

SOOKYUNG KIM, PH.D.

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Lawrence Livermore National Laboratory, 7000 East Ave, Livermore, CA 94550, USA

RESEARCH INTERESTS

Material Science, Machine Learning, Computer Vision, Reinforcement Learning

EDUCATION

Georgia Institute of Technology, Atlanta, Georgia, USA *May 2017*

Ph.D. in Computational Material Science (Advisor: Prof. Hamid Garmestani)

M. S. in Computational Science & Engineering (Advisor: Prof. Richard Fujimoto)

Thesis: Hybrid Computational Modeling of Thermomagnetic Material Systems

Columbia University, New York, New York, USA *May 2009*

M. S. in Electrical Engineering

Ewha Woman's University, Seoul, Korea *Jun 2007*

B. S. in Electrical Engineering, Physics

UC Berkeley, Berkeley, California, USA *Jun - Aug 2005*

Exchange Program

EMPLOYMENT

Lawrence Livermore National Lab., Livermore, CA, USA *Jan 2017 - Present*

Machine Learning Scientist, Center for Applied Scientific Computing

Earth Science and Grid Federation group (Supervisor: Dean N. Williams)

- Predicting extreme climate events using neural networks.

Material Informatics (LDRD) (Supervisor: Dr. Han. T. Yong)

- Predicting density of molecule using Gated Graph Neural Networks.
- Predicting 3D geometry of crystal structure of High Energy Molecule using Reinforcement Learning

Sandia National Lab., Livermore, CA, USA *Jan 2016 - Nov 2016*

Research Scientist Intern, Hydrogen and Materials Science Department

(Supervisor: Dr. Jonathan Zimmerman, Dr. Catalin Spataru)

- Developing Monte-Carlo software based on LSF spin model in C++. Analyzing data from ab-initio DFT using machine learning techniques.
- Studying high temperature Spin-coupling effect to stacking fault energy in stainless steel.

Lawrence Livermore National Lab., Livermore, CA, USA *Jun - Aug 2014, Jun - Dec 2015*

Research Scientist Intern - CCMS program, Physics and Lifescience Division

(Supervisor: Dr. Lorin Benedict, Dr. Mike Surh)

- Developing Monte-Carlo software based on Heisenberg model in C++, statistically simulating spin thermo-dynamics of $FeCo_xB_{(1-x)}$ and $CoPt$.
- GPU-utilized parallelization of the Heisenberg Monte-Carlo software.

Pacific Northwest National Lab., Richland, WA, USA *Oct 2011 - Dec 2012*

Research Student Intern, Advanced Computing, Mathematics and Data Division

(Supervisor: Dr. Kim Ferris)

- Computing thermo-magnetic properties for *MnBi/MnSb* using ab-initio MD (NWChem) and Abinitio DFT.
- Constructing a solvent based carbon capture materials database using SQL to analyze solid sorption materials with their kinetic and thermodynamic parameters.

PUBLICATIONS

1. **Sookyung Kim, Joanne Kim, Brenden K Peterson.** An Interactive Visualization Platform for Deep Symbolic Regression. *IJCAI - demonstration track (submitted)*, 2020.
2. **Sookyung Kim, Sunghyun Park, Kangyeol Kim,** Joonseok Lee, Junsoo Lee, Jiwoo Lee, Jaegul Choo. Hurricane Nowcasting with Irregular Time-step using Neural-ODE and Video Prediction. *Tackling Climate Change with Machine Learning on ICLR*, 2020.
3. Bhavya Kailkhura, Brian Gallagher, **Sookyung Kim,** Anna Hiszpanski, T Yong-Jin Han. Reliable and explainable machine-learning methods for accelerated material discovery. *Nature, NPJ. Computational Material*, 2019.
4. **Sookyung Kim, Yongwoo Cho,** Peggy Li, Mike Surh, Yong Han. Physics-guided Reinforcement Learning for 3D Molecular Structures. *ML for Physical Science on Neurips*, 2019.
5. **Sookyung Kim,** Peggy Li, Joanne Kim, Piyush Karende, Yong Han. Optimizing 3D structure of H₂O molecule using DDPQ. *RL for Real Life on ICML*, 2019.
6. **Sookyung Kim,** Sunghyun Park, Sunghyo-Chung, Yun-sung Lee, Joonseok Lee, Hyojin Kim, Mr Parbhat and Jaegul Choo. Focus and Track: Tracking hurricane events. *Climate Change: How AI can help on ICML*, 2019.
7. **Sookyung Kim,** Sunghyun Park, Sunghyo-Chung, Yun-sung Lee, Joonseok Lee, Hyojin Kim, Mr Parbhat and Jaegul Choo. Focus and Track: Tracking hurricane events. *30 th British Machine Vision Conference (BMVC)*, 2019.
8. **Sookyung Kim,** Hyojin Kim, Sangwoong Yoon, Joonseok Lee, Samira Kahou, Karthik Kashinath, and Mr Prabhat. Deep-Hurricane-Tracker: Tracking and Predicting Extreme Climate Events using ConvLSTM. *IEEE Winter Conference on Applications of Computer Vision (WACV)*, 2019.
9. **Sookyung Kim,** Sangwoong Yoon, Hyojin Kim, Samira Kahou, Karthik Kashinath, and Mr Prabhat. Tracking Extreme Climate Events in Spatio-temporal Climate Data. *European Conference on Computer Vision (ECCV) WiCV Workshop*, 2018.
10. **Sookyung Kim,** Sangwoong Yoon, Hyojin Kim, Samira Kahou, Karthik Kashinath, and Mr Prabhat. Tracking extreme climate events using Neural Networks, *Climate Informatics (with spotlight oral presentation)*, 2018.
11. **Sookyung Kim,** Jungmin. M. Lee, Jiwoo Lee, and Jihoon Seo. Deep-dust: Predicting concentrations of fine dust in Seoul using LSTM, *Climate Informatics*, 2018.
12. **Sookyung Kim,** Mayur Mudigonda, Ankur Mahesh, Samira Kahou, Karthik Kashinath, Dean Williams, Vincent Michalski, Travis O'Brien and Mr Prabhat. Segmenting and Tracking Extreme Climate Events using Neural Networks, *First Workshop Deep Learning for Physical Science on NIPS*, 2017.
13. **Sookyung Kim,** Sasha Ames, Jiwoo Lee, Chengzhu Zhang, Aaron C. Wilson and Dean Williams. Framework for Detection and Localization of Extreme Climate Event with Pixel Recursive Super Resolution, *Seventh Workshop Data Mining on Earth System Science. ICDM on IEEE*, 2017.
14. **Sookyung Kim,** Sasha Ames, Jiwoo Lee, Chengzhu Zhang, Aaron C. Wilson and Dean Williams. Massive Scale Deep Learning For Detecting Extreme Climate Events, *Climate Informatics*, 2017.
15. **Sookyung Kim.** Machine Learning for Earth System Grid Federation (ESGF), *ESGF Proposal Review Meeting*, 2017.

16. **Sookyung Kim**, Robert Lee, Richard Fujimoto. Heisenberg Monte-Carlo Simulation with High Performance Computing, To appear in *International Journal of Computational Materials Science and Engineering*, 2017.
17. **Sookyung Kim**. Massive Scale Deep Learning for Predicting Extreme Climate Events, *Uncertainty Quantification and Data-Driven Modeling*, 2017.
18. **Sookyung Kim**, Robert Lee, Richard Fujimoto. GPU-Accelerated Heisenberg Monte-Carlo Simulation, *The 56th Sanibel Symposium on Quantum Chemistry, Dynamics, Condensed Matter Physics*, 2016.
19. Joonseok Lee, Kisung Lee, Jennifer G. Kim, **Sookyung Kim**. Personalized Academic Research Paper Recommendation System, *Proceedings of the Workshop on Social Recommender Systems in ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2015.
20. Markus Dane1, Lorin Benedict, Mike Surh, **Sookyung Kim**. Density functional theory calculations of magneto-crystalline anisotropy energies for $(Fe_{1-x}Co_x)_2B$, *Journal of Physics: Condensed Matter*, 2014.
21. **Sookyung Kim**, Kim Ferris, Dongsheng Li. Thermo-magnetic Properties of Rare-earth Replacement Critical Magnetic Materials from DFT Calculation, *International Journal of Computational Material Science, Eng. 01, 1250036*, 2012.
22. **Sookyung Kim**. Thermo-magnetic Properties of Rare-earth Replacement Magnetic Materials: $MnBi/Sb$ Compounds and $MnBi/Sb - Co - Fe$ alloys, *Proceedings of International Conference on Materials Research Society, Document Number 1761613, Paper Number U 3.24*, 2013.
23. **Sookyung Kim**, Kim Ferris. Thermo-magnetic Properties of Rare-earth Replacement Magnetic Materials, *The 52nd Sanibel Symposium on Quantum Chemistry, Dynamics, Condensed Matter Physics*, 2012.

OPEN SOURCE SOFTWARE

- **[HMCS] Heisenberg Monte-Carlo Simulator for Spin Dynamics**
 - GPU-utilized parallelization and distributed simulation method for Monte-Carlo many particle simulation. (http://www.prism.gatech.edu/~skim722/open_source_sw.htm)

SKILLS

- **Programming Languages:** C/C++, MPI, CUDA, Python (with Scipy, Numpy), Matlab, HTML, ABS Script, Tensorflow
- **Select Graduate Courses:** Computational Data Analysis and Machine Learning (First place in class), High Performance Computing, Computational Science and Engineering Algorithms, Modeling and Simulation, Computational Methods in Material Science and Engineering, Computational Physics, Genomic Informatics, Stochastic Models in Informatics Systems

INVITED TALKS

- **ESGF Face to Face meeting**, San Francisco C.A, USA.
Deep Learning Application for Community Machine Learning using ESGF *Dec 2017*
- **Data Mining on Earth System Science**, New Orleans L.A, USA, Framework for Detection and Localization of Extreme Climate Event with Pixel Recursive Super Resolution *Dec 2017*
- **KOCSEA(The Korean Computer Scientists and Engineers Association in America) Symposium**, Las Vegas C.A, USA, Deep Learning Application for Climate Science *Nov 2017*
- **Data Analytics Group Seminar in Center for Applied Scientific Computing at LLNL**, Livermore C.A, USA, Detection, Localization and Recursive Super Resolution of Climate Data using Deep Learning *Oct 2017*

- **ESGF Proposal Review Meeting**, Washington D.C., USA, Machine Learning for Earth System Grid Federation (ESGF) *Jun 2017*
- **Uncertainty Quantification and Data-Driven Modeling**, Austin, TX, USA, Massive Scale Deep Learning for Predicting Extreme Climate Events *Mar 2017*
- **US-Korea Conference (UKC)**, Dallas, TX, USA, Monte-Carlo approach for simulate annealing and Applying high performance features using GPU *Aug 2016*
- **NVIDIA GPU Technology Conference(GTC)**, SanJose, CA, USA, Quantum Monte-Carlo Simulation implementing GPU *Apr 2016*
- **The 56th Sanibel Symposium on Quantum Chemistry, Dynamics, Condensed Matter Physics**, Grunswick, GA, USA, GPU-Accelerated Heisenberg Monte-Carlo Simulation *Feb 2016*
- **Workshop on Social Recommender Systems in ACM SIGKDD Conference on Knowledge Discovery and Data Mining**, Sydney, Australia, Personalized Academic Research Paper Recommendation System *Aug 2015*
- **Korea Advanced Institute of Science and Technology (KAIST), Department of Physics**, Daejeon, South Korea, Design Rules for Rare-earth Replacement Magnetic Materials: MnBi and MnSb Families *Dec 2014*
- **Materials Research Society (MRS) Fall Meeting 2014**, Boston, MA, USA, Thermo-magnetic Properties of Rare-earth Replacement Magnetic Materials *Nov 2014*
- **US-Korea Conference (UKC)**, San Francisco, CA, USA, Computational Modeling of Thermo-magnetic Properties of Materials *Aug 2014*
- **The 52nd Sanibel Symposium on Quantum Chemistry, Dynamics, Condensed Matter Physics**, Grunswick, GA, USA, Thermo-magnetic Properties of *MnBi* and *MnSb* Binary Compounds with *NiAs* Structure *Feb 2012*

HONORS AND AWARDS

- R&D 100 Awarded Team Member** *Oct 2017*
Awarded for ESGF(Earth System and Grid Federation) from Federal Laboratory Consortium (FLC) regional competition
- KSEA-KUSCO Graduate Students Scholarship** *Aug 2016*
Korean-American Scientists and Engineers Association (KSEA)
- Best Student Poster Award** *Nov 2015*
Lawrence Livermore National Lab. Poster Competition
- Best Poster Presentation Award**, US-Korea Conference 2014 *Aug 2014*
- Best Poster award**, Sanibel Quantum Chemistry Conference *Feb 2012*
- Summa Cum-Laude**, Ewha Woman's University *Feb 2008*
- Silver Prize Award**, Invention Competition, Korean Intellectual Property Office *Mar 2004*

TEACHING EXPERIENCE

Teaching Assistant, Georgia Institute of Technology

- MSE 2021 Introduction of MSE *Fall 2012, 2013*
- MSE 6404 Scattering Theory *Spring 2012, 2013*

Teaching Assistant, Columbia Univeristy

- E4815 Random Signal and Noise *Fall 2009*
- E4401 Wave Transmission and Fiber Optics *Fall 2010*

Instructor, Ewha Womans University

- Introduction of C Programming

Summer 2006

REFERENCES

- **Dean N. Williams** (williams13@llnl.gov)
Distinguished Member of Technical Staff, Center for Applied Scientific Computing, Lawrence Livermore National Lab (Current Supervisor)
- **Hamid Garmestani** (hamid.garmestani@mse.gatech.edu)
Professor, Material Science and Engineering, Georgia Institute of Technology (Ph.D. Advisor)
- **Jonathan Zimmerman** (jzimmer@sandia.gov)
Manager, Hydrogen and Materials Science Department, Sandia National Lab.
- **Catalin Spataru** (cdspata@sandia.gov)
Research Staff, Materials Physics Department, Sandia National Lab.
- **Lorin Benedict** (benedict5@llnl.gov)
Research Staff, Physics Division, Lawrence Livermore National Lab.
- **Mike Surh** (surh1@llnl.gov)
Research Staff, Computational Materials Science Group, Lawrence Livermore National Lab.
- **Kim Ferris** (kim.ferris@pnnl.gov)
Research Staff, Advanced Computing, Mathematics, and Data Division, Pacific Northwest National Lab.

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