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 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 | 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