Arnaud Allera

Atomic-scale materials modelling expert

Molecular dynamics | Artificial intelligence | Materials science

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Experience

Feb. 2022 – Feb. 2024 **Postdoctoral researcher at CEA Saclay**, *DES-SRMP*, FR.
Developed a new method for structural analysis using deep learning. Developed a Machine-learning force-field fine-tuned on an extended dislocations database, for large-scale free energy calculations. *PI: M.C. Marinica.*

2018 – 2022 **PhD in Physics at Univ. Lyon and IRSN**, *collab. INSA Lyon*, Lyon, FR.
Atomistic modelling of screw dislocations glide and pinning in Fe-C steel.
Used molecular dynamics simulations to identify atomic-scale mechanisms of alloy strengthening. Developed a computationally efficient potential for Fe-C based on DFT calculations. *Supervision: D. Rodney , M. Perez , F. Ribeiro .*

2018 **Master thesis at Deakin University**, *IFM*, Melbourne, Australia.
Modelling and experimental study of novel Al-Sc alloys. *PI: M. Barnett*

Skills

Tools **Python**, C++ 11, F90, JS. Specialized software: **LAMMPS**, VASP, ASE
AI **Tensorflow**, JAX, Torch, Force-Fields models (SNAP, kernels), DeepSpeed
Cloud/HPC Docker, Gitlab/Github CI/CD, Supercomputers usage (5 yrs exp.)
Fluency in French (native), English

Selected Open Source projects

MiLaDy: Machine-learning Interatomic potential package (Fortran /🐍/TF)
PAFI: Anharmonic Free Energy calculations in LAMMPS (C++/🐍)
LAMMPS plugin for VS Code (JS, 22k+ installs), misc. contribs. to LAMMPS, matscipy, atomman, ase.

Selected communications

A. Allera, A. M. Goryaeva, I. Mouton, C. Flament, P. Lafourcade, J-B Maillet, MC. Marinica, Comp. Mat. Sci. 112535 (2024).

P. Lafourcade, J-B Maillet, C. Denoual, E. Duval, A. Allera, A. M. Goryaeva, MC. Marinica, Comp. Mat. Sci. 112534 (2024).

A. Allera, F. Ribeiro, M. Perez, D. Rodney, Phys. Rev. Mater., 013608 (2022).

Teaching

2018–2020 **Physics Teaching Assistant (107h)**, *1^{st} y. bachelors*, INSA Lyon, 2 years.
In charge of practical sessions and tutorials for a group of 25 students, 3 to 6h/week.

Education

2013–2018 **INSA Lyon**, *Engineering Degree in Materials Science*, Lyon, FR.
Metallurgy, Solid state physics, Mechanics of Materials, Finite Elements