GERMAIN SALVATO VALLVERDU

Scientific Computing Developer Engineer

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Inquisitive, exigent scientific computing specialist with 10+ years experience in numerical simulations and scientific programming. Seeking to leverage skills in communication, management and computer science as developer engineer.

EXPERIENCE

Associate Professor in numerical simulations

University of Pau & Pays Adour

2010 – Ongoing Pau, France

- Develop original multi-scale computational strategies adapted to chemical systems in multi-disciplinary teams
- 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 orcid.org/0000-0003-1116-8776

Research Engineer

CEA DAM

2009 – 2010 Bruyères le châtel, France

- Developed parallel, MPI-based, C routines to extend HPC code
- Accomplished the parametrization of advanced models for energetic materials

Ph.D. in computational physical-chemistry

Université Paris Sud 11

2006 – 2009 Orsay, France

Theoretical study of photophysics properties of fluorescent proteins

- Developed novel numerical simulation strategies adapted to biological systems
- Elaborated Fortran routines to produce and analyze high throughput simulations

PROJECTS

Pymatgen - Python Material Genomics — Active contributor

- Use python to implement new features for high throughput production and analyzes of quantum chemistry simulations: `http://pymatgen.org/team.html`

Mass Spectrometry Imaging Software (LA-ICP MS) — Lead programmer

- Build python notebooks for data analyzes that answer experimenters needs
- Plotly-Dash web application: Chemical mapping imaging and data exploration `https://pychemapps.univ-pau.fr/icpms/`

Mosaïca - A nano-materials constructor — Lead programmer

- Use python to implement new algorithms and provide a new library to generate shape deformations on nano-materials
- Develop a plotly-Dash web application to visualize structural data `https://pychemapps.univ-pau.fr/mosaica/`

Mammoth - A molecular force field optimizer — Lead programmer

- Implement algorithms for efficient optimization of force-field parameters `https://mammoth_uppa.gitlab.io/`

HPC SIMULATIONS

Energy storage materials – Li-ion batteries

Surface reactivity of cathode materials from experimental/computational approaches

Petroleum chemistry and complex matrices

Molecular modelling and simulations of crude oil and asphaltens subfractions.

SKILLS

- **Computer science** ●●●●●
- **Mathematics / Modeling** ●●●●○
- **Data Science** ●●●●○
- **HPC** ●●●●○

Computer science details

- **Python** ●●●●●
- **Java** ●●○○○
- **Linux/Unix/Bash** ●●●●○
- **C / Fortran** ●●●●○
- **git** ●●●○○
- **Machine Learning** ●●○○○

OOP · Jupyter · Plotly · Dash · MPI · HTML/CSS · Hugo/Jekyll · Django · Sphinx-doc · LaTeX

LANGUAGES

- **French (native)** ●●●●●
- **English** ●●●●○

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 Arago Perpignan