**Germain Salvato Vallverdu**

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January 6, 2020

Dear Madam, Dear Sir,

I am sending you my application in response to the job offer for Developer AI, reference 19640BR.

Currently as an associate professor at the University of Pau and Pays de l'Adour, I have ten years' experience in numerical simulations and scientific programming in the field of computational chemical-physics as well as high-performance computing. Inquisitive, through my research activities, I contribute to projects linked to miscellaneous scientific domains, such as biological systems and the study of photophysical properties in fluorescent proteins; electrode materials for Li-ion batteries and the chemical reactivity at interfaces; crude oil and the chemical characterization of aggregation processes.

Through the implementation of these projects, I acquired the specificities of the fields to set up and to conduct fruitful exchanges within multidisciplinary teams and supervise the Phd students or post-doctoral researchers of the project. Adapting my skills to each encountered problematic, I designed relevant models, implemented the associated numerical simulations and in particular developed the scientific programs necessary for the production including the analyses and the interpretation of the results obtained from these simulations.

Today, I would like to use my experience and skills for the benefit of new projects within the Total Group. This choice is obvious for two reasons. Firstly, Total is a world leader in the energy sector. Energy production and distribution is a major challenge of the 21st century in both societal and environmental terms. Secondly, Total has for many years been a major international actor in high-performance scientific computing both in terms of hardware, with the Pangea machine ranked among the most powerful supercomputers in the world, and in terms of the development. These two aspects constitute a particularly stimulating context in which I wish to take up new challenges and bring an original perspective from my background.

Yours faithfully.

Germain Salvato Vallverdu

# GERMAIN SALVATO VALLVERDU

## Scientific Computing Developer Engineer

@ germain.vallverdu@gmail.com  +33 6 88 59 08 87  github.com/gvallverdu

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 · C++ · LaTeX · MPI · HTML/CSS · Hugo/Jekyll · Django · Sphinx-doc

## 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