

Myung Chul (Michael) Kim

PhD Candidate, Mechanical Engineering | Stanford University | U.S. Permanent Resident

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Research Summary

PhD candidate in Mechanical Engineering at Stanford developing theory and numerical algorithms for **importance sampling of rare events**, which are transitions too infrequent for direct simulation to reach. I parameterize the committor function with a graph neural network, use it to bias Langevin dynamics toward rare transitions, and recover **unbiased** transition rates and reaction-channel probabilities by reweighting each path with Monte Carlo normalization factors. The central result is **error correction**: the rates stay correct even when the learned committor carries significant approximation error, which is unavoidable in high dimensions. For vacancy migration in bcc Fe ($d=2055$) the rates match brute-force simulation within 3%, whereas the uncorrected estimate is 44% low, and for Pt adatom diffusion on Pt(001) ($d=387$) the method resolves twelve competing diffusion channels. With collaborators I also model strain in Si-Ge-Sn nanowires and dislocation mobility in fcc Cu, and develop Burgers-vector identification for dark-field X-ray microscopy. Two first-author preprints and four manuscripts in preparation.

Education

Stanford University, PhD in Mechanical Engineering [GPA: 3.93/4.0] Sept. 2023 – June 2028

- Advisor: Professor Wei Cai (Micro and Nano Mechanics Group)
- Research area: Monte Carlo methods, molecular dynamics, statistical mechanics, scientific machine learning
- Coursework: Stochastic Differential Equations, Partial Differential Equations, Numerical Linear Algebra, High Performance Computing, Finite Element Analysis, Reinforcement Learning, Machine Learning and the Physical Sciences, Advanced Physical Chemistry, Applied Quantum Mechanics, Quantum Computing, Mathematical Finance

KAIST, BS in Mechanical Engineering and Electrical Engineering (double major) Mar. 2019 – Aug. 2023

Georgia Institute of Technology, Exchange Program in Mechanical Engineering Jan. 2022 – Dec. 2022

Research Experience

Graduate Research Assistant, Stanford University – Stanford, CA Sept. 2023 – Present

Rare event theory and algorithms (primary thesis work)

- Derived an importance sampling framework for overdamped Langevin dynamics that extends kernel biasing (Cai et al., 2002) to the stopped transition kernel: a neural-network committor biases the kernel toward rare transitions while **preserving the relative probabilities** of competing reaction channels. For the exact committor the biased kernel is the **Doob h -transform** of the dynamics, and the path reweighting is the Radon–Nikodym derivative of the corresponding **Girsanov change of measure** (derived in the supplementary information).
- Derived and implemented an **unbiased** estimator of transition rates and channel probabilities that reweights each path by a product of Monte Carlo normalization factors, so the rates remain accurate **despite approximation error in the learned committor**; reading the rates directly off the committor instead errs by 35–44% for the Fe vacancy and 40% for LJ7.
- Adapted a **branching random walk** (stochastic splitting and Russian roulette) to control path-weight variance, and trained committors adaptively on self-generated paths with a replay library, a Polyak-averaged target network, and checkpoint weight averaging.
- Validated on the **Lennard–Jones 7 (LJ7)** benchmark ($d=14$): at 600 K the rate is 2% from brute force and all four rearrangement-channel fractions match it; a committor fine-tuned down to 300 K, where brute force is infeasible, agrees with Kramers theory to about 1%.
- Scaled to **vacancy migration in bcc Fe** ($d=2055$; 685-atom EAM crystal, fully periodic, no atoms fixed) with a SchNet-style graph neural network committor on a 50-atom local cluster: rates at 600–800 K are within 3% of 10^4 -walker brute force, and at 800 K all eight $\langle 111 \rangle$ jump fractions are within 0.004 of the exact $1/8$. Because direct training fails at 800 K ($\beta U_b \approx 9.7$), the committor was bootstrapped at 1600 K and refined at 800 K; reused unchanged, it reaches 500 K (rate $\sim 190\times$ lower), where an earlier brute-force run (800 K lattice) had not finished after 120 GPU-hours.
- Resolved **Pt adatom diffusion on Pt(001)** ($d=387$; 257-atom EAM slab, 129 mobile atoms) into 12 exchange, hopping, and long-jump channels at 1000 K (exchange-to-hopping ratio 6.27, matching brute force, against 11.5

without reweighting) and reused the 1000 K committor at 700–900 K within 4% of the brute-force ranges.

- Engineered the simulation stack in PyTorch: EAM (Pt, Fe) and Lennard–Jones potentials with autograd forces and Hessians, Verlet neighbor lists, string-method minimum energy paths and harmonic Kramers rates, `torch.compile`, memory-aware batch chunking, a CPU/CUDA regression suite, and 100-seed SLURM job arrays on A100/L40S GPUs. A companion discrete-state formulation for Markov chain Monte Carlo is on arXiv.

Application: all-atom alanine dipeptide kinetics (first-author manuscript in preparation)

- Extended the framework to all-atom alanine dipeptide in vacuum (AMBER14), computing $\beta/C5 \leftrightarrow C7_{eq}$ rates in both directions under constrained overdamped (66 Cartesian coordinates) and underdamped (132-dimensional phase space) Langevin dynamics.
- Ported the AMBER14 energy (OpenMM parameters, forces checked against OpenMM) and OpenMM’s Brownian and BAOAB integrators with SHAKE/RATTLE-style constraints to PyTorch, so ensembles of 10^4 walkers run in parallel on GPUs.
- Designed collective-variable-free graph neural network committors on interatomic distances, including a phase-space variant with signed radial-velocity features that distinguishes the direction of motion.
- Matched brute-force rates within 2.5% and 5.8% (overdamped) and came within 12–21% (underdamped, a systematic excess under study), whereas the same networks read directly err by up to $5.8\times$ and $121\times$.

Finite element modeling of semiconductor nanowires (NanoStrain; with Stanford MSE and SLAC)

- Built a 3-D anisotropic elasticity FEM model in FEniCSx/dolfinx with gmsh meshing and PETSc/MUMPS direct solves for a traction-free $\langle 111 \rangle$ Ge/GeSn/SiGeSn core/multishell nanowire lamella, with element-wise cubic stiffness rotated into the growth frame and a Vegard’s-law compositional eigenstrain including bowing terms (650,988 degrees of freedom).
- Drove the model from collaborators’ measured STEM-EDS composition maps, registering the hexagonal cross-section to the map (IoU 0.96) and using a bias-corrected normalized-Gaussian estimator for sparse-count quantification data.
- Verified the FEM core with a uniform-eigenstrain patch test and an analytical core–shell cylinder solution, checked equilibrium on every production solve, and compared predicted strain fields with collaborators’ **4D-STEM** maps.
- Derived the trigonal normal–shear coupling of the $\langle 111 \rangle$ -rotated stiffness behind the three-fold shear pattern, and formulated a two-channel (Sn/Si) EDS composition-error model fit on the in-plane strain deviator, which cancels the Vegard term and the reference offset; the stiffness is factorized once, with one back-substitution per channel.
- Wrote the FEM and composition-error sections of the supporting information of the manuscript in preparation.

Dislocation identification in dark-field X-ray microscopy (co-first author; theory and simulation, with the Dresselhaus-Marais group, Stanford MSE and SLAC)

- Derived the measurement theory that converts per-pixel center-of-mass maps from two goniometer scans into all three components of the projected distortion $\beta^\top \hat{\mathbf{q}}$, showing that the rocking center of mass of a standard rock–roll scan is biased by a resolution-function cross-moment that a rock– 2θ scan cancels.
- Derived a Burgers-circuit formula evaluated directly on measured center-of-mass maps and showed that it is insensitive to pixel blur when the loop encloses the blur kernel, which gives a loop-radius plateau test.
- Validated the protocol with a collaborator’s DFXM forward model (pyDFXM, run with trilinear resolution lookup and an orthonormal crystal frame) on all 12 signed $a/2 \langle 110 \rangle$ Burgers vectors in diamond at two reflections, recovering the Burgers-vector projection with rms error below $0.002a$.
- Reduced reflection choice to an integer separability criterion and identified (139) as the lowest-order allowed single reflection that separates all 12 candidates in diamond-cubic crystals; because it needs 40.8 vs. 12.1 keV and is $\sim 20\times$ weaker than (022), recommended a two-orientation $\{022\}$ measurement instead.

Dislocation mobility from internal-stress statistics (co-first author; collaborators’ ParaDiS data)

- Derived a closed-form (softplus) link-velocity law for dislocation networks from the distribution of internal resolved shear stress, with drag-limited, Orowan, and fluctuation-activated (sinh) limits; through the Orowan relation its short-link limit gives an explicit flow rule in which Taylor hardening enters as an exponential rate suppression.
- Computed internal-stress fields (128^3 grids, ExaDiS, SLURM job arrays) for 117 loading orientations of a collaborator’s discrete dislocation dynamics database of fcc Cu and found no orientation trend in the inverse width of the stress distribution ($c = 0.371 \pm 0.030 \text{ MPa}^{-1}$).
- With a single-length back stress, the resulting 4-parameter law fits simulated link velocities nearly as well as H. Zhai’s 14-coefficient empirical law scored on the same data (R^2 0.955 vs. 0.965).

Mechanics of fibrin fiber networks (in progress; collaborators’ imaging and tensile tests)

- Built a Python/LAMMPS pipeline (sole author of the 2026 rewrite; fiber generator ported from S. Mohanty) that generates 3-D fibrin networks (24,000 beads, 400 fibers, $\sim 8,500$ cross-links), stretches them quasi-statically to 100% strain and back, and adds history-dependent plasticity through per-element rest states for $\sim 32,000$ bonds and $\sim 23,000$ bending angles.
- Tuned the model by parameter sweep to collaborators' load-unload data (peak stress within 6%, hysteresis loop area within 2%; the unloading shape is not yet matched), using a Poisson ratio extracted from the collaborators' test videos by sub-pixel edge tracking, and wrote tabulated LAMMPS bond potentials to compare bond rupture with plasticity as the source of residual strain.
- Earlier (2024), reconstructed 3-D fibrin networks from collaborators' confocal image stacks on top of the open-source Qiber3D skeletonization, adding thresholding variants, periodic-boundary stitching, and volume-fraction and junction-density statistics that parameterized synthetic network models, and built the LAMMPS objective and experimental reference for S. Mohanty's Gaussian-process Bayesian optimization of coarse-grained parameters against a measured stress-strain curve.

Additional materials modeling

- Ran coarse-grained MD (LAMMPS) of cross-linked bead-spring polymer networks under uniaxial tension, extending a group workflow, and used graph analysis (shortest paths, edge betweenness centrality) to test whether rupturing bonds lie on the network's load-bearing shortest paths.
- Benchmarked a pre-trained Ni GAP machine learning interatomic potential (elastic constants, stacking-fault energies, thermal expansion) and computed screw-dislocation cross-slip barriers with a pre-trained tabGAP potential by a string method in LAMMPS, after reproducing published EAM barriers (1.93 vs. 1.92 eV).
- Formulated a population-balance model for dislocation link-length distributions under growth, random splitting, and annihilation, with closed-form solutions in limiting cases and a custom 1-D finite element solver for the general steady state.
- Applied discrete optimal transport (exact and entropic Sinkhorn solvers) to map collaborators' micro-CT grayscale histograms of Berea sandstone, including volumes super-resolved by their pre-trained generative model, onto their SEM reference distributions, lowering Otsu-threshold sensitivity relative to histogram matching (unsubmitted first-author draft).

Undergraduate Research Assistant, Georgia Institute of Technology – Atlanta, GA Jan. 2022 – Dec. 2022

- Conceived, designed, and fabricated a stretchable piezoelectric pressure sensor for tactile sensing, using a curved inter-digitated serpentine geometry to give structural stretchability to an intrinsically brittle piezoelectric material, enabling integration into artificial skin.
- Developed a closed-loop respirator fit-control mechanism driven by facial pressure feedback, yielding a $5\times$ higher fit score, together with flexible gas sensors for humidity monitoring.
- Designed flexible PCBs (Altium) and 3D-printed mechanical housings for wearable soft electronic assembly.

Publications and Preprints

91 citations, *h*-index 3, *i10*-index 3 as of Sept. 2026 at scholar.google.com/citations?user=lzw1uB4AAAAJ

Two articles featured as journal covers.

Accelerated Langevin Dynamics Simulation via Neural Network-Driven Importance Sampling

Mar. 2026

Michael Kim, Wei Cai

chemRxiv preprint | DOI: 10.26434/chemrxiv.15000772 (v1 Mar. 2026, v2 Apr. 2026)

Revised version with the Pt(001) and bcc Fe results in preparation

Accelerated Markov Chain Monte Carlo Simulation via Neural Network-Driven Importance Sampling

Jan. 2026

Michael Kim, Wei Cai

arXiv preprint | arXiv:2602.12294

- Smart Filtering Facepiece Respirator with Self-Adaptive Fit and Wireless Humidity Monitoring** Mar. 2025
Kangkyu Kwon, Yoon Jae Lee, Yeongju Jung, Ira Soltis, Yewon Na, Lissette Romero, Myung Chul Kim, Nathan Rodeheaver, Hodam Kim, Chaewon Lee, Seung-Hwan Ko, Jinwoo Lee, Woon-Hong Yeo
Biomaterials | DOI: 10.1016/j.biomaterials.2024.122866 | 16 citations
- Stretchable Wearable Wireless Bioelectronics Using All Printed Pressure Sensors and Strain Gauges** Feb. 2025
Nathan Zavanelli, Yoon Jae Lee, Myung Chul Kim, Allison Bateman, Matthew Guess, Hyeonseok Kim, Dinesh K. Patel, Woon-Hong Yeo
Advanced Materials Technologies | DOI: 10.1002/admt.202400998 | 12 citations
[Featured as Journal Cover]
- Advances in Electrochemical Sensors for Detecting Analytes in Biofluids** Aug. 2023
Jimin Lee, Myung Chul Kim, Ira Soltis, Sung Hoon Lee, Woon-Hong Yeo
Advanced Sensor Research | DOI: 10.1002/adsr.202200088 | 61 citations
[Featured as Journal Cover]
Manuscripts in preparation ([†]equal contribution)
- Shell-Resolved Elastic Strain Mapping in Radial Group-IV Multishell Nanowires** In prep.
Anis Attiaoui, Michael M. Kim, Áshildur Friðriksdóttir, Wei Cai, Colin Ophus, Paul McIntyre
- Burgers Vector Identification from Center-of-Mass Maps in Dark-Field X-Ray Microscopy** In prep.
Michael M. Kim[†], Brinthan Kanesalingam[†], Yifan Wang, Wei Cai, Leora Dresselhaus-Marais
- Dislocation Mobility from Internal Stress Fluctuations** (tentative title) In prep.
Michael M. Kim[†], Hanfeng Zhai[†], Shaswat Mohanty, Wei Cai
- Error-Correcting Importance Sampling for Descriptor-Free Acceleration of Rare Events: Application to Proteins** (working title) In prep.
Michael M. Kim, Wei Cai

Research Software

- ISLD**: importance-sampled Langevin dynamics Python, PyTorch, SLURM
 - Sole author. Implements the Langevin framework end to end: adaptive neural committor training (replay library, target network, weight averaging), EAM and Lennard–Jones potentials in PyTorch with autograd forces and Hessians, Verlet neighbor lists, string-method minimum energy paths, harmonic Kramers reference rates, branching random walk and Girsanov change-of-measure samplers, a CPU/CUDA regression suite, and brute-force validation across LJ7, Pt(001) adatom, and bcc Fe vacancy systems.
- ISMC**: importance-sampled Markov chain Monte Carlo Python, PyTorch, NumPy
 - Primary author (W. Cai contributed the package skeleton). Implements the discrete-space framework of the Markov chain Monte Carlo preprint (2-D and 14-D model potentials): neural-network and Gaussian bias potentials trained with a simulated-annealing temperature schedule, exact grid solutions of the optimal bias potential, branching random walk rate estimation, and Kramers-theory reference rates, with NumPy and PyTorch backends.
- protein**: accelerated conformational kinetics PyTorch, OpenMM
 - Sole author. Nine-subpackage package for neural-network importance sampling of all-atom peptide transitions: AMBER14 energy and constrained Brownian/BAOAB integrators in PyTorch (forces checked against OpenMM), graph neural network committor training, branching random walk rate estimation, censored brute-force rate estimation, and SLURM/GPU orchestration.
- NanoStrain**: EDS-fed nanowire strain FEM Python, FEniCSx, PETSc
 - Primary author (W. Cai set up the repository and a test stub). EDS-driven anisotropic elasticity pipeline: EDS map ingestion and denoising, hexagonal cross-section registration, gmsh mesh generation, composition-dependent stiffness and eigenstrain assembly, patch-test and analytical verification, and two-channel composition-error fitting

against 4D-STEM strain maps.

netsim: fibrin network simulation

Python, LAMMPS

- Sole author of the 2026 rewrite (the Frenet–Serret fiber generator is ported from S. Mohanty). Fibrin network generation, LAMMPS script generation with per-element plastic rest states and tabulated bond potentials, and SLURM parameter sweeps with provenance logging and automatic scoring against experiment and a straight-line baseline.

reconstruct: 3-D fibrin network reconstruction from confocal images

Python, NetworkX

- Extends the open-source Qiber3D skeletonization (MIT license) with thresholding variants, periodic-boundary stitching, NetworkX graph statistics (volume fraction, junction density), and LAMMPS data files with bond and angle terms for coarse-grained stretching tests.

Agent-Guided Variance Reduction (hackathon project)

Python, Claude Code

- Project for the *Built with Claude: Life Sciences* hackathon (July 2026): used Claude Code in a propose, implement, run, and analyze loop to compare three path-weight control schemes (no resampling, sequential importance resampling, branching random walk) for importance-sampled alanine dipeptide $\beta/\text{C5} \leftrightarrow \text{C7}_{\text{eq}}$ kinetics against brute-force MD; branching matched the brute-force rates within 3–6% in both directions.

Polymer network shortest-path analysis

Python, NetworkX

- Extended S. Mohanty’s parallel Dijkstra shortest-path code for coarse-grained polymer networks: explicit path storage, tracking of individual bond-rupture events across strain steps, and scoring of ruptured bonds against shortest-path membership and edge betweenness centrality.

CS 234 project: importance sampling as value-function learning

Python, PyTorch

- Stanford CS 234 (Reinforcement Learning) course project, Winter 2026, sole author: framed neural-committor training as value-function learning in a Markov reward process with a fixed Langevin policy and a Bellman-residual loss; on 2-D and 14-D model potentials, branching random walk rates agreed with Kramers theory within 3%.

Conference Presentations

HAI Fall Conference 2026: Confronting Our AI Future, Stanford HAI – Stanford, CA Oct. 2026

- Error-Correcting Importance Sampling for Descriptor-Free Acceleration of Rare Events

Empirical Methods in the Age of AI, Stanford Causal Science Center & Stanford Data Science – Stanford, CA Oct. 2026

- Error-Correcting Importance Sampling for Descriptor-Free Acceleration of Rare Events

ChemAI NYC 2026, Simons Center for Computational Physical Chemistry, New York University – New York, NY June 2026

- Accelerated Langevin Dynamics Simulation via Neural Network-Driven Importance Sampling

ICME Research Symposium 2026, Stanford Institute for Computational & Mathematical Engineering – Stanford, CA May 2026

- Accelerating Langevin Dynamics Simulation of Rare Events

AI+Science: Accelerating Discovery, Stanford HAI – Stanford University May 2026

- Accelerating Rare Event Simulations

MRS Spring Meeting, Materials Research Society – Honolulu, HI Apr. 2026

- Neural Network Driven Importance Sampling for Accelerated Kinetic Monte Carlo of Rare Events

DAMOP 2025, 56th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics – Portland, OR June 2025

- Accelerating Monte Carlo Simulation of Rare Events by Importance Sampling using Neural Network

BMES 2022 Annual Meeting, Biomedical Engineering Society – San Antonio, TX Oct. 2022

- Smart Filtering Facepiece Respirator with Adaptive Fit and Wireless Humidity Monitoring

Gordon Research Conference, Multifunctional Materials and Structures – Ventura, CA Sept. 2022

- Stretchable Pressure Sensor using Inter-Digitated Serpentine Structure

Awards and Honors

James D. Plummer Graduate Fellowship , Stanford University	Sept. 2023 – Aug. 2024
Young Engineers Honors Society , National Academy of Engineering of Korea	Mar. 2020 – Aug. 2023
National Science & Technology Scholarship , Korea Ministry of Science and ICT	Mar. 2019 – Aug. 2023
Global Leadership Award , KAIST	Mar. 2023
Student Design Finalist , Biomedical Engineering Society and Medtronic	Oct. 2022
Open Innovation Challenge Award , Korean Society of Mechanical Engineers	Oct. 2022
President's Undergraduate Research Award , Georgia Institute of Technology	Aug. 2022
Guwon Academic Excellence Scholarship , Guwon Scholarship Foundation	Aug. 2020
KAIST Academic Excellence Scholarship , KAIST	Aug. 2020

Teaching and Mentoring

Teaching Assistant , ME 123: Computational Engineering – Stanford University	Spring 2026
Teaching Assistant , ME 346A: Introduction to Statistical Mechanics – Stanford University	Winter 2025
• Wrote the Python (Colab) template and solutions for the transfer-matrix and Monte Carlo problems of the Ising problem set, comparing exact transfer-matrix and Metropolis results for a two-row Ising strip; used by the Winter 2025 class.	
Undergraduate Researchers Mentored , Stanford University	2024 – 2025
• Saul Eduardo Perez Herrera (Stanford SURF, Summer 2025), National Autonomous University of Mexico: transferability of machine learning interatomic potentials for large-scale MD • Eitan Cohen Arazi (Winter 2024), University of Buenos Aires	

Patents

A Method and Apparatus for Classification of Subtypes of Cells with Morphological and Motility Features using Hybrid Learning	Jan. 2025
Hyunjong Shin, Chanhong Min, Minwoo Kang, Hyuntae Jeong, Taeyoon Kwon, <u>Myung Chul Kim</u> KR Patent 10-2762542	

Technical Skills

Programming: Python (NumPy, SciPy), C, MATLAB, Bash
Machine Learning: PyTorch (autograd, <code>torch.compile</code>), graph neural networks (SchNet-style message passing), neural-network committers and bias potentials, replay-buffer and target-network training, pre-trained machine learning interatomic potentials (GAP, tabGAP), Weights & Biases
Computational Methods: Markov chain and kinetic Monte Carlo, importance sampling and variance reduction, Girsanov reweighting, Langevin and molecular dynamics integrators (Euler–Maruyama, BAOAB, constrained dynamics), SDE discretization and simulation, committer analysis, transition rate and pathway-probability estimation, censored-data rate estimation, string-method minimum energy paths, harmonic transition-state and Kramers rate calculation, finite element analysis (anisotropic elasticity, eigenstrain), FFT spectral elasticity, optimal transport, graph algorithms (shortest paths, betweenness centrality), image thresholding and skeletonization, high performance computing
Simulation and Tools: LAMMPS, OpenMM, ASE, FEniCSx/dolfinx, FEniCS, gmsh, PETSc/MUMPS, ExaDiS, SLURM (A100/L40S GPUs), NetworkX, scikit-image, POT, h5py, Git, SolidWorks, AutoCAD, Altium Designer, PSpice
Languages: English (fluent), Korean (native)