

GERMAIN SALVATO VALLVERDU

Researcher in molecular simulations

1983 August 10 – Married, 2 children

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Inquisitive, exigent HPC specialist with 12+ years experience in numerical simulations and scientific programming. Seeking to leverage skills in communication, management and computer science as HPC engineer.

EXPERIENCE

Associate Professor

University of Pau & Pays Adour

📅 2010 – Ongoing

📍 Pau, France

- Develop multi-scale computational strategies adapted to complex systems
 - Develop and distribute data analyses libraries with Python
 - Supervise research projects with Ph.D. and Master students
 - Train UPPA users to HPC and programming languages using active learning
- 18 peer-reviewed articles, h-index 8, 200 citations

Research Engineer

CEA DAM

📅 2009 – 2010

📍 Bruyères le châtel, France

- Used C and MPI to include Dissipative Particle Dynamics algorithms in a massively parallel program
- Parametrization of coarse grain models for molecular simulations

Ph.D. in physical-chemistry

Université Paris Sud 11

📅 2006 – 2009

📍 Orsay, France

Theoretical study of photophysics properties of fluorescent proteins

- Produced molecular simulations of biological systems
- Used Fortran to write simulations and data analysis programs

PROJECTS

Energy storage materials – Li-ion batteries

University of Pau & Pays Adour / RS2E

- Surface reactivity of cathode materials
- Coupled studies between quantum chemistry and experimental surface characterization
- Interfaces: structure, electronic properties and thermochemistry

Petroleum chemistry and complex matrices

University of Pau & Pays Adour / C2MC

- Physico-chemical properties of asphaltenes: solubility, aggregation
- Molecular modelling and molecular dynamics simulations
- Molecular characterization of complex matrices (heavy crude oil)

Python Scientific Libraries

University of Pau & Pays Adour

- Pymatgen: Python Materials Genomics (<http://pymatgen.org/team.html>)
- Mammoth: a molecular force field optimizer (https://mammoth_uppa.gitlab.io/)
- Mosaïca: a generator of nano-materials based on their intrinsic geometry

SKILLS

High Performance Computing ●●●●●

Molecular Modelling ●●●●●

Mathematics / Statistics ●●●●●

Data Visualization ●●●●●

Computer science

Python

Slurm

Linux/Unix/Bash

MPI

Fortran

C

Machine Learning

git

Java

Plotly/Dash

HTML/CSS/PHP

Hugo/Jekyll

Django

Visual Studio Code

Simulations code

Lammps

VASP

Gromacs

Amber

Gaussian

Orca

VMD

LANGUAGES

English ●●●●●

Spanish ●●●●●

EDUCATION

Ph.D. in physical-chemistry

📅 2006 – 2009

📍 Université Paris-Sud 11

M.Sc. in Physical-Chemistry

📅 2004 – 2006

📍 Université Paris-Sud 11

Magistère de Physico-Chimie Moléculaire

📅 2003 – 2006

📍 Université Paris-Sud 11
ENS Cachan

CPGE in Physics & Chemistry

📅 2001 – 2003

📍 Lycée F. Arago Perpignan