Arnaud Allera

Atomic-scale materials modelling and artificial intelligence.

Molecular dynamics | Artificial intelligence | Materials science | HPC | Data science | Force fields

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Experience

Feb. 2022 – **Post-doc. at CEA Saclay**, *DES/ISAS/DMN/SRMP*, FR.
Deep learning-based methods for large-scale molecular dynamics simulations analysis and coarse-graining. Design of a new atomic descriptor to efficiently encode local atomic environments at extreme computational scales. Application to crystal phase and defect identification in highly disturbed atomic systems.
Development of a Machine-learning force-field fine-tuned on a database of DFT dislocations configurations in Fe, to allow for large-scale anharmonic free energy calculations of kink-pair nucleation. *Supervisors: M.-C. Marinica, A. Goryaeva.*

2018 – 2022 **PhD in Physics, at IRSN/Univ. Lyon1**, *collab. INSA Lyon*, Lyon, FR.
Multi-scale modelling of screw dislocations glide and pinning in Fe-C steel.
Molecular dynamics simulations of thermally-activated migration of pinned dislocations. Integration in a Kinetic Monte Carlo model of dislocation pinning. Development of a computationally efficient potential for Fe-C based on DFT calculations. Anharmonic free energy calculations of dislocation glide.
Supervisors: D. Rodney (Lyon1), M. Perez (INSA Lyon), F. Ribeiro (IRSN).
Collaborations: J. Marian (UCLA), T. D. Swinburne (CNRS).
Jury: E. Clouet, C. Becquart, W. Curtin, C. Varvenne, J. Colombani

2018 **Master thesis at Deakin University**, *IFM*, VIC, Australia.
Experimental and modelling study of novel scandium-aluminum alloys. Optimized mean field model, Small-Angle Neutron Scattering, Atom probe tomography, Electron Microscopy. *Supervisor: Matthew Barnett*

Open source software projects

Unseen (sole author): ML/DL simulation data analysis at the atomic scale (, Tensorflow/PyTorch, interfaced with HPC C++/Fortran codes)
MiLaDy: Machine-learning Interatomic potential package (Fortran /)
PAFI: Free Energy calculation beyond the harmonic assumption (C++/)
LAMMPS plugin for VS Code: autocompletion, docs browser (JS, 15k+ installs), KMC dislocation glide model (C++, forked from Marian group)
LAMMPS (Molecular Dynamics, C++), atomman, ase, matscipy ()

Skills

Programming **Python** (packaging and distribution), **C++ 11**, F90, JS

AI **Pytorch, Tensorflow/Keras, Scikit-Learn**, Force-Fields models (SNAP, Milady, kernels), Model Optimization and Parallelism, MLOps

Simulation **LAMMPS** (MD, free energy calculations), KMC, VASP (DFT), ASE

Cloud/HPC 5 years as an HPC user on **4+ Top supercomputers, Docker**, Gitlab/Github CI/CD, cloud (AWS), slurm/SGE, workflow managers

Git, GNU/Linux, LaTeX, Inkscape

Fluency in French (native), English

Publications

- *Neighbors Map: an Efficient Atomic Descriptor for Structural Analysis using Neural Networks.*, A. Allera, A. M. Goryaeva, P. Lafourcade, J-B Maillet, M.-C. Marinica (arXiv:2307.00978).
- *Robust crystal structure identification at extreme conditions using a density-independent spectral descriptor and supervised learning.*, P. Lafourcade, J.-B. Maillet, C. Denoual, E. Duval, A.Allera, A.M. Goryaeva, M.-C. Marinica (arXiv:2307.01560).
- *Carbon-induced strengthening of bcc iron at the atomic scale*, A. Allera, F. Ribeiro, M. Perez, D. Rodney, Physical Review Materials, 6(1) 013608 (2022).

Reviewer for *Computational Materials Science*

Presentations

Conferences (as speaker) MMM10, COSIRES 2022, MRS 2020, GDR IAMAT (2022), Plasticité (2021–2023)

Selected Workshops IPAM@UCLA: "Complex Scientific Workflows at Extreme Computational Scales", IDRIS-CNRS: "Optimized Deep-Learning on Large Models", GdR IAMAT: "Artificial Intelligence for Materials Science", GDR ModMat (2019).

Invited seminar ICAMS, Ruhr University Bochum, Germany, 2021

Teaching

2019–2022 **Numerical tools for research**, Univ Lyon, FR.
In charge of a 16h postgraduate training program including Git, Python, Matlab, GNUplot, data storage and LaTeX skills for PhD students.

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

2014–2018 **Tutoring**, *from high school level to bachelors.*
10+ students, from high school level to bachelors.

Education

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

References

Dr. Mihai-Cosmin Marinica, CEA Saclay — *mihai-cosmin.marinica@cea.fr*
Pr. David Rodney, Univ. Lyon — *david.rodney@univ-lyon.fr*
Dr Thomas D. Swinburne, CINAM – CNRS — *thomas.swinburne@cnrs.fr*