YOUNGGAK SHIN

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PROFESSIONAL PROFILE

Ph.D in Mechanical Engineering with B.S. and M.S. degrees.

Proficient in Molecular Dynamics simulations, code development, and high-performance computing. Focused on simulations of materials for fusion environments and extreme conditions, with a strong passion for developing physics-based simulation and calculation tools.

PolyPal Project: Massive-Scale Parallel Atomistic Structure Generation Code

Project Manager / Core Developer [2022 - present]

- Developed a parallelised code generating massive polycrystalline structures containing billions of atoms for atomistic simulations.
- Developed input-output routines, grain characterisation, load-balancing and atom generation algorithms.
- Designed a unique MPI-IO multi-file output format preserving domain decomposition information enabling fast input reading from parallelised molecular dynamics code by eliminating atom sorting.
- Developed versatile options for polycrystalline structure such as variation in average grain size in certain direction, preferred crystallographic orientation and solute atom mixing.
- Achieved exceptional performance with near-perfect scalability; the generation of a polycrystalline structure containing 10 billions of atoms takes less than 3 minutes with 6,400 computing cores.
- Submitted a manuscript in *Computer Physics Communications* as the first author (accepted, available upon request).
- Available source code upon request.

VITMAS Project: Massive-Scale Parallel Molecular Dynamics Code

Project Manager / Core Developer [2021 - present]

- Developed a parallelised molecular dynamics simulation code for handling massive atomistic systems in primary knock-on atom (PKA) simulations.
- Designed the overall code structure.
- Developed input-output routines, time integration, *Nosé-Hoover* thermostat, interatomic force calculation, and multi-PKA creation routines.
- Tested with a polycrystalline system containing 8 billions of atoms.
- Conducted production runs on a supercomputing cluster, utilising approximately 100,000 cores at the national supercomputing centre (*Nurion-5, Korea Institute of Science and Technology Information*).
- Currently preparing a manuscript for a scientific journal.
- Available source code upon request.

Development of Electron Temperature Model for Molecular Dynamics Collision cascade Simulations

- Modified LAMMPS code to enable the implementation of electron-temperature-dependent two-temperature model (2TM).
- Calculated electronic specific heat and electron-phonon coupling constants over a wide range of electron-temperature based on *ab-initio* calculations.
- Confirmed that the electron-temperature dependent 2TM affects defect production.
- Published a paper in *Nuclear Fusion* (DOI: https://doi.org/10.1088/1741-4326/ad64e7)
- Available source code upon request.

Safety assessment code Development for Commercial Fission Reactor

Solo Developer [2020 - 2023]

- Developed a safety assessment code for pressure tube in Canada Deuterium-Uranium (CANDU) reactor in collaboration with Korea Atomic Energy Research Institute.
- Developed Leak-Before-Break assessment code for pressure tube.
- Developed single-flaw assessment code for pressure tube.
- Integrated assessment codes for Leak-Before-Break and single-flaw analysis in pressure tube into a comprehensive program.
- Verified physics-based calculation functions and probability-model-based prediction functions with sensitivity analysis on key parameters.

- Authored extensive internal reports and manuals related to the project.
- Classified data.

SIDE PROJECTS

Pi-Cluster Build

- Built a small cluster with 4 *RaspberryPi 3* computers configured with OpenMPI and *Slurm* job scheduler.
- Experienced in building and maintaining computing clusters.
- Tested parallel codes on the *RaspberryPi* Cluster for debugging purposes.

Real-Time Rendering in Digital Twin System of Smart Factory

Visiting Developer [2018/7/3 - 2018/7/27] [2019/6/19 - 2019/7/3]

*On-site: German Institute of Artificial Intelligence (DFKI) Smart Factory at Kaiserslautern, Germany

- Visited 2 times as visiting researcher.
- Participated in the development of a digital twin system for monitoring real-time manufacturing processes in Smart Factory at DFKI, Germany.
- Contributed to code tracking and rendering real-time manufacturing process, bridging the physical system and a mixed reality device (*Microsoft HoloLens*).
- Collaborated with colleagues from diverse cultural backgrounds.

WORK EXPERIENCE

Postdoctoral Researcher

Yonsei University, September 2024 - Present

EDUCATION

Philosophical Doctor of Science in Mechanical Engineering

Kyung Hee University, completed August 2024

Thesis: Collision Cascade Molecular Dynamics Simulation with Realistic Test Samples

Master of Science in Mechanical Engineering

Kyung Hee University, completed August 2017

Thesis: First Principles Calculations on Interstitial Defects in W-Re-Ta Ternary System

Bachelor of Science in Mechanical Engineering

Kyung Hee University, completed August 2015

PUBLICATIONS

- Shin, Y., Kang, K., & Lee, B. (in press). PolyPal: A parallel microscale virtual specimen generator. *Computer Physics Communications*.
- Shin, Y., Kang, K., & Lee, B. (2024). Temperature-dependent electron–phonon coupling changes the damage cascades in neutron-irradiation molecular dynamics simulation in W. *Nuclear Fusion*, *64*(10), 106001.
- Moul, V., Shin, Y., & Lee, B. (2023). The Effects of Attractive Interaction on Viscosity in Undercooled Kob–Andersen Liquids. *Multiscale Science and Engineering*, *5*(3), 160-165.
- Shin, Y., Kang, K., & Lee, B. (2021). Reduced interstitial mobility through multicomponent alloying in bcc W. *Fusion Engineering and Design*, *172*, 112745.

INTERNATIONAL CONFERENCES

- Shin, Y., Kang, K., & Lee, B. (2024). Implementation of Electron Temperature Model to W Damage Cascades Molecular Dynamics Simulation under Neutron Irradiation. In *the 11th international conference on MMM*.
- Yoo, S., Shin, Y., Oh, S., Park, H., Kim, Y., Yoo, A., Kwon, O., Kang, K., Lee, B.. (2023). Grain-boundary Effects on the Irradiated Damages in W-Re Alloys. In *TMS annual Meeting*.
- Yoo, S., Oh, S., Shin, Y., Kwon, O., Kang, K., & Lee, B. (2022). Parallel I/O optimization for micrometer-scale atomistic calculations under extreme conditions. In *APS April Meeting Abstracts* (Vol. 2022, pp. S07-009).
- Shin, Y., Lee, B., & Kang, K. (2022). Reduced Interstitial Mobility in W Based Transition Metal Ternary Systems. In *TMS Annual Meeting*.
- Shin, Y., Lee, B. (2018). Defect energetics in W-based transition-metal ternary systems. In *the 9th international conference on MMM*.

ADDITIONAL SKILLS

- **Software**: LAMMPS, DL_POLY, VASP, Ovito, VMD, Git, Jupyter, LaTEX, XMGRACE, Affinity Designer, Keynote, Microsoft Office
- **Programming languages**: C/C++, Python, MATLAB
- **Parallel computing**: Linux/Unix OS, Slurm, SGE, OpenPBS, MPI, OpenMP
- **Machine learning**: Tensorflow, Keras, PyTorch