Anruo Zhong

PhD in Physics

My keywords: machine learning, computational materials science, scientific software development.

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zhonganr

Languages

- English (C1, TOEFL: 102/120)
- French (C1)
- Chinese (native)

Professional skills

Programming languages

- Python (advanced)
- C/C++ (advanced)
- Fortran (advanced)
- Matlab (intermediate)
- SQL (intermediate)
- JavaScript (novice)

Modeling and simulation

- Atomic scale and quantum mechanics: LAMMPS, VASP
- Finite-elements method: HyperMesh, Ansys Mechanical
- Computer-aided design: SolidWorks, CATIA
- Computational fluid mechanics: ICEM CFD, Ansys Fluent

Information technology tools

- HPC and Linux environments
- Parallel computing: OpenMP, MPI
- Git, Docker
- LAPACK/ScaLAPACK

Machine learning

Scikit-Learn, TensorFlow, JAX, Apache TVM.

Other interests

Cycling, hiking, badminton, piano (national grade: 8/10), traveling, bakery.

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WORK EXPERIENCE

2021 – 2024 **Doctoral Researcher at SRMP, CEA Saclay, Gif-sur-Yvette, France** (3 years)
- Contribution to MILADY (Machine Learning Dynamics) and MILADY-LAMMPS packages: implementation of machine learning force fields for molecular dynamics (MD). Design and building of databases. `https://ai-atoms.github.io/milady-docs`
- Development of a Bayesian sampling method for enhanced free energy estimation and its applications: data-driven prediction of thermoelastic properties and defect behaviors for metallic materials (W, Mo, Fe, HEAs) at high temperatures.
- Communication: 3 research papers, 4 oral presentations at national and international conferences, 2 international collaborations.

Skills: solid mechanics and metallurgy, numerical modeling, programming (Python, C++, Fortran), HPC, machine learning, data analysis, oral and written communication, teamwork.

2021 **AI Engineer Intern at OPEN AI Lab, Shenzhen, China** (3 months)
- Feasibility study of machine learning compiler framework Apache TVM: pass infrastructure and quantization.

Skills: machine learning optimization, programming (Python).

2020 - 2021 **Research Intern at Chinese Academy of Sciences (CAS), Guangzhou, China** (6 months)
- Development of micromagnetic simulation software NMD (Nonlinear Magnetoelastic Dynamics): multi-geometry meshing, parallel partial differential equation solvers, graphical user interface and interface to finite-elements method tool. `https://github.com/zhonganr/NMD`
- Numerical simulation of magnetoelastic interaction in chiral magnets (MnSi) for future data storage devices. 2 research papers.

Skills: programming (C/C++), micromagnetic simulation, academic writing.

2020 **Mechanical Engineer Intern at China General Nuclear Power Corporation, Shenzhen, China** (3 months)
- Finite-elements method calculations (Ansys Mechanical) of nuclear island buildings under accident conditions and participation in report writing for Generic Design Assessment in the UK.

Skills: computational mechanics (FEM), structural analysis, technical writing, teamwork.

2019 **Software Engineer Intern at OPEN AI Lab, Shenzhen, China** (2 months)
- Implementation of accelerated matrix multiplication algorithm.

Skills: programming (C).

EDUCATION

2021 – 2024 **PhD in Physics, Paris-Saclay University, Gif-sur-Yvette, France**
- Supervisors: Mihai-Cosmin Marinica (CEA), Manuel Athènes (CEA)
- Thesis: Machine learning and adaptive sampling to predict finite temperature properties in metallic materials at the atomic scale

2019 – 2021 **Master of Engineering in Nuclear Engineering, Sun Yat-sen University (SYSU), Guangzhou, China** | Grade: 87.8/100, top 10%
- Supervisors: Zhipeng Hou (CAS), Yangfan Hu (SYSU)
- Thesis: Dynamics and stability of skyrmions in inhomogeneous elastic fields

2019 – 2020 **Exchange semester, Grenoble INP - Ense3, Grenoble, France**
- Nuclear Energy, *mention très bien*

2015 – 2019 **Bachelor of Engineering in Nuclear Engineering, Sun Yat-sen University, Guangzhou, China** | Grade: 3.4/4, top 25%
- Supervisor: Kan Lai (SYSU)
- Thesis: MD simulations of radiation damage in Ni-based alloys

2015 **National Undergraduate Admission Exam** | Option science, top 0.7%

ANNEXE

PUBLICATIONS

- **Zhong, A.**, Lapointe, C., *et al.* (2024). Unraveling temperature-induced vacancy clustering in tungsten: from direct microscopy to atomistic insights via data-driven Bayesian sampling. *PRX Energy.* Under Review.

- Wróbel, J., **Zhong, A.**, *et al.* (2024). Thermoelasticity, point defect thermodynamics and melting of high-entropy Ta-Ti-V-W alloys: predicting composition dependence using data-driven sampling and machine learning. *Npj Comput. Mater.* Under Review.

- Wan, X., **Zhong, A.**, *et al.* (2024). Discontinuous to continuous transition changeover and magnetic helicity reversal in helimagnet nanodisks under torsion. *New J. Phys.* 26 023009.

- **Zhong, A.**, Lapointe, C., *et al.* (2023). Anharmonic thermo-elasticity of tungsten from accelerated Bayesian adaptive biasing force calculations with data-driven force fields. *Phys. Rev. Mater.* 7 023802.

- **Zhong, A.**, Lan, X., *et al.* (2022). Dynamics and stability of skyrmions in a bent nano-beam. *New J. Phys.* 24 033019.

ORAL PRESENTATIONS

- 2023 TMS Annual Meeting (San Diego, US): Prediction of high-temperature elasticity of tungsten using machine learning and data-driven approach.

- 2023 MRS Spring Meeting (San Francisco, US): Anharmonic thermo-elasticity of tungsten from accelerated Bayesian adaptive biasing force calculations with data-driven force fields.

- 2023 Workshop Probabilistic Sampling for Physics (Orsay, France): Accelerated Bayesian adaptive biasing force method for sampling free energy profile.

- 2022-2023 FOCUS-EJN Annual Seminar (Saint-Rémy-lès-Chevreuse, France): Predicting temperature effects on the microstructural evolution of alloys using high-dimensional regression metamodels.

AWARDS

2015 – 2021	Sun Yat-sen University Excellent Student Scholarship (6 consecutive years)
2019	CGN Excellent Graduate Student Scholarship (top 5%)
2019	Sun Yat-sen University Excellent Bachelor Program & Best Poster Award
2018	CentraleSupélec Jury Excellence Prize for Engineering Degree Program (top 5 in entrance examination)