Curriculum Vitae

Gil Sepúlveda, Víctor Alejandro

19-06-1983

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Work Experience

- **BSC (Barcelona Supercomputing Center), Guallar Lab. Electronic and Atomic Protein Modelling**

  From - To: April 2010 - June 2016

  Position: Research Software Engineer

  Employer: BSC, upon request of Dr. Víctor Guallar Tasies (victor.guallar@bsc.es)

  Description: Coursing Biomedicine PhD program. Some of the tasks performed:
  - Redesigning and translating the in-house software (PELE) from a legacy FORTRAN version to C++.
  - Optimizing the new implementation using modern HPC techniques (multi/manycore and distributed systems).
  - Implementing safer and efficient machine learning methods in Python enabled for High Performance Computing.
  - Implementing and improving novel biophysical simulation algorithms.

- **CRG (Center for Genomic Regulation), Serrano Lab. Systems Biology**

  From - To : February 2009 - August 2009

Position: Research Software Engineer

Employer: CRG, upon request of Dr. Luis Serrano Pubull (luis.serrano@crg.es), supervised by Dr. Raik Grünberg (raik.gruenberg@crg.es).

Description: Coding new features (modules) for the Python package Biskit:
- Designing and implementing a protein domain fusing feature.
- Designing and implementing coiled coil detection algorithms.
- Designing and implementing a *FRET* calculation techniques.

- **BSC (Barcelona Supercomputing Center), Guallar Lab. Electronic and Atomic Protein Modelling**

  From - To: September 2006 - September 2007

  Position: Junior Research Software Engineer

  Employer: BSC, upon request of Dr. Víctor Guallar Tasies (victor.guallar@bsc.es)

  Description: General research and implementation of sampling algorithms:
  - Sampling protein conformations using normal modes (C++ prototype).
  - Implementing and analysing *coarse grain* molecular dynamics algorithms (C++ prototype).
  - Implementing and analysing A.I. based conformational sampling algorithms.

- **MAll Department in UPC (Universitat Politécnica de Catalunya)**

  From - To: January 2006 - June 2006

  Position: Intern

  Employer: UPC, upon request of Dr. Fernando Martínez Sáez (+34 934137690)

  Description: Deployment of a web server for the Cryptography course:
  - Java programming of cryptographic tools.
  - Deploying a secure web server.
  - Scripting for the creation and administration of certificates.
  - Implementing a mail resender with secure MIME parts.

Others:

San Andrés Tennis Club (Barcelona)
From - To: 2000-2006
Position: Tennis coach (<16)

Olimpia Tennis Club (Barcelona)
From - To: 2003-2006
Position: Tennis coach (<16),
Employer: Jordi Díaz (+34 932662395)

Estibarna (Port of Barcelona)

Luggage Servimar S.L. (World Trade Center)

From - To : June-August 2002
Position : Porter

From - To: 2004
Position: Porter

Education and Training

- **PhD in Biomedicine** at Universitat de Barcelona.

  Thesis title: Algorithmic and Technical Improvements in Next Generation *Technical and algorithmical improvement of PELE's conformational sampling*.

  Developed skills:
  - Biochemistry expertise.
  - Conformational sampling techniques
  - Ligand sampling techniques
  - Cluster analysis and PCA techniques

- **MS in Biomedical Engineering** (2 years, European Official Master) at Universitat de Barcelona (UB) and Universitat Politècnica de Barcelona (UPC).

  Project title: *Design and implementation of software to generate complex protein structures*

  Developed skills:
  - Biology and Medicine principles
  - Biomedical signal analysis
  - Biomedical devices
  - Biomedical imaging (image acquisition and analysis)
  - Simulation of natural systems
  - Biomechanics principles
  - Tissue engineering principles

- **Engineer's Degree in Computer Science** (5 years) at Facultat d'Informàtica de Barcelona (FIB), Universitat Politécnica de Catalunya (UPC.

  Project title: *Simulation of a Humanoid Robot* (http://hdl.handle.net/2099.1/5262).

  Developed skills:
  - Analogic and digital electronics
  - Microcontroller and FPGA programming notions
  - General programming
  - Artificial Intelligence
  - Software Engineering

- Robotics
- Computer Vision
- Computer Graphics
- Bioinformatics

Research Stays:

- AstraZeneca, Göteborg, Sweden (1-14 March 2015), supervised by Dr. Anders Hogner.
- LAAS - CNRS, Toulouse, France.(14 May-15 June 2011), supervised by Dr. Juan Cortés (+33 561336345).

Oral communications:

- Implementation of an internal coordinates anisotropic network model in PELE BSC Doctoral Symposium (2015, Barcelona)

Publications:

- “An all-atom, active site exploration of antiviral drugs that target Flaviviridae polymerases“, (Journal of General Virology, 2016)
- “Algorithmic and Technical Improvements for Next Generation Drug Design Software Tools”, PhD Thesis, Biomedicine program (2016).
- “Enhancing backbone sampling in Monte Carlo simulations using Internal Coordinates Normal Mode Analysis” (Bioorganic and Medicinal Chemistry, Special issue 2016)
- “Computational Prediction of HIV-1 Resistance to Protease Inhibitors” (Journal of Chemical Information and Modeling 2016, J. Chem. Inf. Model., 2016, 56 (5), pp 915–923)
- “Nucleoside inhibitors of tick-borne encephalitis virus” (Antimicrob. Agents Chemother.September 2015 vol. 59 no. 95483-5493)
- “Monte Carlo Free Ligand Diffusion with Markov State Model Analysis and Absolute Binding Free Energy Calculations” (J. Chem. Theory Comput., 2014, 10 (1), pp 282-288)
- “pyProCT: Automated Cluster Analysis for Structural Bioinformatics” (J. Chem. Theory Comput., 2014, 10 (8), pp 3236-3243)
- “pyRMSD: a Python package for efficient pairwise RMSD matrix calculation and handling” (Bioinformatics (2013) 29 (18):2363-2364.)

Posters:

- “PyProCT: Accurate Conformational Cluster Analysis in Python” at VI International Conference of

the Institute for Biocomputation and Physics of Complex Systems (BIFI) 2014, Zaragoza, Spain.

- ”pyProCT: Automatic Clustering in Python” at Frontiers in Dynamics Simulations of Biological Molecules, 2013, Barcelona, Spain.

- “Parallelization of non bonding calculations gradient calculation in PELE++”, PUMPS Summer School 2012 , 2012, Barcelona, Spain.

Courses and Conferences:

- Programming Distributed Computing Platforms with COMPSs (19 February 2015), Barcelona, Spain.

- International Summer School in Parallel Patterns (9 - 12 June 2014), National College of Ireland, Dublin, Ireland.

- Iberian Google Cloud Platform Tour, (9 May 2014), Barcelona, Spain.

- Introduction to Unified Parallel C and Co-Array Fortran (14-15 April 2014), Stuttgart (HLRS), Germany.

- VI International Conference of the Institute for Biocomputation and Physics of Complex Systems (BIFI) (22-24 January 2014), Zaragoza, Spain.

- Frontiers in dynamics simulations of biological molecules (4-6 November 2013), Barcelona, Spain.

- PRACE HPC Numeric Libraries 2013 (8-12 July 2013), Bologna (CINECA), Italy.

- International Summer School on HPC Challenges in Computational Sciences (23-28 June 2013) XSede-PRACE-RIKEN, New York, USA.

- Parallel Programming Workshop (26-30 November 2012), Barcelona, Spain.

- PUMPS Summer School 2012 (2-6 July 2012), Barcelona, Spain.

- Heterogeneous Programming on GPUs with MPI + OmpSs (23-24 May 2012), Barcelona, Spain.

- ICREA conference on Network Medicine Approaches to Human Disease: from Computers to the Clinic (21-23 November 2011), Barcelona, Spain.

- PRACE Autumn School (25-27 October 2011), GENCI/CEA (TGCC), Bruyères-le-Châtel, Paris, France.

- PUMPS Summer School 2011 (18-22 July 2011), Barcelona, Spain.

- Exascale Challenges in Computational Biology (13-15 December 2010), Barcelona, Spain.

- PRACE Autumn School 2010 (25-29 October 2010), Barcelona, Spain.
- PRACE Tutorial (6-9 August 2010), Barcelona, Spain.
- PUMPS Summer School 2010 (5-9 July 2010), Barcelona, Spain

Teaching Experience:

- Director of the Bachelor's Thesis *Optimization of the cluster analysis tool pyProCT with pyCOMPSs* by Pol Alvarez Vecino. Engineer's Degree in Computer Science (UPC, Barcelona), 2015 (http://hdl.handle.net/2117/79993).
- Director of the Bachelor's Thesis *Protein vibrational analysis using internal coordinates ANM* by Alba Rincón. Engineer's Degree in Computer Science (UPC, Barcelona), 2012- 2014 (http://hdl.handle.net/2099.1/24417).
- Director of the Bachelor's Thesis *PELE++ Software parallelization through GPUs* by Xavier Orò. Engineer's Degree in Computer Science (UPC, Barcelona), 2012 (http://hdl.handle.net/2099.1/15498).

Prizes and Grants:

- "Severo Ochoa 2015" Travel Grant (Gothenburg, Sweden).
- "International Summer School 2013" Travel Grant (New York, USA)
- "Best Poster Award" (PUMPS Summer School 2012, Barcelona, Spain)
- "PRACE Autumn School 2011" Housing Grant (Paris, France)

Personal Skills

Languages:

Mother tongue : Spanish, Catalan

Foreign languages:

	Listening	Reading	Speaking	Writing
English	●●●●	●●●●	●●●○	●●●○
Italian	●●●○	●●●○	●●○○	●○○○

Computer skills :

- Great knowledge of Unix environments and its ecosystem. SVN and git version control.
- Use of SQL and noSQL databases.
- Most frequently used programming languages:

Python	●●●●●
C / C++	●●●●●
Javascript (+HTML5)	●●●●○○
Java (+JavaME)	●●●●○○
FORTRAN	●●●●○○
Octave	●●●○○○
R	●●●●○○

- Excellent ability to learn new programming languages.
- Great knowledge of high performance computing techniques (e.g. OpenMP, MPI, CUDA/OpenCL).
- Creation and deployment of virtual machines with Vagrant.
- Great interest in software engineering (production methodologies, testing, etc.) and good coding practices (software craftsmanship).

Organizational and social skills:

- Ability to work individually and as a part of a team.
- Good communication skills.
- Perseverance and resolution.
- Fast learner.

Others

- Spanish car driving license (B license)
- “National Tennis Coach” title issued by the Catalan Tennis Federation (FCT, 2001).