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 and 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

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 simulations 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 https://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

SKILL

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

Computer science details

Python	●●●●●
Linux/Bash/Unix	●●●●○
C / Fortran	●●●●○
git	●●●○○
Java	●●○○○
Maching Learning	●●○○○

OOP · Jupyter · pandas · MPI · numpy/scipy · Plotly · HTML/CSS · Dash · C++ · LaTeX · Django · github/gitlab · Sphinx-doc · Hugo / Jekyll

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