# Ankit Agrawal

CURRENT
POSITION

**Research Professor**
*Department of Electrical and Computer Engineering*
*McCormick School of Engineering and Applied Science*
*Northwestern University*

**Affiliate Faculty**
*International Institute for Nanotechnology*
*Northwestern University*

**Affiliate Faculty**
*Paula M. Trienens Institute for Sustainability and Energy*
*Northwestern University*

**Honorary Professor**
*Amity School Of Engineering And Technology*
*Amity University*

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CUCIS: http://cucis.ece.northwestern.edu/members/ankitag
Google Scholar: http://scholar.google.com/citations?user=5e7JslgAAAAJ
Northwestern Scholar: https://www.scholars.northwestern.edu/en/persons/ankit-agrawal
DBLP: https://dblp.org/pid/55/5176-1.html
Scopus: https://www.scopus.com/authid/detail.uri?authorId=24604939500
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ScholarGPS: https://scholargps.com/scholars/45723753753118/ankit-agrawal
Loop: https://loop.frontiersin.org/people/2137579
LinkedIn: https://www.linkedin.com/in/ankit-agrawal-iitr-isu-nu/
AD Scientific Index: https://www.adscientificindex.com/scientist/ankit-agrawal/833110
TopSciNet: https://topscinet.com/scientist_profile/Agrawal,%20Ankit/2005/?stype=single_year

RESEARCH
INTERESTS

Artificial Intelligence, High Performance Data Mining, Materials Informatics, Healthcare Informatics, Social Media Analytics, Bioinformatics

RESEARCH
OUTPUT
SUMMARY

- 200+ peer-reviewed publications (100+ as first/last author)
- 17,000+ citations (h-index: 50+)
- 20+ software
- 100+ invited/keynote talks
- 20+ research projects as PI/Co-PI
- 1 patent granted, 2 pending

EDUCATION

- Ph.D in Computer Science (with Minor in Bioinformatics and Computational Biology), Iowa State University, USA. 2006 - 2009.

    - GPA: 4.0/4.0

- Dissertation: Sequence-Specific Sequence Comparison Using Pairwise Statistical Significance
- Advisor: Dr. Xiaoqiu Huang

- B.Tech. in Computer Science and Engineering, Indian Institute of Technology, Roorkee, INDIA. 2002 - 2006.

  - GPA: 9.43/10.0

**APPOINTMENTS**

- *Research Professor*, Northwestern University, 2020 - present
- *Affiliate Faculty*, Northwestern Paula M. Trienens Institute for Sustainability and Energy, 2024 - present
- *Affiliate Faculty*, Northwestern International Institute for Nanotechnology (IIN), 2021 - present
- *Honorary Professor*, Amity University, India, 2020 - present
- *Research Associate Professor*, Northwestern University, 2013 - 2020
- *Research Assistant Professor*, Northwestern University, 2010 - 2013
- *Postdoctoral Fellow*, Northwestern University, 2009 - 2010
- *Research Assistant*, Iowa State University, 2007 - 2009
- *Graduate Assistant*, Iowa State University, 2006 - 2007

**RESEARCH GRANTS**

1. **Senior Personnel**, "Center for Hierarchical Materials Design (CHiMaD): Phase III", *National Institute of Standards and Technology (NIST)*, $700,000, 2025-2025. (PI: Peter Voorhees) [70NANB24H136]

2. **PI**, "AI-Driven Nanocombinatorics for Accelerated Structural Characterization: Automated High-Throughput Nanoparticle Library Screening and Analytics (Renewal)", *Center for Nanocombinatorics, Northwestern University*, $100,000, 2024-2026.

3. **Co-PI**, "EAGER: XAISE: Explainable Artificial Intelligence for Science and Engineering", *National Science Foundation (NSF)*, $300,000, 2023-2026. (PI: Alok Choudhary) [OAC-2331329]

4. **PI**, "AI-Driven Nanocombinatorics for Accelerated Structural Characterization: Automated High-Throughput Nanoparticle Library Screening and Analytics (Renewal)", *Center for Nanocombinatorics, Northwestern University*, $100,000, 2023-2024.

5. **Co-PI**, "Nitrogen Activation at Catalyst Surfaces to Catalyze Net-Zero: An AI-Driven Approach", *Center for Nanocombinatorics, Northwestern University*, $100,000, 2023-2024.

6. **PI**, "AI-Driven Nanocombinatorics for Accelerated Structural Characterization: Automated High-Throughput Nanoparticle Library Screening and Analytics", *Center for Nanocombinatorics, Northwestern University*, $100,000, 2021-2022.

7. **PI**, "AI-Driven Nanocombinatorics for Functional Characterization and Optimization: Predictive Modeling and Active Learning of Catalysis in Megalibraries", *Center for Nanocombinatorics, Northwestern University*, $90,000, 2021-2022.

8. **PI**, "Collaborative Research: AI-Driven Multi-Scale Design of Materials under Processing Constraints", *National Science Foundation (NSF)*, $379,022 (Total $651,462), 2021-2025. (Lead PI: Pinar Acar) [CMMI-2053929]

9. **Co-PI**, "RAPIDS2: A SciDAC Institute for Computer Science, Data, and Artificial Intelligence", *Department of Energy (DOE)*, $650,000 (Total $28,750,000), 2020-2025. (PI: Wei-keng Liao; Lead PI: Rob Ross) [DE-SC0021399]

10. **PI**, "Center for Hierarchical Materials Design (CHiMaD): Phase II" (Agrawal Subproject), *National Institute of Standards and Technology (NIST)*, $953,221 (Total $25,000,000), 2019-2023. (Lead PI: Peter Voorhees) [70NANB19H005]

11. **PI**, "Data-driven Analytics for Understanding Materials Properties", *Toyota Motor Corporation*, $300,000, 2019-2020.

12. **PI**, "Digital Innovation Design (DID)", *Defense Logistics Agency via Steel Founders Society of America*, $200,000, 2019-2020. (Original PI: Greg Olson)

13. **Co-PI**, "PROTEUS: Machine Learning Driven Resilience for Extreme-scale Systems", *Department of Energy (DOE)*, $1,248,115, 2018-2023. (PI: Alok Choudhary) [DE-SC0019358]

14. **PI**, "The investigation of machine learning for material development", *Toyota Motor Corporation*, $200,000, 2017-2018.

15. **Senior Personnel**, "BD Spokes: SPOKE: MIDWEST: Collaborative: Integrative Materials Design (IMaD): Leverage, Innovate, & Disseminate", *National Science Foundation (NSF)*, $123,847 (Total $989,700), 2017-2022. (PI: Peter Voorhees; Lead PI: Ian Foster) [IIS-1636909]

16. **Co-PI**, "Scalable, In-situ Clustering and Data Analysis for Extreme Scale Scientific Computing", *Department of Energy (DOE)*, $1,219,899, 2015-2021. (PI: Alok Choudhary) [DE-SC0014330]

17. **Co-PI**, "SHF:Medium:Collaborative Research: Scalable Algorithms for Spatio-temporal Data Analysis", *National Science Foundation (NSF)*, $709,342 (Total $934,342), 2014-2019. (PI: Alok Choudhary) [CCF-1409601]

18. **PI**, "Advanced Materials Center for Excellence: Center for Hierarchical Materials Design (CHiMaD)" (Agrawal Subproject), *National Institute of Standards and Technology (NIST)*, $505,358 (Total $25,000,000), 2014-2018. (Lead PI: Peter Voorhees) [70NANB14H012]

19. **PI**, "Social Media mining of caregiver experiences: Opportunity for preventing caregiver burnout", *Northwestern Data Science Initiative*, $25,000, 2017-2017.

20. **PI**, "Data-driven analytics for understanding processing-structure-property-performance relationships in steel alloys", *Northwestern Data Science Initiative*, $45,000, 2016-2017.

21. **Co-PI**, "Scaling up the screening of molecular networks in the rational design of optically active materials", *Northwestern Data Science Initiative*, $9,000 (Total $45,000), 2016-2017. (PI: Kevin Kohlstedt)

22. **PI**, "Analyzing caregiving experience on Twitter", *Feinberg School of Medicine*, $14,246, 2015-2016.

23. **Co-PI**, "SIMPLEX: Data-driven Discovery of Novel Thermoelectric Materials", *Defense Advanced Research Projects Agency (DARPA)*, $601,250 (Total $1,559,999), 2015-2018. (PI: Alok Choudhary; Lead PI: Greg Olson) [N66001-15-C-4036]

24. **Co-PI**, "EAGER: Scalable Big Data Analytics", *National Science Foundation (NSF)*, $300,000, 2013-2016. (PI: Alok Choudhary) [IIS-1343639]

25. **Co-PI**, "MURI: MANAGING THE MOSAIC OF MICROSTRUCTURE: Image analysis, data structures, mathematical theory of microstructure, and hardware for the structure-property relationship", *Air Force Office of Scientific Research (AFOSR), Department of Defense (DOD)*, $750,000 (Total $5,658,616), 2012-2018. (PI: Alok Choudhary; Lead PI: Marc De Graef) [FA9550-12-1-0458]

26. **Co-PI**, "Scalable Data Management, Analysis, and Visualization (SDAV) Institute", *Department of Energy (DOE)*, $750,000 (Total $25,000,000), 2012-2019. (PI: Alok Choudhary; Lead PI: Arie Shoshani) [DE-SC0007456]

27. **Senior Researcher**, "Expeditions in Computing: Understanding Climate Change: A Data Driven Approach", *National Science Foundation (NSF)*, $900,000 (Total $10,000,000), 2010-2016. (PI: Alok Choudhary; Lead PI: Vipin Kumar) [CCF-1029166]

28. **Co-PI**, "EAGER: Discovering Knowledge from Scientific Research Networks", *National Science Foundation (NSF)*, $256,000, 2011-2014. (PI: Alok Choudhary) [ACI-1144061]

29. **Research Participant**, "Scalable and Power Efficient Data Analytics for Hybrid Exascale Systems", *Department of Energy (DOE)*, $705,000, 2010-2014. (PI: Alok Choudhary) [DE-SC0005340]

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| **HONORS AND AWARDS** | • Featured in Stanford/Elsevier's list of top 2% scientists worldwide (single-year), 2025, 2024, 2023, 2022, 2021, 2020 |
| | • Featured in Stanford/Elsevier's list of top 2% scientists worldwide (career-wide), 2025, 2024, 2023 |
| | • Named a Top Scholar by ScholarGPS for being in top 0.5% of scholars worldwide in the fields of machine learning, deep learning, and informatics, 2024 |
| | • Hind Rattan Award, 2023 (translated as "Jewel of India", one of the highest Indian diasporic awards conferred to NRIs on the eve of Republic Day, for outstanding services, achievements, and contributions for keeping the "Flag of India High") |
| | • Honorary Professor, Amity School of Engineering and Technology (ASET), Amity University, 2020-present |
| | • Best Paper Finalist, HiPC 2017 |
| | • Northwestern Data Science Initiative Award, 2017 |
| | • Northwestern Data Science Initiative Award, 2016 |
| | • Best Paper Award at IEEE Cluster 2016 |
| | • Gordon Betty Moore Foundation (GBMF) Data-Driven-Discovery Competition Finalist, 2014 |
| | • Outstanding Paper Award awarded by Tata Consultancy Services for joint work published in IMMI, 2014 |
| | • Best Paper Award at KDD Workshop on Big Data, Streams and Heterogeneous Source Mining: Algorithms, Systems, Programming Models and Applications (BigMine), 2013 |
| | • Design Contest Winner at 25th International Conference on VLSI Design, 2012 |
| | • Research Excellence Award for Summer 2009 at ISU (to recognize up to 10% graduating students for outstanding research accomplishments) |
| | • Graduate and Professional Student Senate Peer Research Award for Spring 2009 at ISU (based on research conducted at ISU) |
| | • Best student paper award at International Conference on Information Technology, ICIT 2008 |
| | • Institute Silver Medal for obtaining the highest C.G.P.A. (9.43/10) amongst the students graduating with B.Tech. (Computer Science and Engineering) at IIT Roorkee, 2006 |
| | • Institute Silver Medal for Best Project in B.Tech. (Computer Science and Engineering) at IIT Roorkee, 2006 |
| | • Offered branch change at the end of B.Tech. first year at IIT Roorkee for being in top 1% of students, 2003 |
| **TEACHING** | • Co-instructor: CE/CS 395/495/396/496: AI for Science and Business, Spring 2025. |
| | • Co-instructor: CE/CS 395/495: AI for Science, Spring 2024. |
| | • Co-instructor: TMS Online Course on Artificial Intelligence in Materials Science and Engineering, April 03-05, 2023, November 02-04, 2021. |
| | • Co-instructor: PSED 510-1: Predictive Science & Engineering Design Cluster Seminar, Fall 2024, Fall 2020, Fall 2017, Northwestern University. |
| | • Co-instructor: CE/EECS 510: Social Media Mining, Spring 2024, Spring 2022, Spring 2021, Spring 2020, Spring 2019, Spring 2018, Spring 2017, Spring 2016, Spring2015, Spring 2014, Northwestern University. |
| | • Invited Speaker: BiGmax Summer School on Harnessing Big Data in Materials Science from Theory to Experiment, September 15, 2021, Max Plank Institute, Germany (Virtual). |
| | • Co-instructor: EECS 100: Electrons, Photons, and Bits: Adventures in Electrical and Computer Engineering, Spring 2019, Spring 2018, Spring 2017, Spring 2016, Spring 2015, Spring 2011, Northwestern University. |
| | • Co-instructor: MSIT 423: Data Mining and Business Intelligence, Spring 2011, Northwestern University. |
| | • Teaching Assistant: ComS/BCB 567: Bioinformatics I - Fundamentals of Genome Informatics, Fall 2008, Iowa State University. |
| | • Teaching Assistant: ComS 309: Software Engineering, Fall 2006, Iowa State University. |
| **PATENTS** | *Granted* |

1. Ankit Agrawal and Alok Choudhary, "System and method for predicting fatigue strength of alloys." U.S. Patent No. 10,830,747. 10 Nov. 2020.

*Pending*

1. Alexandra Lauren Day, Carolin Barbara Wahl, Roberto M. dos Reis, Alok Nidhi Choudhary, Chad A. Mirkin, Vinayak P. Dravid and Ankit Agrawal, "Rapid image segmentation pipeline for scanning transmission electron microscopy" US Application No.: 19/207,977, 2025.

2. Alexandra Lauren Day, Carolin Barbara Wahl, Roberto M. dos Reis, Wei-keng Liao, Chad A. Mirkin, Vinayak P. Dravid, Alok Nidhi Choudhary, and Ankit Agrawal, "Nanoparticle Image Processing Pipeline for Structure Characterization" US Application No.: 63/710,371, 2024 (Provisional).

PUBLICATIONS

*Book Chapters*

1. **A. Agrawal** and A. Choudhary, "Artificial Intelligence for Accelerating Materials Discovery," in Artificial Intelligence for Science: A Deep Learning Revolution, A. Choudhary, T. Hey, and G. Fox, Eds. World Scientific, 2023, pp. 431–443.

2. **A. Agrawal**, K. Gopalakrishnan, and A. Choudhary, "Materials Image Informatics Using Deep Learning," in Handbook on Big Data and Machine Learning in the Physical Sciences, vol. 1: Big Data Methods in Experimental Materials Discovery, World Scientific, 2020, pp. 205–230.

3. D. Han, **A. Agrawal**, W. Liao, and A. Choudhary, "A Fast DBSCAN Algorithm with Spark Implementation," in Big Data in Engineering Applications, S. S. R. et al., Ed. Springer Nature Singapore, 2018, pp. 173–192.

4. **A. Agrawal** and A. Choudhary, "Health Services Data: Big Data Analytics for Deriving Predictive Healthcare Insights," in Data and Measures in Health Services Research, B. Sobolev, A. Levy, and S. Goring, Eds. Springer US, 2016, pp. 1–17.

5. **A. Agrawal**, M. Patwary, W. Hendrix, W. Liao, and A. Choudhary, "High performance big data clustering," in Advances in Parallel Computing, Volume 23: Cloud Computing and Big Data, L. Grandinetti, Ed. IOS Press, 2013, pp. 192–211.

6. **A. Agrawal**, A. Choudhary, and X. Huang, "Sequence-Specific Sequence Comparison Using Pairwise Statistical Significance," in Software Tools and Algorithms for Biological Systems, vol. 696, H. R. Arabnia, Ed. Springer, 2011, pp. 297–306.

*Journal Publications*

7. M. M. Billah, M. N. T. Kilic, M. M. Hasan, Z. E. Eger, Y. Mao, K. Wang, A. Choudhary, **A. Agrawal**, V. Sundararaghavan, and P. Acar, "MicroProcSim: A Software for Simulation of Microstructure Evolution," Integrating Materials and Manufacturing Innovation, pp. 1–17, 2025.

8. A. L. Day, C. B. Wahl, R. D. Reis, W. Liao, Y. Li, M. N. T. Kilic, C. A. Mirkin, V. P. Dravid, A. Choudhary, and **A. Agrawal**, "Automated image segmentation for accelerated nanoparticle characterization," Scientific Reports, vol. 15, no. 1, pp. 1–13, 2025.

9. A. J. Esposito, A. Peltekian, K. Grudzinski, M. Zhu, N. S. Markov, B. C. Bemiss, M. Carns, K. Aren, A. Soriano, M. Dapas, A. N. Gundersheimer, K. C. Selvan, M. E. Hinchcliff, K. Warrior, C. L. Richardson, J. E. Dematte, C. A. Gao, G. S. Budinger, A. N. Choudhary, A. V. Misharin, and **A. Agrawal**, "Machine Learning Predicts Mortality in Patients With Systemic Sclerosis-Associated Interstitial Lung Disease From Electronic Health Record Data," American Journal of Respiratory and Critical Care Medicine, vol. 211, no. Abstracts, pp. A3234–A3234, 2025.

10. S. W. Fenske, A. Peltekian, M. Kang, N. S. Markov, M. Zhu, K. Grudzinski, M. J. Bak, A. Pawlowski, V. Gupta, Y. Mao, S. Bratchikov, T. Stoeger, L. V. Rasmussen, A. N. Choudhary, A. V. Misharin, B. D. Singer, G. R. S. Budinger, R. G. Wunderink, **A. Agrawal**, C. A. Gao, and N. U. S. S. Investigators, "Developing and validating machine learning models to predict next-day extubation," Scientific Reports, vol. 15, no. 1, p. 27552, 2025.

11. V. Guggilla, M. Kang, A. Pawlowski, P. Nannapaneni, L. Rasmussen, D. Schneider, H. Donnelly, **A. Agrawal**, D. Liebovitz, R. G. Wunderink, C. Gao, T. Walunas, and N. U. S. C. R. I. P. T. S. Investigators, "Identifying Immunosuppressive Medication Use From Clinical Notes Using GPT-4o," American Journal of Respiratory and Critical Care Medicine, vol. 211, no. Abstracts, pp. A3289–A3289, 2025.

12. S. Keshavarz, Y. Mao, A. C. E. Reid, and **A. Agrawal**, "Advancing material simulations: Physics-Informed Neural Networks and Object-Oriented Crystal Plasticity Finite Element Methods," International Journal of Plasticity, vol. 185, p. 104221, 2025.

13. Y. Li, V. Gupta, M. N. T. Kilic, K. Choudhary, D. Wines, W. Liao, A. Choudhary, and **A. Agrawal**, "Hybrid-LLM-GNN: integrating large language models and graph neural networks for enhanced materials property prediction," Digital Discovery, vol. 4, pp. 376–383, 2025.

14. Y. Mao, M. Hasan, M. M. Billah, Y. Li, S. Chakrabarty, C. S. Lee, K. Wang, M. N. T. Kilic, V. Gupta, W.-keng Liao, A. Choudhary, P. Acar, and **A. Agrawal**, "An AI framework for time series microstructure prediction from processing parameters," Scientific Reports, vol. 15, no. 1, p. 24074, 2025.

15. Y. Mao, S. Keshavarz, M. N. T. Kilic, K. Wang, Y. Li, A. C. E. Reid, W. Liao, A. Choudhary, and **A. Agrawal**, "A deep learning-based crystal plasticity finite element model," Scripta Materialia, vol. 254, p. 116315, 2025.

16. A. Yan, M. N. T. Kilic, G. Nolze, **A. Agrawal**, R. dos Reis, and V. Dravid, "Towards Extracting Space Group Information From Experimental EBSD Patterns Using Unsupervised Domain Adaptation," Microscopy and Microanalysis, vol. 31, no. 7, pp. 497–499, 2025.

17. K. Choudhary, D. Wines, K. Li, K. F. Garrity, V. Gupta, A. H. Romero, J. T. Krogel, K. Saritas, A. Fuhr, P. Ganesh, P. R. C. Kent, K. Yan, Y. Lin, S. Ji, B. Blaiszik, P. Reiser, P. Friederich, **A. Agrawal**, P. Tiwary, E. Beyerle, P. Minch, T. D. Rhone, I. Takeuchi, R. B. Wexler, A. Mannodi-Kanakkithodi, E. Ertekin, A. Mishra, N. Mathew, M. Wood, A. D. Rohskopf, J. Hattrick-Simpers, S.-H. Wang, L. E. K. Achenie, H. Xin, M. Williams, A. J. Biacchi, and F. Tavazza, "JARVIS-Leaderboard: A large scale benchmark of materials design methods," npj Computational Materials, vol. 10, no. 1, p. 93, 2024.

18. A. L. Day, C. B. Wahl, V. Gupta, R. D. Reis, W. Liao, C. A. Mirkin, V. P. Dravid, A. Choudhary, and **A. Agrawal**, "Machine Learning-Enabled Image Classification for Automated Electron Microscopy," Microscopy and Microanalysis, p. ozae042, 2024.

19. A. L. Day, C. B. Wahl, R. dos Reis, W. Liao, Y. Li, M. N. T. Kilic, C. A. Mirkin, V. P. Dravid, A. Choudhary, and **A. Agrawal**, "Rapid Image Segmentation Pipeline to Support Multimodal STEM Acquisition," Microscopy and Microanalysis, vol. 30, no. Supplement 1, pp. 442–443, 2024.

20. V. Gupta, K. Choudhary, B. DeCost, F. Tavazza, C. Campbell, W. Liao, A. Choudhary, and **A. Agrawal**, "Structure-aware graph neural network based deep transfer learning framework for enhanced predictive analytics on diverse materials datasets," npj Computational Materials, vol. 10, p. 1, 2024.

21. V. Gupta, Y. Li, A. Peltekian, M. N. T. Kilic, W. Liao, A. Choudhary, and **A. Agrawal**, "Simultaneously improving accuracy and computational cost under parametric constraints in materials property prediction tasks," Journal of Cheminformatics, vol. 16, no. 1, p. 17, 2024.

22. C. Lee, V. Hewes, G. Cerati, K. Wang, A. Aurisano, **A. Agrawal**, A. Choudhary, and W. Liao, "Addressing GPU Memory Limitations for Graph Neural Networks in High-Energy Physics Applications," Frontiers in High Performance Computing, vol. 2, p. 1458674, 2024.

23. K. Wang, V. Gupta, C. S. Lee, Y. Mao, M. N. T. Kilic, Y. Li, Z. Huang, W. Liao, A. Choudhary, and **A. Agrawal**, "XElemNet: Towards explainable AI for deep neural networks in materials science," Scientific Reports, vol. 14, p. 25178, 2024.

24. A. Yan, M. N. T. Kilic, **A. Agrawal**, R. dos Reis, and V. Dravid, "Neural Network Models Towards Space Group Determination Using Dynamically Simulated EBSD and TKD Patterns," Microscopy and Microanalysis, vol. 30, no. Supplement 1, pp. 388–390, 2024.

25. V. Gupta, K. Choudhary, Y. Mao, K. Wang, F. Tavazza, C. Campbell, W. Liao, A. Choudhary, and **A. Agrawal**, "MPpredictor: An Artificial Intelligence-Driven Web Tool for Composition-Based Material Property Prediction," Journal of Chemical Information and Modeling, vol. 63, no. 7, pp. 1865–1871, 2023.

26. K. Gumpula, N. Koloskov, D. Grzenda, V. Hewes, A. Aurisano, G. Cerati, A. Day, J. Kowalkowski, C. Lee, K. Wang, W. Liao, M. Spiropulu, **A. Agrawal**, J. Vlimant, L. Gray, T. Klijnsma, P. Calafiura, S. Conlon, S. Farrell, X. Ju, and D. Murnane, "Graph Neural Network for Object Reconstruction in Liquid Argon Time Projection Chambers," Journal of Physics: Conference Series, vol. 2438, p. 012091, 2023.

27. V. Gupta, W. Liao, A. Choudhary, and **A. Agrawal**, "Evolution of artificial intelligence for application in contemporary materials science," MRS Communications, pp. 1–10, 2023.

28. V. Gupta, A. Peltekian, W. Liao, A. Choudhary, and **A. Agrawal**, "Improving deep learning model performance under parametric constraints for materials informatics applications," Scientific Reports, vol. 13, no. 1, p. 9128, 2023.

29. Y. Mao, M. Hasan, A. Paul, V. Gupta, K. Choudhary, F. Tavazza, W. Liao, A. Choudhary, P. Acar, and **A. Agrawal**, "An AI-driven microstructure optimization framework for elastic properties of titanium beyond cubic crystal systems," npj Computational Materials, vol. 9, p. 111, 2023.

30. Y. Mao, H. Lin, C. X. Yu, R. Frye, D. Beckett, K. Anderson, L. Jacquemetton, F. Carter, Z. Gao, W. Liao, A. N. Choudhary, K. Ehmann, and **A. Agrawal**, "A deep learning framework for layer-wise porosity prediction in metal powder bed fusion using thermal signatures," Journal of Intelligent Manufacturing, vol. 24, pp. 315–329, 2023.

31. C. Wahl, A. Day, V. Gupta, R. R. dos Reis, W. Liao, C. Mirkin, A. Choudhary, V. P. Dravid, and **A. Agrawal**, "Machine Learning Enabled Image Classification for Automated Data Acquisition in the Electron Microscope," Microscopy and Microanalysis, vol. 29, pp. 1909–1910, 2023.

32. K. Choudhary, B. DeCost, C. Chen, A. Jain, F. Tavazza, R. Cohn, C. W. Park, A. Choudhary, **A. Agrawal**, S. J. L. Billinge, E. Holm, S. P. Ong, and C. Wolverton, "Recent advances and applications of deep learning methods in materials science," npj Computational Materials, vol. 8, p. 59, 2022.

33. M. Hasan, Y. Mao, K. Choudhary, F. Tavazza, A. Choudhary, **A. Agrawal**, and P. Acar, "Data-Driven Multi-Scale Modeling and Optimization for Elastic Properties of Cubic Microstructures," Integrating Materials and Manufacturing Innovation, vol. 11, pp. 230–240, 2022.

34. D. Jha, V. Gupta, W. Liao, A. Choudhary, and **A. Agrawal**, "Moving closer to experimental level materials property prediction using AI," Scientific Reports, vol. 12, p. 11953, 2022.

35. S. Lee, K.-yuan Hou, K. Wang, S. Sehrish, M. Paterno, J. Kowalkowski, Q. Koziol, R. B. Ross, **A. Agrawal**, A. Choudhary, and W. Liao, "A case study on parallel HDF5 dataset concatenation for high energy physics data analysis," Parallel Computing, vol. 110, p. 102877, 2022.

36. S. Lee, Q. Kang, R. Al-Bahrani, **A. Agrawal**, A. Choudhary, and W. Liao, "Improving scalability of parallel CNN training by adaptively adjusting parameter update frequency," Journal of Parallel and Distributed Computing, vol. 159, pp. 10–23, 2022.

37. Y. Mao, Z. Yang, D. Jha, A. Paul, W. Liao, A. Choudhary, and **A. Agrawal**, "Generative Adversarial Networks and Mixture Density Networks-Based Inverse Modeling for Microstructural Materials Design," Integrating Materials and Manufacturing Innovation, vol. 11, pp. 637–647, 2022.

38. V. Gupta, K. Choudhary, F. Tavazza, C. Campbell, W. Liao, A. Choudhary, and **A. Agrawal**, "Cross-property deep transfer learning framework for enhanced predictive analytics on small materials data," Nature Communications, vol. 12, no. 6595, 2021.

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## Peer-Reviewed Workshop Publications

196. D. Jha, K. V. L. V. Narayanachari, R. Zhang, J. Liao, D. T. Keane, W. Liao, A. Choudhary, Y.-W. Chung, M. J. Bedzyk, and **A. Agrawal**, "An Incremental Phase Mapping Approach for X-ray Diffraction Patterns using Binary Peak Representations," in SDM Workshop on Domain-Driven Data Mining (DDDM), 2021, p. 11.

197. Z. Yang, T. Watari, D. Ichigozaki, A. Mitsutoshi, H. Takahashi, Y. Suga, W. Liao, A. Choudhary, and **A. Agrawal**, "Heterogeneous feature fusion based machine learning on shallow-wide and heterogeneous-sparse industrial datasets," in ICPR Workshop on Industrial Machine Learning (IML), 2021, pp. 566–577.

198. Z. Yang, D. Jha, A. Paul, W. Liao, A. Choudhary, and **A. Agrawal**, "A General Framework Combining Generative Adversarial Networks and Mixture Density Networks for Inverse Modeling in Microstructural Materials Design," in Proceedings of 2020 NeurIPS workshop on Machine Learning for Engineering Modeling, Simulation, and Design (ML4Eng), 2020, pp. 1–8.

199. Q. Kang, **A. Agrawal**, A. Choudhary, A. Sim, K. Wu, R. Kettimuthu, P. Beckman, Z. Liu, and W. Liao, "Spatiotemporal Real-Time Anomaly Detection for Supercomputing Systems," in Proceedings of IEEE BigData Workshop on Big Data Predictive Maintenance using Artificial Intelligence, 2019, pp. 4381–4389.

200. Z. Yang, T. Watari, D. Ichigozaki, K. Morohoshi, Y. Suga, W. Liao, A. Choudhary, and **A. Agrawal**, "Data-driven insights from predictive analytics on heterogeneous experimental data of industrial magnetic materials," in Proceedings of 2019 ICDM Workshop on Learning and Mining with Industrial Data (LMID), 2019, pp. 806–813.

201. K. Hou, R. Al-Bahrani, E. Rangel, **A. Agrawal**, R. Latham, R. Ross, A. Choudhary, and W. Liao, "Integration of Burst Buffer in High-level Parallel I/O Library for Exa-scale Computing Era," in Proceedings of SC workshop on Parallel Data Storage and Data Intensive Scalable Computing Systems (PDSW-DISCS 2018), 2018, pp. 1–12.

202. Q. Kang, **A. Agrawal**, A. Choudhary, and W. Liao, "Optimal Algorithms for Half-Duplex Inter-Group All-to-All Broadcast on Fully Connected and Ring Topologies," in Proceedings of 2018 SC Workshop on Exascale MPI (ExaMPI), 2018, pp. 1–11.

203. R. Kettimuthu, Z. Liu, I. Foster, P. Beckman, A. Sim, K. Wu, W. Liao, Q. Kang, **A. Agrawal**, and A. Choudhary, "Towards Autonomic Science Infrastructure: Architecture, Limitations, and Open Issues," in Proceedings of the 1st International Workshop on Autonomous Infrastructure for Science, 2018.

204. S. Lee, **A. Agrawal**, P. Balaprakash, A. Choudhary, and W. Liao, "Communication-Efficient Parallelization Strategy for Deep Convolutional Neural Network Training," in Proceedings of SC workshop on Machine Learning in HPC Environments (MLHPC 2018), 2018, pp. 47–56.

205. A. Paul, D. Jha, R. Al-Bahrani, W. Liao, A. Choudhary, and **A. Agrawal**, "CheMixNet: Mixed DNN Architectures for Predicting Chemical Properties using Multiple Molecular Representations," in Proceedings of 2018 NIPS workshop on Machine Learning for Molecules and Materials (MLMM), 2018, pp. 1–13.

206. R. Al-Bahrani, M. K. Danilovich, W. Liao, A. Choudhary, and **A. Agrawal**, "Analyzing Informal Caregiving Expression in Social Media," in IEEE ICDM Workshop on Sentiment Elicitation from Natural Text for Information Retrieval and Extraction (SENTIRE), 2017, pp. 342–349.

207. Q. Kang, W. Liao, **A. Agrawal**, and A. Choudhary, "A Hybrid Training Algorithm for Recurrent Neural Network Using Particle Swarm Optimization-based Preprocessing and Temporal Error Aggregation," in IEEE ICDM Workshop on Optimization Based Techniques for Emerging Data Mining Problems (OEDM), 2017, pp. 812–817.

208. D. Han, **A. Agrawal**, W. Liao, and A. Choudhary, "A novel scalable DBSCAN algorithm with Spark," in Proceedings of 5th IEEE IPDPS Workshop on Parallel and Distributed Computing for Large Scale Machine Learning and Big Data Analytics (ParLearning), 2016, pp. 1393–1402.

209. A. Krishna, **A. Agrawal**, and A. Choudhary, "Predicting the Outcome of Startups: Less Failure, More Success," in Proceedings of IEEE ICDM Workshop on Data Market for Co-evolution of Sciences and Business (MoDAT), 2016, pp. 798–805.

210. R. Liu, **A. Agrawal**, W. Liao, M. D. Graef, and A. Choudhary, "Materials Discovery: Understanding Polycrystals from Large-Scale Electron Patterns," in Proceedings of IEEE BigData Workshop on Advances in Software and Hardware for Big Data to Knowledge Discovery (ASH), 2016, pp. 2261–2269.

211. S. Lee, W. Liao, **A. Agrawal**, N. Hardavellas, and A. Choudhary, "Evaluation of K-Means Data Clustering Algorithm on Intel Xeon Phi," in Proceedings of IEEE BigData Workshop on Advances in Software and Hardware for Big Data to Knowledge Discovery (ASH), 2016, pp. 2251–2260.

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214. A. Paul, **A. Agrawal**, W. Liao, and A. Choudhary, "AnonyMine: Mining anonymous social media posts using psycho-lingual and crowd-sourced dictionaries," in Proceedings of ACM SIGKDD Workshop on Issues of Sentiment Discovery and Opinion Mining (WISDOM), 2016.

215. S. Gupta, D. Palsetia, M. M. A. Patwary, **A. Agrawal**, and A. Choudhary, "A New Parallel Algorithm for Two-Pass Connected Component Labeling," in Proceedings of IEEE IPDPS Workshop on Multithreaded Architectures and Applications (MTAAP), 2014, pp. 1355–1362.

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217. R. Liu, **A. Agrawal**, W. Liao, and A. Choudhary, "Search Space Preprocessing in Solving Complex Optimization Problems," in Proceedings of IEEE BigData Workshop on Complexity for Big Data (C4BD), 2014, pp. 1–5.

218. Y. Xie, Y. Cheng, **A. Agrawal**, and A. Choudhary, "Estimating online user location distribution without GPS location," in Proceedings of ICDM Workshop on Connecting Online and Offline Social Network Analysis (COOL-SNA), 2014, pp. 936–943.

219. **A. Agrawal**, R. Al-Bahrani, R. Merkow, K. Bilimoria, and A. Choudhary, "Colon Surgery Outcome Prediction Using ACS NSQIP Data," in Proceedings of the KDD Workshop on Data Mining for Healthcare (DMH), 2013, pp. 1–6.

220. **A. Agrawal**, R. Al-Bahrani, J. Raman, M. J. Russo, and A. Choudhary, "Lung Transplant Outcome Prediction using UNOS Data," in Proceedings of the IEEE Big Data Workshop on Bioinformatics and Health Informatics (BHI), 2013, pp. 1–8.

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224. C. Jin, Q. Fu, H. Wang, **A. Agrawal**, W. Hendrix, W. Liao, M. M. A. Patwary, A. Banerjee, and A. Choudhary, "Solving Combinatorial Optimization Problems using Relaxed Linear Programming: A High Performance Computing Perspective," in Proceedings of the KDD Workshop on Big Data, Streams and Heterogeneous Source Mining: Algorithms, Systems, Programming Models and Applications (BigMine), 2013, pp. 39–46. **Won the best paper award**.

225. C. Jin, M. M. A. Patwary, **A. Agrawal**, W. Hendrix, W. Liao, and A. Choudhary, "DiSC: A Distributed Single-Linkage Hierarchical Clustering Algorithm using MapReduce," in Proceedings of the 4th International SC Workshop on Data Intensive Computing in the Clouds (DataCloud) 2013, 2013, pp. 1–6.

226. K. Lee, **A. Agrawal**, and A. Choudhary, "Real-Time Digital Flu Surveillance using Twitter Data," in Proceedings of the SDM Workshop on Data Mining for Medicine and Healthcare (DMMH), 2013, pp. 19–27.

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228. Y. Cheng, Y. Xie, K. Zhang, **A. Agrawal**, and A. Choudhary, "How Online Content is Received by Users in Social Media: A Case Study on Facebook. com Posts," in Proceedings of the KDD Workshop on Social Media Analytics (SOMA), 2012, pp. 1–8.

229. D. Palsetia, M. M. A. Patwary, K. Zhang, K. Lee, C. Moran, Y. Xie, D. Honbo, **A. Agrawal**, W. Liao, and A. Choudhary, "User-Interest based Community Extraction in Social Networks," in Proceedings of the KDD Workshop on Social Network Mining and Analysis (SNAKDD), 2012, pp. 1–4.

230. Y. Xie, Y. Cheng, D. Honbo, K. Zhang, **A. Agrawal**, A. Choudhary, Y. Gao, and J. Gou, "Probabilistic macro behavioral targeting," in Proceedings of the CIKM workshop on Data-driven user behavioral modelling and mining from social media (DUBMMSM), 2012, pp. 7–10.

231. Y. Xie, Y. Cheng, D. Honbo, K. Zhang, **A. Agrawal**, and A. Choudhary, "Crowdsourcing recommendations from social sentiment," in Proceedings of KDD Workshop on Issues of Sentiment Discovery and Opinion Mining (WISDOM), 2012, pp. 9:1–9:8.

232. **A. Agrawal** and A. Choudhary, "Identifying HotSpots in Lung Cancer Data Using Association Rule Mining," in 2nd IEEE ICDM Workshop on Biological Data Mining and its Applications in Healthcare (BioDM), 2011, pp. 995–1002.

233. **A. Agrawal**, S. Misra, R. Narayanan, L. Polepeddi, and A. Choudhary, "A lung cancer outcome calculator using ensemble data mining on SEER data," in Proceedings of the Tenth International Workshop on Data Mining in Bioinformatics (BIOKDD), New York, NY, USA, 2011, pp. 1–9.

234. Y. Cheng, K. Zhang, Y. Xie, **A. Agrawal**, W. Liao, and A. Choudhary, "Learning to Group Web Text Incorporating Prior Information," in 6th IEEE ICDM Workshop on Optimization Based Techniques for Emerging Data Mining Problems, (OEDM), 2011, pp. 212–219.

235. W. Hendrix, I. Tetteh, **A. Agrawal**, F. Semazzi, W. Liao, and A. Choudhary, "Community Dynamics and Analysis of Decadal Trends in Climate Data," in 3rd IEEE ICDM Workshop on Knowledge Discovery from Climate Data, (ClimKD), 2011, pp. 9–14.

236. K. Lee, D. Palsetia, R. Narayanan, M. Patwary, **A. Agrawal**, and A. Choudhary, "Twitter Trending Topic Classification," in 6th IEEE ICDM Workshop on Optimization Based Techniques for Emerging Data Mining Problems, (OEDM), 2011, pp. 251–258.

237. N. Nakka, **A. Agrawal**, and A. N. Choudhary, "Predicting Node Failure in High Performance Computing Systems from Failure and Usage Logs," in IEEE International Symposium on Parallel and Distributed Processing Symposium (IPDPS) Workshops, 2011, pp. 1557–1566.

238. L. Polepeddi, **A. Agrawal**, and A. Choudhary, "Poll: A Citation-Text-Based System for Identifying High-Impact Contributions of an Article," in IEEE ICDM Workshop on Data Mining in Networks, (DaMNet), 2011, pp. 965–968.

239. K. Zhang, Y. Cheng, Y. Xie, **A. Agrawal**, D. Palsetia, K. Lee, and A. Choudhary, "SES: Sentiment Elicitation System for Social Media Data," in IEEE ICDM Workshop on Sentiment Elicitation from Natural Text for Information Retrieval and Extraction, (SENTIRE), 2011, pp. 129–136.

240. Y. Zhang, M. Patwary, S. Misra, **A. Agrawal**, W. Liao, and A. N. Choudhary, "Enhancing parallelism of pairwise statistical significance estimation for local sequence alignment," in HiPC Workshop on Hybrid Multi-core Computing (WHMC), 2011, pp. 1–8.

241. **A. Agrawal**, S. Misra, D. Honbo, and A. Choudhary, "MPIPairwiseStatSig: Parallel Pairwise Statistical Significance Estimation of Local Sequence Alignment," in Proceedings of the HPDC Workshop on Emerging Computational Methods for the Life Sciences (ECMLS), 2010, pp. 470–476.

242. **A. Agrawal** and X. Huang, "Pairwise Statistical Significance of Local Sequence Alignment Using Multiple Parameter Sets," in Proc. of ACM 2nd International Workshop on Data and Text Mining in Bioinformatics (DTMBIO), 2008, pp. 53–60.

SCIENTIFIC PRESENTATIONS AND TALKS

1. (Invited) Artificial Intelligence for Accelerating Materials Science and Engineering: Leveraging GNNs, LLMs, XAI, GenAI, Nanocombinatorics, and More, *4th World Symposium on Materials Sciences and Engineering (SMSE) 2025*, December 02, 2025, Singapore.

2. (Keynote) AI for Science and Engineering: Leveraging GNNs, LLMs, XAI, Nanocombinatorics, and More, *International Conference on Artificial Intelligence and Emerging Technology 2.0 (Global AI Summit) 2025*, November 19, 2025, Bennett University, Greater Noida, UP, India.

3. (Invited) AI + HPC to Accelerate Science and Engineering, *International Conference on Artificial Intelligence (AI 2025)*, October 30, 2025, Tokyo, Japan.

4. (Invited) Introduction to Machine Learning and Deep Learning for Materials Science, *TMS Online Course: Artificial Intelligence in Materials Science and Engineering*, October 27, 2025 (Virtual).

5. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Science and Engineering, *International Guest Lecture Series 2025*, September 22, 2025, Amity University Tashkent, Uzbekistan.

6. (Invited) Towards AI-Driven Discovery of Renewable Energy Materials: Thermoelectrics, Semiconductors, Catalysts, and More, *3rd Global Summit on Renewable and Sustainable Energy (GSRSE 2025)*, September 11, 2025, Barcelona, Spain.

7. (Keynote) AI and High-Performance Data Mining for Accelerating Science and Engineering, *International Conference on Sustainability, Innovation &Technology (ICSIT 2025)*, August 23, 2025, Symbiosis Institute of Technology, Nagpur, Maharashtra, India.

8. (Invited) Towards AI-Driven Discovery for Renewable Energy Materials: Thermoelectrics, Semiconductors, Catalysts, and More, *3rd Biennial International Symposium on Fluids and Thermal Engineering (FLUTE 2025)*, August 07, 2025, Amity University, Noida, Delhi NCR, India.

9. (Invited) AI and High-Performance Data Mining for Accelerating Science and Engineering, *KIET Distinguished Lecture Series*, July 24, 2025, KIET Group of Institutions, Ghaziabad, Delhi NCR, India.

10. (Invited) Artificial Intelligence for Accelerating Materials Science and Engineering: Leveraging GNNs, LLMs, XAI, Nanocombinatorics, and More, *Artificial Intelligence for Materials Science Workshop (AIMS)*, National Institute of Standards and Technology, July 09, 2025, Rockville, MD, USA.

11. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *AI for Science and Business*, May 29, 2025, Evanston, IL, USA.

12. (Keynote) AI+HPC for Accelerating Science and Engineering, *2nd International Conference on Recent Advances in Artificial Intelligence, Computer Vision & Smart Systems (ICRACS)*, April 16, 2025, Poornima Institute of Engineering & Technology (PIET), Jaipur, Rajasthan, India.

13. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Science, *5th International Conference on AI, Machine Learning and Applications (AIMLA 2025)*, February 15, 2025, Chennai, India.

14. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Science, *15th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2025*, January 17, 2025, Amity University, Noida, Delhi NCR, India.

15. (Invited) AI for Materials: Research Landscape of AI and Design", *IIN Workshop on AI for Materials*, November 22, 2024, Evanston, IL, USA.

16. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Science, *SciX 2024*, October 21, 2024, Raleigh, NC, USA.

17. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *Predictive Science and Engineering Design (PSED) Interdisciplinary Cluster Initiative Seminar*, October 10, 2024, Evanston, IL, USA.

18. (Keynote) AI+HPC for Accelerating Science and Engineering, *International Conference on Artificial Intelligence and Emerging Technology (Global AI Summit) 2024*, September 06, 2024, Bennett University, Greater Noida, UP, India.

19. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *AI for Science*, May 23, 2024, Evanston, IL, USA.

20. (Keynote) AI+HPC for Accelerating Science and Engineering, *14th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2024*, January 19, 2024, Amity University, Noida, Delhi NCR, India.

21. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *10th International Symposium on Fusion of Science and Technology (ISFT) 2024* and *1st International Workshop on Sustainable Technologies for a Better Planet: Challenges & Preparedness for 2050 (STBP) 2024*, January 05, 2024, J.C. Bose University of Science and Technology, Faridabad, Haryana, India.

22. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Science and Engineering, *Computers, Materials & Continua (CMC) Webinar*, December 21, 2023 (Virtual).

23. A Deep Learning Framework for Time-Series Processing-Microstructure-Property Prediction, *22nd IEEE International Conference on Machine Learning and Applications (ICMLA) 2023*, December 15, 2023, Jacksonville, FL, USA.

24. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Science and Engineering, *7th International Conference on Image Information Processing (ICIIP) 2023*, November 23, 2023, Jaypee University of Information Technology, Solan, HP, India.

25. Physics-based Data-Augmented Deep Learning for Enhanced Autogenous Shrinkage Prediction on Experimental Dataset, *International Conference on Contemporary Computing (IC3 2023)*, August 04, 2023, Noida, Delhi NCR, India.

26. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *Freudenberg Visit*, July 11, 2023, Evanston, IL, USA.

27. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *JARVIS School and CHiMaD Training*, June 15, 2023, Lemont, IL, USA.

28. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *JARVIS School and CHiMaD Training*, June 14, 2023, Evanston, IL, USA.

29. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *7th World Congress on Integrated Computational Materials Engineering (ICME 2023)*, May 22, 2023, Orlando, FL, USA.

30. (Invited) Introduction to Machine Learning and Deep Learning for Materials Science, *TMS Online Course: Artificial Intelligence in Materials Science and Engineering*, April 03, 2023 (Virtual).

31. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *6th Forum of Materials Genome Engineering (ForMGE)*, February 18, 2023, Hangzhou City, Zhejiang Province, China.

32. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Science and Engineering, *13th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2023*, January 20, 2023, Amity University, Noida, Delhi NCR, India.

33. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Science and Engineering, *Accelerated Materials Design and Additive Manufacturing: Scientific and Technological Perspectives (AMDAM), 76th Annual Technical Meeting of The Indian Institute of Metals*, November 13, 2022, Hyderabad, Telangana, India.

34. Artificial Intelligence and High-Performance Data Mining: Overview and Updates, *CHiMaD Annual Meeting*, November 08, 2022, University of Chicago, Chicago, IL, USA.

35. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *3rd International Conference on Advances and Applications of Artificial Intelligence & Machine Learning (ICAAAIML 2022)*, September 16, 2022, Sharda University, Greater Noida, Delhi NCR, India.

36. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *9th International Conference Signal Processing and Integrated Networks(SPIN 2022)*, August 26, 2022, Amity University, Noida, Delhi NCR, India (Virtual).

37. Machine Learning for Materials Science (MLMS), *28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2022)*, August 15, 2022, Washington DC, USA.

38. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *3rd Biennial International Conference on Future Learning Aspects of Mechanical Engineering (FLAME 2022)*, August 04, 2022, Amity University, Noida, Delhi NCR, India.

39. AI/ML/DL for Forward and Inverse Problems in Science and Engineering, *International Conference on Dynamical Systems, Control and their Applications (ICDSCA 2022)*, July 01, 2022, Indian Institute of Technology Roorkee (IITR), Roorkee, Uttarakhand, India.

40. (Keynote) AI + HPC for Accelerating Science, *IEEE International Conference on Machine Learning, Big Data, Cloud and Parallel Computing: Trends, Perspectives and Prospects (Com-IT-Con 2022)*, May 26, 2022, Manav Rachna International Institute of Research and Studies, Faridabad, Delhi NCR, India.

41. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Materials Discovery and Design, *Workshop on Data-driven Modeling and Optimization*, May 19, 2022, Fraunhofer Institute for Mechanics of Materials, IWM, Germany.

42. (Invited) AI/ML/DL Approaches for Accelerating Materials Discovery and Design, *TMS 2022: AI/Data Informatics*, February 28, 2022, Anaheim, CA, USA.

43. (Invited) Harnessing the Power of FAIR Materials Data, *MaRDA Annual Meeting*, February 23, 2022 (Virtual).

44. (Invited) AI-Driven Learning of the Science and Engineering of Materials from Simulations, *NAFEMS Seminar on AI, Data Driven Models & Machine Learning*, February 23, 2022 (Virtual).

45. (Keynote) AI + HPC for Accelerating Science, *12th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2022*, January 28, 2022, Amity University, Noida, Delhi NCR, India (Virtual).

46. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *AI for Interdisciplinary Scientific Discovery*, January 27, 2022, Institute of Advanced Studies, Loughborough University, England, UK.

47. Artificial Intelligence and High-Performance Data Mining: Overview and Updates, *CHiMaD Annual Meeting*, January 24, 2022, Northwestern University, USA (Virtual).

48. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *US Army DEVCOM CBC Seminar on AI/ML Applications*, November 10, 2021 (Virtual).

49. (Invited) Introduction to Machine Learning and Deep Learning for Materials Science, *TMS Online Course: Artificial Intelligence in Materials Science and Engineering*, November 02, 2021 (Virtual).

50. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *BiGmax Summer School on Harnessing Big Data in Materials Science from Theory to Experiment*, September 15, 2021, Max Plank Institute, Germany (Virtual).

51. (Invited) AI for Accelerating Materials Discovery and Design, *Nanocombinatorics Workshop on Science of AI*, August 19, 2021, Northwestern University, USA (Virtual).

52. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *ULTRA DOE-EFRC Seminar*, June 28, 2021, Arizona State University, USA (Virtual).

53. (Invited) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *NSF Workshop on Accelerating Materials Discovery, Design, and Synthesis: A Grand Challenge for Artificial Intelligence (AIMS): AI Panel*, April 09, 2021, Pennsylvania State University, USA (Virtual).

54. CHiMaD AI and High Performance Data Mining: Tool Group Updates, *CHiMaD Executive Meeting*, February 12, 2021, Northwestern University, USA (Virtual).

55. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *TMS Webinar Series: Artificial Intelligence in Materials: Research, Design, and Manufacturing*, February 04, 2021, Virtual.

56. (Keynote) Artificial Intelligence and High-Performance Data Mining for Accelerating Scientific Discovery, *11th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2021*, January 29, 2021, Amity University, Noida, Delhi NCR, India (Virtual).

57. (Invited) AI and High-Performance Data Mining: Illustrative Applications in Materials Science, *Indian Symposium on Machine Learning (IndoML)*, December 16, 2020, Indian Institute of Technology (IIT) Gandhinagar, India (Virtual).

58. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *MS&T 2020: Materials Design through AI Composition and Process Optimization*, November 02, 2020 (Virtual).

59. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *Predictive Science and Engineering Design (PSED) Interdisciplinary Cluster Initiative Seminar*, October 22, 2020, Evanston, IL, USA (Virtual).

60. Data-Driven Analytics on Navy Hull Steels Data, *DLA/SFSA Naval Structural Steels Review*, July 24, 2020 (Virtual).

61. Artificial Intelligence and High-Performance Data Mining, *CHiMaD Annual Meeting*, June 09, 2020, Northwestern University, USA (Virtual).

62. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *CHiMaD Phase Field Workshop 2020*, April 21, 2020, Northwestern University, USA (Virtual).

63. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *TMS 2020: ICME Gap Analysis in Materials Informatics*, February 26, 2020, San Diego, CA, USA.

64. (Keynote) High Performance Data Mining: An Essential Paradigm for AI and Big Data Analytics, *10th International Conference on Cloud Computing, Data Science & Engineering (CONFLUENCE) 2020*, January 29, 2020, Amity University, Noida, Delhi NCR, India.

65. Data-driven Analytics for Understanding Materials Properties, *Toyota Visit*, Toyota Motor Corporation, January 23, 2020, Nagoya, Aichi, Japan.

66. A Real-time Iterative Machine Learning Approach for Temperature Profile Prediction in Additive Manufacturing Processes, *6th IEEE International Conference on Data Science and Advanced Analytics (DSAA) 2019*, October 07, 2019, Washington DC, USA.

67. Martensite Start Temperature Predictor for Steels Using Ensemble Data Mining, *6th IEEE International Conference on Data Science and Advanced Analytics (DSAA) 2019*, October 07, 2019, Washington DC, USA.

68. CHiMaD Data Mining and Analytics, *CHiMaD Annual Meeting and Phase II Kickoff*, September 24, 2019, Chicago, IL, USA.

69. (Keynote) Materials Image Informatics Using Deep Learning: Challenges and Opportunities, *LANL Workshop on Advanced Probes and Materials for Enabling 3-D Imaging,* , Los Alamos National Laboratory, August 27, 2019, Santa Fe, NM, USA.

70. (Keynote) High Performance Data Mining: An Essential Paradigm for Big Data Analytics and AI, *5th International Conference on Artificial Intelligence and Security (ICAIS) 2019*, July 27, 2019, Brooklyn, NY, USA.

71. (Invited) Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *CHiMaD Materials Design & Data Informatics Workshop*, July 26, 2019, Evanston, IL, USA.

72. Deep Materials Informatics: Illustrative Applications of Deep Learning in Materials Science, *5th World Congress on Integrated Computational Materials Engineering (ICME 2019)*, July 22, 2019, Indianapolis, IN, USA.

73. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *KAIST Faculty Visit*, May 16, 2019, Evanston, IL, USA.

74. (Invited) Illustrative Microstructure Analytics @CHiMaD, *NIST/NSF Microstructures Workshop*, May 14, 2019, National Cybersecurity Center of Excellence, Rockville, MD, USA.

75. (Invited) CHiMaD Data Analytics, *SRG 2019*, March 25, 2019, Evanston, IL, USA.

76. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *TMS 2019: Computational Approaches for Big Data, Artificial Intelligence and Uncertainty Quantification in Computational Materials Science - Big Data*, March 13, 2019, San Antonio, TX, USA.

77. (Invited) High Performance Data Mining: An Essential Paradigm for Interdisciplinary Big Data Analytics, *SRMAP Visit*, February 26, 2019, SRM University, Amaravati, Andhra Pradesh, India.

78. (Invited) High Performance Data Mining: An Essential Paradigm for Interdisciplinary Big Data Analytics, *IEEE International Conference on Machine Learning, Big Data, Cloud and Parallel Computing: Trends, Perspectives and Prospects (Com-IT-Con 2019)*, February 16, 2019, Faridabad, Haryana, India.

79. (Invited) High Performance Data Mining: An Essential Paradigm for Applied Mathematics and Interdisciplinary Big Data Analytics, *RAMSA 2019*, January 18, 2019, Noida, Delhi NCR, India.

80. Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *ACS Midwest Regional Meeting (MWRM 2018)*, October 23, 2018, Ames, IA, USA.

81. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *XXVII International Materials Research Congress (MRS-Mexico)*, August 20, 2018, Cancun, Mexico.

82. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Artificial Intelligence for Materials Science Workshop (AIMS)*, National Institute of Standards and Technology, August 07, 2018, Gaithersburg, MD, USA.

83. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *13th World Congress on Computational Mechanics (WCCM)*, July 25, 2018, New York City, NY, USA.

84. (Invited) High Performance Data Mining: An Essential Paradigm for Interdisciplinary Big Data Analytics, *Tata Consultancy Services Visit*, TRDDC/TCS, July 18, 2018, Pune, Maharashtra, India.

85. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Toyota Visit*, Toyota Motor Corporation, June 13, 2018, Toyota-shi, Japan.

86. The investigation of machine learning for material development, *Toyota Visit*, Toyota Motor Corporation, June 13, 2018, Toyota-shi, Japan.

87. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Machine Learning in Science & Engineering*, Carnegie Mellon University, June 08, 2018, Pittsburgh, PA, USA.

88. Deep Transfer Learning Based Pavement and Structural Health Monitoring , *Machine Learning in Science & Engineering*, Carnegie Mellon University, June 08, 2018, Pittsburgh, PA, USA.

89. Big Data Analytics in Medicine and Healthcare: Analyzing Electronic Healthcare Records, Sequence Data, Social Media, and More, *Machine Learning in Science & Engineering*, Carnegie Mellon University, June 07, 2018, Pittsburgh, PA, USA.

90. CHiMaD Data Mining, *CHiMaD Site-Visit*, April 16, 2018, Evanston, IL, USA.

91. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Machine Learning in Materials Science Workshop*, University of Utah, April 06, 2018, Salt Lake City, UT, USA.

92. Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *MRS Spring Meeting & Exhibit*, April 04, 2018, Phoenix, AZ, USA.

93. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *6th NU-NIMS Materials Genome Workshop*, March 28, 2018, Evanston, IL, USA.

94. (Invited) CHiMaD Data Mining, *SRG 2018*, March 27, 2018, Evanston, IL, USA.

95. (Invited) Data-Driven Approaches for Steel Fatigue Strength Prediction, *TMS 2018: Fatigue in Materials: Fundamentals, Multiscale Modeling and Prevention - Data-driven Investigations of Fatigue*, March 12, 2018, Phoenix, AZ, USA.

96. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Materials Science Division Colloquium, Argonne National Lab*, February 15, 2018, Lemont, IL, USA.

97. Deep Learning Models for Structure-Property Linkages in High Contrast Composites, *MURI Final Review*, December 18, 2017, Arlington, VA, USA.

98. Learning Crystal Orientations of Polycrystalline Materials from Electron Backscatter Diffraction Experiments using Convolutional Neural Networks, *MURI Final Review*, December 18, 2017, Arlington, VA, USA.

99. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *Predictive Science and Engineering Design (PSED) Interdisciplinary Cluster Initiative Seminar*, November 30, 2017, Evanston, IL, USA.

100. (Invited) Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *International Conference on Nano and Functional Materials (NFM 2017)*, November 17, 2017, BITS Pilani, Rajasthan, India.

101. (Invited) Materials Informatics on Images: Structure Characterization, Crack Detection, Localization, and More, *Machine Learning Applied to Materials Imaging Workshop, Northwestern-Argonne Institute of Science and Engineering*, October 30, 2017, Evanston, IL, USA.

102. (Invited) High Performance Data Mining: An Essential Paradigm for Interdisciplinary Big Data Analytics, *2017 IEEE Region 4 Workshop on Big Data*, October 25, 2017, Evanston, IL, USA.

103. Materials Informatics and Big Data: Realization of "Fourth Paradigm" of Science in Materials Science, *MS&T 2017: Data and Tools for Materials Discovery and Design: Data Science Methods in Materials Discovery and Development*, October 11, 2017, Pittsburgh, PA, USA.

104. Data-Driven Approaches for Predicting Thermoelectric Properties, *MS&T 2017: In-situ Characterization of Energy Materials*, October 10, 2017, Pittsburgh, PA, USA.

105. Classification of Scientific Journal Articles to Support Automated Data Extraction and Curation, *MS&T 2017: Recent Advances in Computer-aided Materials Design: Emerging Approaches of Material Design*, October 10, 2017, Pittsburgh, PA, USA.

106. Data-Driven Approaches for Predicting Fatigue Strength of Steels, *MS&T 2017: Shaping & Forming of Advanced High Strength Steels: Performance*, October 10, 2017, Pittsburgh, PA, USA.

107. Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *Materials Research and Data Science Conference*, September 25, 2017, Rockville, MD, USA.

108. (Invited) Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *MAPEX Symposium 2017, University of Bremen*, September 15, 2017, Bremen, Germany.

109. (Keynote) Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *Materials Genome Symposium, Chinese Materials Conference (CMC 2017), Chinese Materials Research Society (C-MRS)*, July 11, 2017, Yinchuan, Ningxia, China.

110. Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *4th World Congress on Integrated Computational Materials Engineering (ICME 2017), ICME Success Stories and Applications*, May 24, 2017, Ypsilanti, MI, USA.

111. (Invited) Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *SJTU/MaGIC Faculty Visit*, April 27, 2017, Evanston, IL, USA.

112. (Invited) Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science: Steel Fatigue Strength Predictor, *5th NU-NIMS Materials Genome Workshop*, March 28, 2017, Evanston, IL, USA.

113. CHiMaD Data Mining, *CHiMaD Annual Meeting*, March 27, 2017, Evanston, IL, USA.

114. (Invited) CHiMaD Data Mining: Fatigue, *SRG 2017*, March 23, 2017, Evanston, IL, USA.

115. Data Science Approaches for Predicting Fatigue Strength of Steels, *TMS 2017*, February 27, 2017, San Diego, CA, USA.

116. Data Science Approaches for Predicting Thermoelectric Properties, *TMS 2017*, February 27, 2017, San Diego, CA, USA.

117. Parallel Implementation of Lossy Data Compression for Temporal Data Sets, *23rd Annual International Conference on High Performance Computing, Data, and Analytics (HiPC)*, December 20, 2016, Hyderabad, India.

118. Five Year Life Expectancy Calculator for Older Adults, *IEEE International Conference on Data Mining (ICDM)*, December 13, 2016, Barcelona, Spain.

119. A Formation Energy Predictor for Crystalline Materials Using Ensemble Data Mining, *IEEE International Conference on Data Mining (ICDM)*, December 13, 2016, Barcelona, Spain.

120. Predicting the Outcome of Startups: Less Failure, More Success, *IEEE ICDM Workshop on Data Market for Co-evolution of Sciences and Business (MoDAT)*, December 12, 2016, Barcelona, Spain.

121. (Invited) Materials Informatics and Big Data: Realization of the "Fourth Paradigm" of Science in Materials Science, *CHiMaD Summit on Data & Analytics for Materials Research*, November 02, 2016, Evanston, IL, USA.

122. A Fatigue Strength Predictor for Steels Using Ensemble Data Mining, *25th ACM International Conference on Information and Knowledge Management (CIKM)*, October 26, 2016, Indianapolis, IN, USA.

123. (Invited) High Performance Data Mining: An Essential Paradigm for Big Data Analytics and Knowledge Discovery, *3M Visit*, October 19, 2016, Evanston, IL, USA.

124. Identifying HotSpots in Five Year Survival Electronic Health Records of Older Adults, *6th IEEE International Conference on Computational Advances in Bio and Medical Sciences (IC-CABS)*, October 13, 2016, Atlanta, GA, USA.

125. Software tools for sequence comparison, sequence mapping, and patient-specific healthcare outcome prediction, *7th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM BCB)*, October 05, 2016, Seattle, WA, USA.

126. Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *International Conference on Fatigue Damage of Structural Materials (FATD)*, September 22, 2016, Hyannis, MA, USA.

127. CHiMaD Data Mining: An Update, *CHiMaD Executive Meeting*, September 12, 2016, Evanston, IL, USA.

128. Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science, *Theory and Applications of Computational Chemistry (TACC)*, August 30, 2016, University of Washington, Seattle, WA, USA.

129. Deep Learning Based Big Data Analytics in Materials Science, *MURI Annual Meeting*, August 22, 2016, Caltech, Pasadena, CA, USA.

130. (Invited) Data-driven materials science enabling large-scale property prediction and optimization, *APS/CNM Users Meeting 2016*, May 10, 2016, Argonne National Lab, Chicago, IL, USA.

131. (Invited) High Performance Data Mining: An Essential Paradigm for Big Data Analytics and Knowledge Discovery, *Invited seminar*, May 05, 2016, Golden, CO, USA.

132. (Invited) Big data analytics in medicine and healthcare: Analyzing electronic healthcare records, sequence data, social media, and more, *Outcomes Research Workshop*, April 27, 2016, University of Chicago, Chicago, IL, USA.

133. CHiMaD Data Mining, *CHiMaD Annual Meeting*, March 23, 2016, Evanston, IL, USA.

134. (Invited) CHiMaD Data Mining: Fatigue, *SRG 2016*, March 21, 2016, Evanston, IL, USA.

135. (Invited) High Performance Data Mining: An Essential Paradigm for Big Data Analytics and Knowledge Discovery, *Invited seminar*, March 02, 2016, Auburn, AL, USA.

136. (Invited) Towards Better Efficiency and Accuracy: Data Mining for Prediction and Optimization in Materials System Design, *TMS 2016*, February 16, 2016, Nashville, TN, USA.

137. CHiMaD Data Mining: An Update, *CHiMaD Executive Meeting*, October 19, 2015, Evanston, IL, USA.

138. Parallel Distributed-Memory Based Community Detection for Large Graphs, *DARPA GRAPHS / SIMPLEX Workshop: Data, Algorithms and Problems on Graphs (DAPG) 2015*, September 28, 2015, New York, NY, USA.

139. (Invited) Big Data Analytics and Discovery in Medicine and Healthcare, *NUS Surgical Faculty Visit*, September 18, 2015, Chicago Innovation Exchange, Chicago, IL, USA.

140. Pruned Search: A Machine Learning Based Meta-Heuristic Approach for Constrained Continuous Optimization, *8th International Conference on Contemporary Computing (IC3) 2015*, August 20, 2015, Noida, Delhi NCR, India.

141. All Your Google and Facebook Logins are Belong to Us: A Case for Single Sign-off, *8th International Conference on Contemporary Computing (IC3) 2015*, August 20, 2015, Noida, Delhi NCR, India.

142. (Invited) Towards an Infrastructure for Materials Data Analytics: An Overview of Tools and Platforms for Code Development, Collaboration, and Data Analytics, *Materials Research Collaboration Environment Workshop*, August 13, 2015, Dayton, OH, USA.

143. Application of Machine Learning to Materials Discovery and Development, *MURI 3-Year Review*, June 23, 2015, Arlington, VA, USA.

144. Optimization of Microstructures in Magnetoelastic Alloys, *MURI 3-Year Review*, June 23, 2015, Arlington, VA, USA.

145. Mining of Process-Structure-Property Linkages Using Data Science Tools, *MURI 3-Year Review*, June 23, 2015, Arlington, VA, USA.

146. Towards Better Efficiency and Accuracy: Data Mining for Optimization and Prediction in Materials System Design, *AFOSR Program Review*, May 21, 2015, Arlington, VA, USA.

147. CHiMaD Data Mining, *CHiMaD Annual Meeting*, May 01, 2015, Evanston, IL, USA.

148. Data-driven Analytics for Materials Science: Realization of the Fourth Paradigm of Science, *DARPA SIMPLEX Pre-Kickoff Meeting*, April 14, 2015, Evanston, IL, USA.

149. (Invited) CHiMaD Data Mining: Fatigue, *SRG 2015*, March 23, 2015, Evanston, IL, USA.

150. (Invited) High Performance Data Mining: An Essential Paradigm for Big Data Analytics and Knowledge Discovery, *Invited seminar*, March 09, 2015, Lawrence, KS, USA.

151. CHiMaD Data Mining, *CHiMaD Executive Meeting*, December 01, 2014, Evanston, IL, USA.

152. (Invited) High Performance Big Data Analytics for Data-Driven Discovery in Natural Sciences, *GBMF Symposium*, July 29, 2014, Palo Alto, CA, USA.

153. (Invited) CHiMaD Data Mining, *MTL/SRG 2014*, March 24, 2014, Evanston, IL, USA.

154. High Performance Big Data Clustering, *SDAV All-Hands Meeting*, February 25, 2013, Atlanta, GA, USA.

155. (Invited) An Overview of Essential Concepts in Data Mining, *MURI Program Review*, January 21, 2014, Dayton, OH, USA.

156. Multi-objective Optimization and Multimodal Prediction in the Design of Materials System, *MURI Program Review*, January 21, 2014, Dayton, OH, USA.

157. (Invited) Data-Driven Analytics and Discovery in Medicine and Healthcare, *Research Mela*, November 23, 2013, Rush Hospital, Chicago, IL, USA.

158. An Analysis of Variation in Hospital Billing Using Medicare Data, *KDD Workshop on Data Mining for Healthcare (DMH)*, August 11, 2013, Chicago, IL, USA.

159. Heart Transplant Outcome Prediction using UNOS Data, *KDD Workshop on Data Mining for Healthcare (DMH)*, August 11, 2013, Chicago, IL, USA.

160. Colon Surgery Outcome Prediction Using ACS NSQIP Data, *KDD Workshop on Data Mining for Healthcare (DMH)*, August 11, 2013, Chicago, IL, USA.

161. High Performance Big Data Clustering, *SDAV All-Hands Meeting*, February 20, 2013, San Fransisco, CA, USA.

162. Parallel Hierarchical Clustering on Shared Memory Platforms, *International Conference on High Performance Computing (HiPC)*, December 19, 2012, Pune, Maharashtra, India.

163. Data-driven Analytics and Applications - Realization of the Fourth Paradigm of Science, *MURI Kickoff Meeting*, October 19, 2012, Carnegie Mellon University, Pittsburgh, PA, USA.

164. Supporting Computational Data Model Representation with High-performance I/O in Parallel netCDF, *International Conference on High Performance Computing (HiPC)*, December 19, 2011, Bangalore, Karnataka, India.

165. Enhancing Parallelism of Pairwise Statistical Significance Estimation for Local Sequence Alignment, *2nd HiPC Workshop on Hybrid Multi-Core Computing*, December 18, 2011, Bangalore, Karnataka, India.

166. Identifying HotSpots in Lung Cancer Data Using Association Rule Mining, *2nd IEEE ICDM Workshop on Biological Data Mining and its Applications in Healthcare, BioDM 2011*, December 11, 2011, Vancouver, Canada.

167. Community Dynamics and Analysis of Decadal Trends in Climate Data, *3rd IEEE ICDM Workshop on Knowledge Discovery from Climate Data, ClimKD 2011*, December 11, 2011, Vancouver, Canada.

168. Derived Distribution Points Heuristic for Fast Pairwise Statistical Significance Estimation, *ACM International Conference on Bioinformatics and Computational Biology (ACM-BCB) 2010*, August 03, 2010, Niagara, NY, USA.

169. MPIPairwiseStatSig: Parallel Pairwise Statistical Significance Estimation of Local Sequence Alignment, *HPDC ECMLS 2010*, June 22, 2010, Chicago, IL, USA.

170. Pairwise Statistical Significance of Local Sequence Alignment Using Substitution Matrices with Sequence-Pair-Specific Distance, *IEEE International Conference on Information Technology (ICIT 2008)*, December 20, 2008, Bhubaneswar, Orissa, India.

171. Pairwise DNA Alignment with Sequence Specific Transition-Transversion Ratio Using Multiple Parameter Sets, *IEEE International Conference on Information Technology (ICIT 2008)*, December 20, 2008, Bhubaneswar, Orissa, India.

172. Conservative, Non-Conservative and Average Pairwise Statistical Significance of Local Sequence Alignment, *IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2008)*, November 5, 2008, Philadelphia, PA, USA.

173. Pairwise Statistical Significance of Local Sequence Alignment Using Multiple Parameter Sets, *2nd International Workshop on Data and Text Mining in Bioinformatics (DTMBIO 2008)*, October 30, 2008, Napa Valley, CA, USA.

174. DNAlignTT: Pairwise DNA Alignment with Sequence Specific Transition-Transversion Ratio, *IEEE International Conference on EIT 2008*, May 21, 2008, Ames, IA, USA.

175. Pairwise Statistical Significance Versus Database Statistical Significance for Local Alignment of Protein Sequences, *International Symposium on Bioinformatics Research and Applications (ISBRA 2008)*, May 7, 2008, Atlanta, GA, USA.

176. Estimating Pairwise Statistical Significance of Protein Local Alignments Using a Clustering-Classification Approach Based on Amino Acid Composition, *International Symposium on Bioinformatics Research and Applications (ISBRA 2008)*, May 7, 2008, Atlanta, GA, USA.

177. Identifying Temporal Gene Networks Using Signal Processing Metrics on Time-Series Gene Expression Data, *IEEE Third International Conference on Intelligent Sensing and Information Processing*, December 14, 2005, Bangalore, Karnataka, India.

178. Identifying Temporal Gene Networks by Mining Gene Expression Data, *IEEE 12th International Conference on Advanced Computing and Communications (ADCOM) 2004*, December 17, 2004, Ahmedabad, Gujarat, India.

SOFTWARE

1. Parallel Data Clustering Algorithms: Software for parallel DBSCAN clustering in MPI and OpenMP, along with sample dataset is available at [http://cucis.ece.northwestern.edu/projects/Clustering](http://cucis.ece.northwestern.edu/projects/Clustering)

2. Pruned Search Optimization: A general optimization package that performs search space reduction given an objective function and mathematical constraints, available at [http://cucis.ece.northwestern.edu/projects/MURI/workopt.html](http://cucis.ece.northwestern.edu/projects/MURI/workopt.html)

3. Parallel MEP: A parallel community detection algorithm for graphs, based on idea of maximizing equilibrium and purity of communities, available at [http://cucis.ece.northwestern.edu/projects/PMEP/](http://cucis.ece.northwestern.edu/projects/PMEP/)

4. Steel Fatigue Strength Predictor: The online steel fatigue strength predictor is available at [http://info.eecs.northwestern.edu/SteelFatigueStrengthPredictor](http://info.eecs.northwestern.edu/SteelFatigueStrengthPredictor)

5. Formation Energy Predictor: The online formation energy predictor is available at [http://info.eecs.northwestern.edu/FEpredictor](http://info.eecs.northwestern.edu/FEpredictor)

6. ThermoEl Toolkit: The online thermoelectric toolkit for predicting thermoelectric properties is available at http://info.eecs.northwestern.edu/ThermoEl

7. Seebeck Coefficient Predictor: The online Seebeck coefficient predictor is available as part of the ThermoEl toolkit at http://info.eecs.northwestern.edu/SeebeckCoefficientPredictor

8. Bulk Modulus Predictor: The online bulk modulus predictor is available as part of the ThermoEl toolkit at http://info.eecs.northwestern.edu/BulkModulusPredictor

9. Martensite Start Temperature (MsT) Predictor: The online MsT predictor is available at http://info.eecs.northwestern.edu/MsTpredictor

10. Organic Photovoltaic Predictor: The online OPV predictor is available at http://info.eecs.northwestern.edu/OPVPredictor

11. Macroscale (Effective) Stiffness Predictor: The macroscale (effective) stiffness predictor of high-contrast two-phase three-dimensional composite materials is available at http://cucis.ece.northwestern.edu/projects/MURI/workpred.html

12. Stress-Strain Curve Predictor: The online stress-strain curve predictor is available at http://info.eecs.northwestern.edu/StressStrainCurvePredictor

13. Materials Property Predictor: The online materials property predictor is available at http://ai.eecs.northwestern.edu/MPpredictor

14. Five Year Life Expectancy Calculator: The online five year life expectancy calculator for older adults is available at http://info.eecs.northwestern.edu/FiveYearLifeExpectancyCalculator

15. Lung Cancer Outcome Calculator: The online lung cancer outcome calculator is available at http://info.eecs.northwestern.edu/LungCancerOutcomeCalculator

16. Colon Cancer Outcome Calculator: The online colon cancer outcome calculator is available at http://info.eecs.northwestern.edu/ColonCancerOutcomeCalculator

17. Analyzing the Variation in Hospital Billing using Medicare Data: Visually depicted results in the form of US state heat maps can be found at http://users.eecs.northwestern.edu/~ankitag/hospitalbilling/

18. Sentiment Analysis for Social Media Data: An API for sentiment analysis service and benchmark data is available at http://cucis.ece.northwestern.edu/projects/Social/sentiment_api.html

19. Real-Time Digital Flu Surveillance: The real-time disease surveillance tool for flu is available at http://pulse.eecs.northwestern.edu/~kml649/flu/

20. Real-Time Digital Cancer Surveillance: The real-time disease surveillance tool for cancer is available at http://pulse.eecs.northwestern.edu/~kml649/cancer/

21. Real-Time Digital Allergy Surveillance: The real-time disease surveillance tool for allergy is available at http://pulse.eecs.northwestern.edu/~kml649/allergy/

22. Pairwise Statistical Significance Estimation: Sequential codes for pairwise statistical significance estimation and its variants are available at http://www.cs.iastate.edu/~ankitag/projects.html. Parallel codes for optimized HPC implementations (on MPI, OpenMP, Hybrid, GPU) of pairwise statistical significance estimation are available at http://cucis.ece.northwestern.edu/projects/PSSE/

23. AGILE: Long Read Sequence Mapping: Software and data for AGILE are available at http://cucis.ece.northwestern.edu/projects/NGS/agile.html

24. DNAlignTT: DNA Alignment with Sequence-Specific Transition-Transversion Ratio: Source code for DNAlignTT is available at http://www.cs.iastate.edu/~ankitag/DNAlignTT.html

25. FATBEP: Fuzzy Adaptive Thresholding Based Exon Predictor: An implementation of the approach as a user friendly GUI in MATLAB is available at http://www.cs.iastate.edu/~ankitag/FATBEP.html

RESEARCH
SUPERVISION

*Postdoctoral Fellows and/or Research Associates*
- Jagat Sesh Challa (2020-2021)
- Reda Al-Bahrani (2018-2019)
- Dianwei Han (2015-2017)
- Al'ona Furmanchuk (2015-2016)
- Lu Liu (2013-2014)
- Zhengzhang Chen (2012-2014)
- Mostofa Patwary (2011-2013)
- William Hendrix (2011-2012)

*Graduate Students (as Advisor/Co-advisor/Preceptor/Committee Co-Chair)*
- Sayak Chakrabarty, PhD (2024-present)
- Youjia Li, PhD (2023-present)
- Muhammed Nur Talha Kilic, PhD (2022-present)
- Alec Peltekian, PhD (2022-present)
- Alexandra Day, Dissertation Title: "Development of Artificial Intelligence Techniques for Automated Nanoparticle Characterization" PhD (2020-2025)
- Yuwei Mao, PhD, Dissertation Title: "Artificial Intelligence Methodologies for Prediction and Optimization Problems in Materials Informatics" (2020-2025)
- Kewei Wang, PhD, Dissertation Title: "Scalable Training Strategy for Parallel Neural Network and Interpretable Materials Modeling" (2019-2025)
- Vishu Gupta, PhD, Dissertation Title: "Deep Learning Methodologies for Limited Resources Scenarios in Materials Informatics" (2019-2023)
- Zijiang Yang, PhD, Dissertation Title: "Deep Learning for Computer Vision and Applications in Materials Informatics" (2016-2021)
- Dipendra Jha, PhD, Dissertation Title: "Deep Learning Methodologies for Scientific Knowledge Discovery" (2016-2019)
- Arindam Paul, PhD, Dissertation Title: "Machine Learning and Data-driven Optimization for Applications in Scientific Discovery" (2015-2019)
- Reda Al-Bahrani, PhD, Dissertation Title: "Knowledge Discovery for Health Informatics from Structured and Textual Data" (2012-2018)
- Kathy Lee, PhD, Disseration Title: "Mining Social Media for Healthcare Intelligence" (2010-2017)
- Ruoqian (Rosanne) Liu, PhD, Dissertation Title: "Multi-Contextual Representation and Learning with Applications in Materials Knowledge Discovery" (2012-2016)
- Yusheng (Yves) Xie, PhD, Dissertation Title: "Recommender Systems for Social Networks" (2011-2015)
- Diana Palsetia, PhD, Dissertation Title: "High Quality, Scalable Community Detection for Large Graphs" (2010-2015)

*Graduate Students (Other)*
- Zanhua Huang, PhD (2023-2024)
- Claire Lee, PhD, Dissertation Title: "Data Management Challenges for Scaling Graph Neural Networks in Scientific Workflows" (2019-2024)
- Kai Yuan Hou, PhD, Dissertation Title: "Scalable Parallel I/O in the Exa-scale Era" (2016-2022)
- Qiao Kang, PhD, Dissertation Title: "Scalable Communication and I/O Algorithms for High Performance Computing Systems" (2015-2020)
- Sunwoo Lee, PhD, Dissertation Title: "Scalable Parallelization Strategy for Large-Scale Deep Learning" (2015-2020)
- Esteban (Steve) M. Rangel, PhD, Dissertation Title: "High Performance Algorithms for Data Analysis in Computational Cosmology" (2012-2018)
- Chen Jin, PhD (2013-2018)

- Amar Krishna, MS (2013-2016)
- Sharifah Ummu Kulthumm, MS (2015)
- Zheng (Dobbie) Yuan, PhD (2015-2016)
- Yu Cheng, PhD, Dissertation Title: "Mining and Understanding Professional Social Network: Challenges and Solutions" (2010-2015)
- Yuhong Zhang, PhD (2009-2011)
- Daniel Honbo, PhD (2009-2014)
- Kunpeng Zhang, PhD, Dissertation Title: "Big Social Media Data Mining for Marketing Intelligence" (2010-2013)
- Sanchit Misra, PhD, Dissertation Title: "High Throughput Sequence Mapping for Next Generation DNA Sequencing" (2009-2011)

## Undergraduate Students

- Justin Liao (2018-2018)
- Pranjal Daga (2015-2015)
- Siddharth Gupta (2013-2013)
- Lalith Polepeddi (2009-2010)

## Graduate Student Exam Committees

- Youjia Li, PhD Research Proposal (2025)
- Kevin Yao (Chemical and Biological Engineering Major), PhD Research Proposal (2024)
- Sayak Chakrabarty, PhD Qualifying Examination (2024)
- Alexandra Day, PhD Research Proposal (2024), PhD Thesis Defense Exam (2025)
- Yuwei Mao, PhD Research Proposal (2023), PhD Thesis Defense Exam (2024)
- Kewei Wang, PhD Research Proposal (2023), PhD Thesis Defense Exam (2024)
- Claire Lee, PhD Research Proposal (2023), PhD Thesis Defense Exam (2024)
- Vishu Gupta, PhD Research Proposal (2022), PhD Thesis Defense Exam (2023)
- Kai Yuan Hou, PhD Research Proposal (2020), PhD Thesis Defense Exam (2022)
- Zijiang Yang, PhD Research Proposal (2019), PhD Thesis Defense Exam (2021)
- Yu-Chin Chan (Mechanical Engineering Major), PhD Qualifying Examination (2019), PhD Thesis Defense Exam (2022)
- Wenyu Han (Mechanical Engineering Major), MS Thesis Defense Exam (2019)
- Qiao Kang, PhD Research Proposal (2018), PhD Thesis Defense Exam (2020)
- Sunwoo Lee, PhD Research Proposal (2018), PhD Thesis Defense Exam (2020)
- Dipendra Jha, PhD Research Proposal (2017), PhD Thesis Defense Exam (2019)
- Arindam Paul, PhD Research Proposal (2017), PhD Thesis Defense Exam (2019)
- Xiaolin Li (Mechanical Engineering Major), PhD Qualifying Examination (2016), PhD Thesis Defense Exam (2018)
- Reda Al-Bahrani, PhD Qualifying Examination (2015), PhD Research Proposal (2017), PhD Thesis Defense Exam (2018)
- Ruoqian (Rosanne) Liu, PhD Research Proposal (2015), PhD Thesis Defense Exam (2016)
- Yusheng (Yves) Xie, PhD Research Proposal (2014), PhD Thesis Defense Exam (2015)
- Yu Cheng, PhD Research Proposal (2014), PhD Thesis Defense Exam (2015)
- Esteban (Steve) M. Rangel, PhD Qualifying Examination (2014), PhD Research Proposal (2015, 2016), PhD Thesis Defense Exam (2018)
- Diana Palsetia, PhD Research Proposal (2014), PhD Thesis Defense Exam (2015)
- Chen Jin, PhD Research Proposal (2013)
- Kathy Lee, PhD Qualifying Examination (2013), PhD Research Proposal (2014), PhD Thesis Defense Exam (2017)
- Kunpeng Zhang, PhD Qualifying Examination (2012), PhD Research Proposal (2012), PhD Thesis Defense Exam (2013)
- Daniel Honbo, PhD Research Proposal (2011), PhD Thesis Defense Exam (2014)
- Sanchit Misra, PhD Research Proposal (2011), PhD Thesis Defense Exam (2011)

PROFESSIONAL
SERVICE

*Editorial board and organizing committees*

- Editor-in-Chief, Computers, Materials & Continua, 2019-present
- Specialty Chief Editor, Frontiers in High Performance Computing: HPC Applications, 2022-present
- Guest Editor, MRS Communications, Special Issue on Artificial Intelligence, 2019
- Guest Editor, Integrating Materials and Manufacturing Innovation (IMMI), Special Issue on "Using Digital Data in Materials Science and Engineering", 2013
- Editorial Oversight Committee Member, Integrating Materials and Manufacturing Innovation (IMMI), 2020-present
- Editorial Board, Integrating Materials and Manufacturing Innovation (IMMI), 2022-present
- Editorial Board, Scientific Reports, 2023-present
- Editorial Board, Journal of Materials Informatics, 2024-present
- Editorial Board, AI & Materials, 2025-present
- Editorial Board, BMC/Springer Big Data Analytics, 2016-2020
- Organizing Committee Member, First Workshop on Machine Learning for Materials Science (MLMS) in conjunction with 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, August 15, 2022
- Organizing Committee Member, Data & Analytics for Materials Research Summit, hosted by the National Institute of Standards and Technology and its Center of Excellence for Hierarchical Materials Design (CHiMaD), October 31 - November 2, 2016.
- Advisory Committee Member, Materials Data Analytics: A Path-Finding Workshop, hosted by ASM International's CMD Network and OSU with support from NIST, October 8-9, 2015.
- Session Chair, TMS 2019, 2016

*Invited program committee member*

- IEEE International Conference on Data Mining (ICDM) 2025, 2024, 2023, 2022, 2021, 2020, 2019, 2018, 2017, 2016, 2015, 2014
- IEEE International Conference on Big Data (BigData) 2025, 2024, 2023, 2022, 2021, 2020, 2019, 2018, 2017, 2016, 2015, 2014, 2013
- ACM International Conference on Information and Knowledge Management (CIKM) 2022, 2021, 2020, 2019, 2013, 2012
- IEEE International Conference on Machine Learning and Applications (ICMLA) 2022, 2021
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) 2016
- IEEE International Conference on Machine Learning and Data Science (ICMLDS) 2017
- ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis (SC) 2017
- IEEE International Parallel & Distributed Processing Symposium (IPDPS) 2016, 2015
- IEEE IPDPS Workshop on Parallel and Distributed Processing for Computational Social Systems (ParSocial) 2022, 2021, 2020, 2018, 2017, 2016
- IEEE ICDM Workshop on Data Mining in Networks (DaMNet) 2019, 2017, 2016, 2015, 2014, 2013, 2012
- ACM/IEEE SC Workshop on Big Data Analytics: Challenges and Opportunities (BDAC) 2015
- IEEE International Conference on Systems, Man, Cybernetics (SMC) 2015
- IEEE International Conference on Big Data Science and Engineering (BDSE) 2014, 2013

*Invited grant proposal reviewer/panelist*

- US National Science Foundation (NSF)
- US Department of Energy (DOE)
- US Air Force Office of Scientific Research (AFOSR)
- US Army Research Office (ARO)
- Northwestern Data Science Initiative (DSI)
- Singapore Agency for Science, Technology and Research (A*STAR)

- European Research Council (ERC)
- Dutch Research Council (NWO)
- Austrian Science Fund (FWF)
- Mitacs Canada

*Invited paper reviewer*
- ACM Computing Surveys
- ACM Transactions on Knowledge Discovery from Data (TKDD)
- ACS Combinatorial Science
- ARC American Institute of Aeronautics and Astronautics Journal (AIAA)
- BMC Big Data Analytics
- BMC Bioinformatics
- BMC Medical Informatics and Decision Making
- BMC Research Notes
- Cambridge MRS Advances
- Cambridge MRS Communications
- Elsevier Acta Materialia
- Elsevier Additive Manufacturing (AM)
- Elsevier Calphad (Computer Coupling of Phase Diagrams and Thermochemistry)
- Elsevier Computers in Biology and Medicine (CBM)
- Elsevier Computer Methods and Programs in Biomedicine (CMPB)
- Elsevier Computer Communications (COMCOM)
- Elsevier Computational Materials Science (COMMAT)
- Elsevier Current Opinion in Solid State & Materials Science (COSSMS)
- Elsevier Composites Science and Technology (CSTE)
- Elsevier Data and Knowledge Engineering (DKE)
- Elsevier Digital Signal Processing (DSP)
- Elsevier Information Sciences
- Elsevier Journal of Computational Science (JOCS)
- Elsevier Journal of Parallel and Distributed Computing (JPDC)
- Elsevier Materials Science and Engineering: A (MSEA)
- Elsevier Neural Networks (NEUNET)
- Hindawi BioMed Research International
- Hindawi Scientifica
- IEEE Transactions on Computational Biology and Bioinformatics (TCBB)
- IEEE Transactions on Emerging Topics in Computing (TETC)
- IEEE Transactions on Knowledge and Data Engineering (TKDE)
- IEEE Transactions on Parallel and Distributed Systems (TPDS)
- IEEE Transactions on Very Large Scale Integration Systems (TVLSI)
- IET Healthcare Technology Letters
- Inderscience International Journal of Computer Aided Engineering and Technology (IJCAET)
- Inderscience International Journal of High Performance Computing and Networking (IJHPCN)
- MDPI Algorithms
- MDPI Crystals
- MDPI Entropy
- Nature Communications
- npj Computational Materials
- OxfordUP Bioinformatics
- PLOS One
- Springer Artificial Intelligence Review
- Springer Data Mining and Knowledge Discovery (DMKD)
- Springer Integrating Materials and Manufacturing Innovation (IMMI)
- Springer International Journal of Precision Engineering and Manufacturing (IJPEM)
- Springer Journal of Materials Science (JMSC)

- Springer Language Resources and Evaluation (LREV)
- T&F International Journal of Parallel, Emergent and Distributed Systems (IJPEDS)
- T&F Journal of Civil Engineering and Management (JCEM)
- T&F Transport
- Wiley Concurrency and Computation: Practice and Experience (CCPE)
- World Scientific Journal of Circuits, Systems, and Computers (JCSC)
- SC 2013
- ICDM 2012
- ICDM DaMNet 2011
- IPDPS 2011
- PAKDD 2010

REFERENCES    Available upon request