Chemistry) with a thesis entitled: ”Innovative computational strategies for ab-initio Quantum Chemistry: Grid Computing and novel Green’s function techniques”

Università degli Studi di Perugia (Italy)
Bachelor's degree in chemistry (Chemical Physics) with a score of 110/110 cum laude discussing a thesis entitled” Double Molecular Ionization: effects of ’Foreign Imaging’ and nuclear dynamics hexa-halide of sulfur”

Qualified as Full Professor in General and Inorganic Chemistry (ASN - MIUR)

Summary

- Over 20 years of experience in programming. Programming languages include, but not limited to, C/C++, Python, Fortran 77/90. Developing both commercial and academic/research software.

- Over 20 years of experience in High Performance Computing, Parallel, and Distributed Computing. I work in various fields such as: Machine Learning techniques, Chemoinformatic, Ab-Initio Quantum Chemistry, Computational Chemistry, Computational Physics, and High Energy Physics. Experience in Computational Finance

- Over 20 years of Research activity with a multidisciplinary background that is reflected both in the list of my scientific interest, diversification of publications, and as well in my working experience and teaching activity.

- **Languages include** Italian (mother language), English (advanced), French (basic knowledge)

- **Computer skills include** Deep knowledge of programming languages: C/C++, Python, Fortran77/90. Good knowledge of Java, Pascal, Basic, and x86 assembly. Deep knowledge of Linux and Unix in general. Excellent knowledge of Microsoft operating systems. Deep knowledge of networks, network protocols, and cloud computing. Deep knowledge of computational architecture (such as modern CPU architecture and memory). Deep knowledge of HPC (High-performance computing), including part of the calculation parallel/multithreaded (MPI, Posix Thread, OpenMP, other shared memory techniques and framework like GlobalArray, ScaLAPACK and other HPC libraries and framework), GPGPU platforms (CUDA, OpenCL), and code optimization. Participation in numerous projects in HPC, Parallel Computing, Grid computing, Cloud Computing, managing both systems engineering, network, and programming. Deep knowledge of Cheminformatics and Machine-Learning (Deep-Learning) techniques

My multidisciplinary background is reflected both in the list of my scientific interests, diversity of my publications, and surely in my approach to research. My work activity is mainly devoted to computer simulation in both chemical and physical science. In this way I have acquired wide competences in several programming languages and computational and numerical methods, Machine and Deep Learning techniques, HPC High Performance Computing, parallel and distributed programming, computational architecture (e.g. modern CPU and memory architectures), networks and network protocols.

Soon after my degree in Chemistry (110/110 cum laude), my first work experience was at the Dept. of Chemistry and CNR-ISTM. I have worked mainly as a programmer in various fields, mainly focusing on the parallelization of computational chemistry programs with different techniques and paradigms. I worked with the Dept. of Computer Science (Pisa), being involved in many computational projects. In 2003 I started my PhD in Chemistry, which I successfully completed in 3 years. During this period, in addition to the research activities, I also worked as a system and network administrator. In 2007 I received a 3-year research grant entitled "Theoretical study of lifetimes of ionized states through Green Functions and non-Hermitian techniques", working also in the field of Relativistic DFT. I also started working as a scientific consultant and programmer with: Molecular Discovery, developing several commercial programs and with CRC (optimization and porting in HPC environments of atmospheric science codes). In 2010 I worked with INFN to evaluate the computational needs for the Einstein Telescope project, developing codes for gravitational signal analysis. In 2011 I got a 1-year research grant at the ISTM aiming to implement methods for the simulation and characterization of TiO_2 nanostructured materials. I am now Associate Professor at the Univeristy of Chieti, and I also started working with INFN in Cloud computing and as Software Engineer at CERN working in the L1 Track Finding activity (reconstruction Real-time trace of charged particles using FPGA).

Professional Experience

University G. D'Annunzio Chieti-Pescara Associate Professor June 2020 – present	I am an Associate Professor in General and Inorganic Chemistry at the University of Chieti-Pescara, teaching General and Inorganic Chemistry. During this period, I worked also as System and Network administrator for the Theoretical Inorganic Chemistry Group, managing network, servers and HPC resources. And collaborating within the local group in the field of Machine and Deep Learning, bio and cheminformatics Institutional Leadership & Governance: Serves as an appointed Member of the University IT Committee (Comitato Informatico di Ateneo) and the strategic Working Group defining the official Guidelines for the Use of Artificial Intelligence at the University of Chieti-Pescara. Official Member of the Faculty Board for the PhD Program in Business and Behavioral Sciences from 2016 - Present
University G. D'Annunzio Chieti-Pescara Researcher, Assistant Professor December 2011 – June 2020	I worked as a researcher in General and Inorganic Chemistry at the University of Chieti-Pescara, teaching General and Inorganic Chemistry. During this period, I worked also as System and Network administrator for the Theoretical Inorganic Chemistry

Group, managing network, servers and HPC resources. And collaborating within the local group in the field of bio and cheminformatics in the very last period, I also started a collaboration with a group of Computational Finance mainly involved in the development of High-Performance Computing code related to the evaluation of the Financial Risk.

CNR SCITEC **Researcher**
January 2017 - present

I am collaborating with the Department of Chemistry of the University of Perugia on projects related to the development of relativistic DFT software. In addition, I am still collaborating as associated researcher also with the ISTM (CNR) acting within the projects related to hybrid and organic
Photovoltaics (Computational Laboratory for Hybrid and Organic Photovoltaics http://www.clhyo.org).

INFN (National Institute of Nuclear Physics)
Researcher
March 2013 – present

I am collaborating with the INFN (National Institute of Nuclear Physics) involved in the research activity belonging to the CMS experiment. The collaboration is specifically focused on the aspects of computing related to innovative infrastructure solutions based on the CLOUD paradigm, necessary for the deployment of the future computing model. The activity is part of the Cloud computing Working Group INFN Commission for Computing and Networking (local affiliate). During this period, I have been involved in **OCP projects.** Member of the BM team that has been granted an Iron Medal at the **"Innovate FPGA2018" (http://www.innovatefpga.com, under the name "Reconfigurable Computing") I** am currently working on Machine-Learning techniques applied both to the HEP as well as medical data.

CERN (European Organization for Nuclear Research)
Software Engineer
March 2014 – present

I am collaborating as a software engineer at CERN as part of the group CMS (Compact Muon Solenoid) of Perugia. In this context, I am actively engaged in the development and testing of track fitting algorithms. Following the upgrade of the LHC (Large Hadron Collider) to prevent the loss of interesting events, it will be necessary to use new approaches. In this context the reconstruction Real-time trace of charged articles, may be carried out using Associative Memory and FPGA (Field - Programmable Gate Array). My work is mainly focused on the study and implementation of track fitting algorithms of interest in the project of L1 Track Triggering of the CMS experiment. The study is facing the testing and optimization of algorithms to implement them on a FPGA. As a CERN associated Software Engineer I've been at

CERN (Genève) numerous times (Tracker week Phase II upgrade days) to attend meetings and present the results. (Developing a PCA fitter for the L1 track Finding https://github.com/lstorchi/pca_fit and its integration on the CMSSW framework https://github.com/lstorchi/cmssw)

Molecular Discovery Ltd., London UK
Programmer Scientific Consultant
March 2004 - present **(after 2011 present scientific collaboration)**

In this period, I worked as a scientific consultant and programmer for Molecular Discovery Ltd., London, UK, participating in the development of many commercial programs, a complete review of which can be found at: http://www.moldiscovery.com/. The following list is a subset of the software and scientific contribution that I consider the most significant:

- libgrid/grid: thread safe library and a subsequent (parallel) program inspired by the original GRID developed by Dr. Peter Goodford, a computational procedure for determining energetically favorable binding sites on molecules of known structure. It may be used to study individual molecules such as drugs, molecular arrays such as membranes or crystals, and macromolecules such as proteins, nucleic acids, glycoproteins or polysaccharides. The library is used in several other commercial programs, such as VolSurf+, MetaSite, Almond, Shop, Pentacle, Flap, and more.
- MoKa : in-silico computation of pKa values using a novel approach that provides accurate and fast calculations using an algorithm based on descriptors derived from GRID molecular interaction fields.
- Kibitzer: an automatic and expert tool to expand the MoKa internal database with a corporate database of pKa values.
- libtaut/tauthor: a computational procedure for the enumeration of tautomers and the estimation of their stability in the aqueous medium solution.
- liblogd : a library for logD and logP prediction.
- MoKaBio : in-silico computation of protein pKa values by environmental similarity.
- fixpdb : a procedure for filtering PDB files based also on a PDB residues dictionary.
- DeepGrid: a CBB model to predict various drug-like molecule properties starting from the GRID MIF

(Many of the procedures/libraries mentioned above are used by other commercial programs to which I contributed)
During this period, and this collaboration, I also worked on several scientific publications in international journals. Acquisition of competences in using the Qt framework also belongs to this collaboration.

ISTM-CNR (Institute of Molecular Science and Technologies)
Staff Scientist
June 2011 – December 2011

I have done research activities at the (ISTM (Institute of Molecular Science and Technology) – CNR of Perugia as holder of a research grant aiming to achieve the ”Implementation and optimization of non-relativistic and relativistic DFT codes of parallel computer architectures and multi and many cores (GPU) for advanced simulations materials and processes in organic and hybrid photovoltaics.”. In this period, I improved my skills in Python programming language, and I acquired the skills of VTK (The Visualization Toolkit). The research project involved the development of software and computational techniques for the simulation of TiO2 nanostructured materials and their characterization, acquiring also skills on computational geometry.

2b Solutions S.R.L.
Programmer Consultant
February 2011 – September 2011

During this period, I worked as a programmer developing a tool for database synchronization in Python Joomla! in relation to the project ”Tazebao of the XXI century”.

CRC (Center for Research on Climate and Climate Change)
Programmer Scientific Consultant
May 2011 – December 2011

I worked as a scientific consultant and programmer for the CRC (Center for Research on Climate and Climate Change) in Perugia with object” Porting and optimization of code meteorological platforms multi and many cores”

INFN (National Institute of Nuclear Physics)
Staff Scientist
May 2010 – May 2011

I worked as a collaborator with the I.N.F.N. (National Institute of Nuclear Physics) section of Perugia, evaluating the computational needs for the Einstein Telescope project using the Many-Core (GPU) environment. During this period, I developed and optimized codes for gravitational signal analysis, therefore I acquired the basic skills of the DSP (Digital Signal Processing), as well as in the field of Many-Core programming (GPGPU and beyond). Contemporaneously, during this cooperation, I co-wrote the Design Study for the Einstein Telescope. At the same time, I also worked as a consultant for the SCI (Italian Chemical Society) as a staff organizer of the HOPV2010.

Department of Chemistry University of Perugia
Staff Scientist
January 2007 – December 2009

Grant holder at the University of Perugia entitled” Theoretical study of lifetimes of ionized states through technical and non-Hermitian Green functions”, with involvement in developing and parallelizing code. In the same period, I carried out activities as a Systems and Network Administrator at the ISTM (Institute of Molecular Sciences and Technologies) and the Department of

	Chemistry. In the early months of 2009 to carry out activities as a scientific consultant and programmer with The CRC (Center for Research on Climate and Climate Change) of Perugia with object ”Optimizing, porting and management in HPC environments of parallel codes for the simulation of convective weather phenomena in static equilibrium ”played in Project ”AMMA - African Monsoon Multidisciplinary Analysis”. My research activity starting from this period has been devoted also to Relativistic Density Functional Theory. With a specific focus on simulation of big structures involving heavy and super heavy atoms. Contributing to the implementation, optimization, and parallelization of BERTHA (Four-Component Relativistic DFT code).
Department of Chemistry University of Perugia Ph.D. Student November 2003 – December 2006	I am a holder of a PhD scholarship at the Department of Chemistry at the University of Perugia. During this period in addition to the research activities I have worked also at the ISTM (CNR) and the Department Chemistry as a System and Network administrator, managing and configuring network and servers (DNS, mail server, DHCP server, web server, and more) and resources clustered HPC Beowulf. Two of the most significant software contributions of this period are the method not-Dyson ADC (3) (Integral Driven) for the simulation of molecular ionization spectra. As well as a portal based on Java Servlet technology for the simulation of potential energy surfaces on a computing grid. During this time, I also realized the Chemgrid project (in collaboration with several Italian institutions), of which I have studied both the architectural (i.e., sysadmin) and the software aspects.
Department of Computer Science University of Pisa Research Grant June 2003 – November 2003	During this period, I worked with the Department of Computer Science University of Pisa for the” Developing Codes ASSIST parallel environment for chemical applications in the strategic project MIUR (High-performance distributed platform)”. Developing a methodology for dynamic memory allocation within the ASSIST framework.
ISTM (Institute of Molecular Science and Technologies) Department of Chemistry University of Perugia Research Grant	This period belongs to the first practical work experience immediately following my graduation. During these years I have done activities as a programmer in various fields in addition to supporting skilled people in system management and networking.

January 2001 – June 2003	I have done research activities having as its object:" Parallelization of computational chemistry programs using Message Passing and Shared Memory techniques"," Development of ASSIST patterns" and" Development of parallel programs (MPI and ASSIST Programming)". Most of my research activity of this period has been essentially carried out in collaboration with ASI (Italian Space Agency) and the Department of Computer Science (University of Pisa).

Publications list

- Matteo De Santis, Edoardo Mosconi, Leonardo Pacifici, Valerie Vallet, Andre' Severo Pereira Gomes, Loriano Storchi, Leonardo Belpassi, "Environmental Effects via Frozen Density Embedding in Real-Time Time-Dependent Dirac-Kohn-Sham Theory: Solvation of Lead Halides", Journal of Chemical Theory and Computation, DOI: 10.1021/acs.jctc.5c01980 (2026)
- L. Storchi within CMS, "Evaluation of 3D pixel silicon sensors for the CMS Phase-2 Inner Tracker", Nucl. Instrum. Meth.A, DOI: 10.1016/j.nima.2026.171359 (2026)
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- L. Belpassi, L. Storchi, "Foreword to special issue on the 13th international conference on relativistic effects in heavy-element chemistry and physics (REHE-2022) held in Assisi, Italy" Molecular Physics, DOI: 10.1080/00268976.2025.2468591 (2025)
- L. Storchi within CMS collaboration, "Beam Test Performance Studies of CMS Phase-2 Outer Tracker Module Prototypes", Journal of Instrumentation, DOI: 10.1088/1748-0221/19/10/P10032 (2024)
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- D. Ciangottini, G. Bianchini, M. Mariotti, D. Spiga, L. Storchi, G. Surace, "KServe inference extension for an FPGA vendor-free ecosystem", CHEP2023, REF (2023)
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aerospace technology", Rendiconti Lincei. Scienze Fisiche e Naturali, DOI: 10.1007/s12210-019-00805-9 (2019).

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- GEMS EXPRESSION OF INTEREST FOR THE EGI, EUDAT AND INDIGO-DATACLOUD H2020 PROJECT PROPOSAL EINFRA12 (A) Antonio Laganà, Sergio Rampino, Loriano Storchi, Ernesto Garcia, Cecilia Coletti, Edward Blurock, Carles Bo, Mirco Mariotti, Giuseppe Vitillaro
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Proceedings

- R. Di Staso, L. Aragão, E. Ronchieri, L, Storchi,;D, Spiga, S. Cutini, D. Salomoni, P. Lubrano, “TIME SERIES ANALYSIS OF METEOROLOGICAL PARAMETERS AND AIR POLLUTION CONCENTRATIONS IN EMILIA-ROMAGNA, ITALY, DURING COVID-19 INFECTION”, 21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, HARMO 2022 , 152-156, 2022.
- Guglielmo D’Amico, Filippo Petroni, Philippe Regnault, Stefania Scocchera, Loriano Storchi, A copula based Markov Reward approach to the credit spread in European Union, 19th Applied Stochastic Models and Data Analysis International Conference (ASMDA2019)
- Mariangela Agamennone, Roberto Paciotti, Loriano Storchi, Federica Sommonte, Alessandro Marrone, “DRUGGING THE UNDRUGGABLE: THE PRION PROTEIN AS A CASE STUDY OF AGGREGATING PROTEINS”, CDDD 2019
- Matteo de Santis, Loriano Storchi, Francesco Tarantelli, Leonardo Belpassi, “Charge-displacement analysis: a simple tool to reveal charge transfer effects throughout the whole periodic table (from Helium to Oganesson)”, 2018
- Carla Maria Coppola, Alessandro Marrone, Cecilia Coletti, Iogann Tolbatov, Loriano Storchi, Nazzareno Re Pietro Di Profio, Gaastra Nedea S.V., Ionut Claudiu Tranca, Silvia V. Nedea, Simone Arca, Emilio D'Alessandro, J. Longo, “Hydrates and Mofs as candidate Materials for Hydrogen Storage in Telecommunication Satellites”, Space Propulsion 2018

- Guglielmo D'Amico, Filippo Petroni, Philippe Regnault, Stefania Scocchera and Loriano Storchi, Investigating the financial risk: information theory and break detection approach, AMASES 2018
- Marrone A, Paciotti R , Re N , and Storchi L. A computational workflow to investigate the molecular interaction properties and aggregation propensity of prion proteins. Prion20128
- Leonardo Belpassi, Loriano Storchi, "Bond analysis in the four-component relativistic framework: Charge-Displacement analysis via natural spinors for chemical valence" , REHE2017 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics
- Guglielmo D'Amico, Stefania Scocchera, Loriano Storch, "Financial Risk Distribution in European Union", 17th Applied Stochastic Models and Data Analysis International Conference with Demographics Workshop ASMDA2017
- L. Storchi, F. Nunzi, S. Fantacci, F. De Angelis, "Modeling dye-sensitized TiO2 interfaces in dye-sensitized solar cells models", SimOEAP, International Conference on Simulation of Organic Electronics and Photovoltaics, 10-14 June 2012, Spain.
- Gabriele Cruciani, Francesca Milletti, Loriano Storchi, Gianluca Sforna, "Do pKa predictions matter anymore?", QSAR 2008, Uppsala, Sweden.
- P. Linusson, L. Storchi, F. Heijkenskjld, E. Andersson, M. Elshakre, J.H.D. Eland, L. Karlsson, M. Larsson, J.-E. Rubensson, F.Tarantelli and R. Feifel, "Double photoionisation of thiophene and bromine substituted thiophenes", International workshop on photoionization, 2008, Uppsala, Sweden.
- F. Milletti, L. Storchi, G. Cruciani, "New tools for pKa prediction: from small molecules to proteins", Proceedings of Drug Discovery and Selection, International Conference on Medicinal Chemistry 2007, Lille, France.
- F. Milletti, L. Storchi, G. Sforna, G. Cruciani, "A new software for pka predictions", Proceedings of TUMA 2006, Camerino, Italy.
- Leone B. Bosi, Loriano Storchi, "Impact of GPU Technology on gravitational wave physics and signal detection systems", E4 Workshop 2010, Bologna, Italy, 16-17 September 2010.
- Alessandro Marrone, Loriano Storchi, Gianpiero Marconi, Emidio Albertini, The gene APOSTART: theoretical and computational study of the binding domain of phytosterols, "Chemistry Innovation and ...", University Chieti-Pescara 14 May 2013

Presentation at Conferences and Workshops

- **Invited speaker at:** Accademia dei Lincei, Rome, Quantum Chemistry One Hundred Years After the Schrödinger Equation, May 2026, "BERTHA and PyBERTHA: An HPC-enabled four-component Dirac-Kohn-Sham framework"
- **Invited speaker at:** Accademia dei Lincei, Rome, Quantum chemistry and cheminformatics - 26-27 September 2024, "Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator"
- **Invited speaker at:** University Perugia, Dpt. Chemistry, "Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator", May, 2024
- **Invited speaker at:** VISTEC Vidyasirimedhi Institute of Science and Technology , School of Molecular Science and Engineer 31/05/2022 (Thailand)
- **Invited speaker at:** Shoolini Science Web Series Lecture IX - "Four-component Dirac-Kohn-Sham Calculations" 30/06/2021

- **Featured Speaker at the OPEN ACCELERATED COMPUTING SUMMIT** "ERTHA and PyBERTHA: state of the art for full four-component Dirac-Kohn-Sham calculations", October 7th
- Loriano Storchi, Paolo Campeti, Massimiliano Lattanzi, Enrico Calore, Pasquale Lubrano "gCAMB: A GPU-accelerated Boltzmann solver for next-generation cosmological surveys", The Universe in a Chip: Final ICSC Spoke-3 Meeting on HPC & Big Data in Astrophysics, Sexten Center for Astrophysics Riccardo Giacconi December 15-19, 2025
- "A walkthrough Machine and Deep Learning techniques in chemistry", One Day Workshop 8 October 2025 Artificial Intelligence for Molecular & Materials Systems Experiments vs Theory, Accademia Nazionale delle Scienze detta dei XL
- "BERTHA and PyBERTHA: state of the art for full four-component Dirac-Kohn-Sham calculations", 2nd Southern European Conference on the Science of Molecules, Madrid, 16-18 September 2025
- "Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator", Southern European Conference on the Science of Molecules Perugia, 27-29 September 2023
- "Applications of Machine and Deep Learning techniques: from DeepGRID to a simple formula generator", Center for Advanced Studies and Technology University «G. d'Annunzio», Chieti-Pescara, December 19, 2023
- *BERTHA* and *PyBERTHA*: *State* of the *Art* for *Full Four-Component Dirac-Kohn-Sham Calculations*. *PARCO* 2019: 354-363.
- "Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator", Experiment-Theory: a round trip, Chieti, Sept 14th 2023
- "The Track Fitter for L1 Tracking", First H-Team Workshop - Higgs precision physics at LHC with Trigger, Electronics and Advanced Methods Thursday 07 April 2016 – Friday 08 April 2016 Cortona – Italy
- "Computing molecular energy surfaces on a grid", (ICCSA06), Glasgow, 8-11 May 2006.
- "SUPSIM: Computing electronic potential energy surfaces on a GRID", Tutorial on grid technologies, (ICCSA04), Assisi, 13-14 May 2004
- "Computing electronic PES on a GRID", V Edizione del Congresso del Gruppo Italiano di Chimica Computazionale, Siena, 6-18 December 2003

Congress organization

- **Co-Chair** of the REHE – 2020/2022 - 13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Assis - Italy (2022) https://www.rehe2020.it/
- Part of the organizing committee of the MES 2024 - Molecular Electronic Structure 2024, Pescara - Italy, 2024 https://www.mes2024.it/
- Part of the organizing committee of the HOPV 2010 - International Conference on Hybrid and Organic Photovoltaics, Assisi - Italy, 2010

Schools

- "Summer School of Advanced Calculus - Second Edition", Castel Gandolfo (Roma), 28 agosto – 8 September 2006.

- ”First Specialization School on Parallel Computing”, CINECA Casalecchio di Reno (Bologna), 24-28 October 2005.
- ”The 2nd International Summer School on grid computing 2004”, Vico Equense (Napoli), 18-30 July 2004

Workshops and Tutorials

- ”ICT security Day 2012”, University of G. D’Annunzio Chieti-Pescara.
- ”NVIDIA Cuda Workshop”, Roma, Institute of Applied Mathematics (CNR), 19-20 July 2010.
- ”Modeling Winter 2010”, Pisa, Scuola Normale Superiore, February 26, 2010
- ”HPC with CUDA”, Department of Electrical Systems and Automation of the University of Pisa, September 7, 2009.
- ”Developing for Multi-core Intel seminar”, Roma, Italy, November 20, 2008
- ”Joint ICTP-KFAS Workshop on Nanoscience for Solar Energy Conversion”, ICPT, Trieste, Italy, 27-29 October 2008.
- ”Cluster OpenMP Workshop”, CASPUR, Roma, December 7, 2006.
- ”QCDOC and BlueGene Workshop Next Generation of HPC architectures”, EPCC, Edinburgh, 4-6 October 2005.
- ”ASSIST Tutorial”, Department of Computer Science, University of Pisa, 5-7 May 2004.
- ”ENACTS (European Network for Advanced Computing Technology for Science) 4rd Annual Meeting”, Prague, 11-13 March 2004.
- ”Tutorial on Grid Computing”, Swiss National Supercomputing Center, 25-26 October 2003.
- ”ENACTS (European Network for Advanced Computing Technology for Science) 3rd Annual Meeting”, Dublin, 14-15 March 2003.
- ”Performance Tuning for Microprocessor-Based Systems Workshop”, CINECA Casalecchio di Reno (Bologna), January 17, 2002
- ”INFN-GRID/EDG User Tutorial”, Turin, 5-6 December 2002.
- I also participated with numerous contributions to workshops conducted within the projects: ”ASIPQE2000”, ”GRID.IT”.
- ”High Performance Computing in Chemistry”, NNL, Lecce, 2009.

Periods of study abroad and Invited Prfessor

- **Invited Professor**: “Université de Lorraine, 54000 Nancy” at the “Laboratoire de Physique et Chimie Théoriques (UMR) CNRS”, Academic Year 2021/22
- Visting researcher at the “Centro de Investigación y de Estudios Avanzados Av. Instituto Politécnico Nacional” as a Member of the Cooperation project Mexico-Italy, June-July 2025
- Heidelberg (Germania) at: ”Physikalisch-Chemisches Institut (Theoretische Chemie)”. February-March 2005 and April - May 2006
- Budapest (Hungary) at the ”MTA SZTAKI - Computer and Automation Research Institute of the Hungarian Academy of Sciences”, and “The Chemical Research Center of the Hungarian Academy of Sciences (CRC HAS)”. November - December 2004

Awards

- Member of the BondMachine project that has been granted an Iron Medal at the Innovate FPGA 2018 grand final (http://www.innovatefpga.com, under the name Reconfigurable Computing). Part of the presenter team at Intel San Jose, CA, USA (2018)
- Awarded with a consultancy contract (consultancy topic: Machine and Deep Learning techniques) within the project VITALITY at the University of Perugia (2024/2025).

Teaching

- Invited speaker for the seminar 'Machine Learning and Deep Learning', presented as part of a Python training series for researchers at the National Research Council's Institute of Biophysics (CNR-IBF) and Institute of Chemical Sciences and Technologies (CNR-SCITEC), held online on March 11, 2026
- Teacher at the Multiscale, Machine Learning and QSAR methods applied to biomolecules: “Introduction to Machine and Deep Learning using python”, Aspet, France, 25-29, November 2024
- Teacher at the Multiscale, Machine Learning and QSAR methods applied to biomolecules: “Introduction to Machine and Deep Learning using python”, Aspet, France, 24-28, November 2025
- ANALYSIS AND MACHINE LEARNING TECHNIQUES WITH BASICS OF COMPUTER SCIENCE AND STATISTICAL LEARNING, Course Degree in C.T.F. (University of Chieti-Pescara) - From 2025/26 - Present
- Material Chemistry, Course Degree in Biomedical Engineering, (University of Chieti-Pescara) - From 2021/22 - Present
- Basics of computer science - Course Degree in TESTA (University of Chieti-Pescara) - From 2021/22 - To Present
- General Chemistry - Course Degree in TESTA (University of Chieti-Pescara) - From 2021/22 - To Present
- Statistics and computer science - Course Degree in TPALL (University of Chieti-Pescara) - From 2014/2015 - To Present
- Computational Chemistry, Course Degree in C.T.F (University of Chieti-Pescara) - From 2018/19 - To 2021/22
- Computer programming & Data Analysis using Python - PhD Course Degree Business and Behavioral Sciences (University of Chieti-Pescara) - From 2016/2017 - To Present
- Introduction to Chemo and Bioinformatics - Course Degree in C.T.F, (University of Chieti-Pescara) - From 2015/2016 - To 2016/17
- General Chemistry - Course Degree in TPALL (University of Chieti-Pescara) - From 2014/2015 - To 2019/20
- General Chemistry - Course Degree in Assistenza Sanitaria - (University of Chieti-Pescara) - From 2015/2016 - To 2016/2017
- General and Inorganic Chemistry - Course Degree in Pharmacy (University of Chieti-Pescara) - From 2012/2013 - To 2019/20
- General and Inorganic Chemistry - Course Degree in C.T.F. (University of Chieti-Pescara) - 2011/2012 (20 hours)

- Computational Chemistry - Course Degree in C.T.F. (University of Chieti-Pescara) – (few hours) From 2014/2015 - To 2016/2017
- Advanced Computational Methods - Course Degree in Computer Science (University of Perugia) - From 2010/2011 - To 2011/2012
- Applications and Computing with Network - Course Degree in Computer Science (University of Perugia) - From 2007/2008 - To 2010/2011
- Applications and Computing with Network II - Course Degree in Computer Science (University of Perugia) - Academic Year 2005/2006
- Computer Science - Degree in Technology for Conservation and Restoration of Cultural Heritage (University of Perugia) - From 2004/2005 - To 2007/2008
- Operating Systems Laboratory 3 - Course Degree in Computer Science (University of Perugia) - 2005/2006
- General Laboratory of Computer Science - Course Degree in Computer Science (University of Perugia) - From 2005/2006 - To 2008/2009
- "Introductiopn to Parallel programming, the Message Passing Interface" - Lecturer at the TCCM 06 - European Master in Theoretical Chemistry and Computational Modeling - Year 2006
- Atomic and Molecular structures - Course Degree in Computer Science (University of Perugia) -Support to teaching - 2003/2004
- One year contract professor for the course "Applications and Computing with Networks" Degree in Computer Science University of Perugia academic year 2010/2011

Projects

- **Principal Investigator** of the "PaGUSci" project (Parallelization and GPU Porting of Scientific Codes) within the Cascading Call issued by Spoke 3 and relating to the implementation of the Research "National Centre for HPC, Big Data and Quantum Computing"
- Open City Platform (OCP) intends to research, develop and test new technology solutions that are open, interoperable and usable on-demand on the Cloud, as well as innovative organizational models that will be sustainable over time. The aim of the project is to innovate, with scientific results and new standards the delivery of services by Local Government Administrations (LGA).
- ASI-PQE2000 within that project I developed and integrated methods for the dynamic allocation of memory in the framework of ASSIST.
- GRID.IT (technical board member) within the project I worked mainly on the activity about ChemGrid.
- ChemGrid I worked as a project coordinator, giving the basis and guidelines for its realization.
- LIGTHS (LIgand to interfere with Human TS).
- DEISA Project" Chemical Characterization of Super Heavy Elements (E112 and E114) by 4-component relativistic DFT."
- Many-cores Computing for future Gravitational Observatories (MaCGO). Within this project I worked mainly in developing the basic structure of a general purpose library for computation using many cores.

- H-team The discovery of the Higgs boson opens de-facto' the phase of the precision measurement of its couplings. The aim of this research project is to develop the most advanced trigger, selection and analysis techniques to allow the LHC experiments to gain an order of magnitude with respect to the current levels of accuracy. In such a way it would become possible to explore the existence of new physics over a wide energy regime.

Posters

- "Chemical Characterization of Super Heavy Elements by four-component relativistic DFT. (CC-SHE)", Leonardo Belpassi, Loriano Storchi, Francesco Tarantelli, Molecular Properties 2009, Oslo.
- "Chemical Characterization of Super Heavy Elements by four-component relativistic DFT. (CC-SHE)", Leonardo Belpassi, Loriano Storchi, Francesco Tarantelli, DEISA Meeting 2009.
- "An all-electron 4-component Dirac-Kohn-Sham procedure for large molecules and clusters containing heavy elements." Leonardo Belpassi, Francesco Tarantelli, Antonio Sgamellotti, Loriano Storchi,Harry M. Quiney, "Joint ICTP-KFAS Workshop on Nanoscience for Solar Energy Conversion", ICPT, Trieste Italy, 27-29 Ottobre 2008.
- "Characterization of inner shell excitation, ionization and decay of pyrimidine", S. Veronesi, P. Bolognesi, E. Fainelli, V.Feyer, K.C.Prince, P.O.Kudelic, M.Coreno, F. Tarantelli, L. Storchi and L. Avaldi., IX School on Synchrotron Radiation: Fundamentals, Methods and Applications, 2007
- "New tools for pKa prediction - from small molecules to proteins" F. Milletti, L. Storchi, G. Sforna, G. Cruciani. Drug Discovery and Selection, International Conference on Medicinal Chemistry 2007, Lille, France.
- "MoKa - pKa prediction software", M. Shalaeva, Z. Zhu, R. Stanton, D. Li, F. Milletti, L. Storchi, G. Sforna, G. Cruciani. Euro QSAR 2006, Italy, 10-16 September 2006.
- "Parallelization of a relativistic DFT code", L. Belpassi, L. Storchi, F. Tarantelli, A. Sgamellotti, H. M. Quiney. V Edition of the Congress of the Italian Group of Computational Chemistry, Siena, 6-18 December 2003

Thesis Supervisor

- Matteo Picciolini, "Postprocessing and Display in theoretical simulations of Molecular Spettrosopy", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Francesco Muscarà, "DHCP: virtualization and management", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Andrea Lauri, "Using ScaLAPACK and Adaptive MPI in a Relativistic DFT code", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Daniele Bocciolini," Use and management of SMARTCARD for authentication procedures", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi

- Matteo De Bonis," Pseudo-Random number generators on GPU", University of Perugia, Course Degree in Computer Science, Supervisors: Leonello Servoli, Loriano Storchi, Leone Bosi
- Fabio Andrea Petrini," Authentication, Authorization, Accounting for a secure wireless network" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Lanfranco Fontana," Using MPI and Pthreads for parallelization on multi-GPU platform of gravitational signals identification algorithms" University of Perugia, Course Degree in Computer Science, Supervisors: Leonello Servoli, Loriano Storchi, Leone Bosi
- Matteo Picciolini," GPGPU and multithreading in molecular ionization spectra computation" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Antonio Nigro," Study and implementation of algorithms for spheres packing in Simulation of nanoporous materials" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi
- Andrea Lauri," Development of a gesture controller for a Python molecular visualization system", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Loriano Storchi, Massimiliano Pippi
- Ermanna Fabbri," Algorithms for the packing of spheres and polyhedra in the simulation of nanoporous materials of potential pharmaceutical interest", University of Chieti-Pescara, Course degree in Pharmacy, Supervisors: Loriano Storchi
- Matteo Pergolesi," Design and implementation of a monitoring system for federated cloud infrastructure", University of Perugia, Corse degree in Computer Engineering, Supervisors: Prof. Gianluca Reali, Dr. Loriano Storchi
- Gabriele Galli, "AI-based intelligent caching system for the CMS experiment", University of Perugia, Corse degree in Physics, Supervisors: Prof. Loriano Storchi, Prof. Livio Fanò, Dr. Daniele Spiga
- Giandomenico Terrenzio, "Study, use and implementation of numerical procedures (Machine Learning algorithms) for the prediction of the logD of molecular structures of potential chemical-pharmaceutical interest", University of Chieti-Pescara, Course degree in CTF, Supervisors: Prof. Loriano Storchi
- Giacomo Surace, "FPGA accelerators userspace library development", University of Perugia, Course Degree in Computer Science, Supervisors: Giovanni Ambros, Mirko Mariotti, Loriano Storchi
- Luna Di Marco, "PROCESSES AND CHEMICAL COMPOSITIONS FOR STORAGE IMPROVED MOLECULAR HYDROGEN IN HYDRATE CLATHRATES", Pietro Di Profio, Loriano Storchi
- Giuseppe Prudente, "Use of Machine Learning techniques to study the possible role of air pollutants in the spread of COVID-19", University of Perugia, Corse degree in Physics, Supervisors: Prof. Loriano Storchi, Prof. Livio Fanò, Dr. Daniele Spiga

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Tutor (Stages)

- Marco Di Maio, Served as an Academic Tutor for a Training and Orientation Project within the Department of Engineering and Geology at Università degli Studi 'G. D'Annunzio', mentoring a student in the application of Machine Learning and Deep Learning techniques (Random Forests, Artificial Neural Networks) to predict Blood-Brain Barrier permeability for drug discovery.
- Chiara Sofia Di Lorenzo, Served as the Academic Tutor for a Biomedical Engineering internship at Università degli Studi 'G. D'Annunzio'. The project focused on structuring large quantum mechanical

databases generated via the Fragment Molecular Orbital (FMO) method and developing Machine Learning (ML) models to accelerate the discovery of new materials and drugs.

- Matteo De Bonis," Test and porting of code on GPU", at INFN Perugia.
- Metteo Picciolini," Implementation of a url shortening service by the development environment provided by google apps using python language", at Evonove s.r.l.
- Antonio Nigro," Implementation using Python language of an online system storing on Google Blobstore backend including client desktop in a transparent manner that supports the symmetric key encryption methodology", at Evonove s.r.l.
- Andrea Lauri," Construction of a gesture-based controller using Microsoft Kinect device", at Evonove s.r.l.

Institutional Service

- Member, University IT Committee (Comitato Informatico di Ateneo) | G. d'Annunzio University of Chieti-Pescara
- Member, Working Group on Guidelines for the Use of Artificial Intelligence in the University (Gruppo di lavoro sulle Linee Guida per l'uso dell'Intelligenza Artificiale in Ateneo) | G. d'Annunzio University of Chieti-Pescara
- Member of the Faculty Board, Ph.D. Program in Business and Behavioural Sciences | G. d'Annunzio University of Chieti-Pescara