Kipton Barros

Los Alamos National Laboratory
P.O. Box 1663, Mail Stop B221
Los Alamos, NM 87545

kbarros@lanl.gov
http://cnls.lanl.gov/~kbarros
Phone: 505 667 6870

Education

2004-2009, **Boston University**
Ph.D. in Physics
Advisor: William Klein
Thesis: *Phase Transition Kinetics in Long-Range Systems*

1997–2001, **Carnegie Mellon University**
B.S. Computer Science, Minor in Discrete Mathematics

Professional Experience

2014–Present, **Los Alamos National Laboratory**,
Staff Scientist in Physics and Chemistry of Materials, Theoretical Division

2010–2014, **Los Alamos National Laboratory**,
Postdoc. in CNLS and Theoretical Division
Organizer of the CNLS postdoc. seminar
Mentors: Turab Lookman, Timothy Germann, and Cristian D. Batista

2010, **Northwestern University**, Evanston, IL
Postdoc. in the Departments of Materials Science and Engineering
and Applied Mathematics
Mentor: Erik Luijten

2007 Summer, **NIST**, Gaithersburg, MD
NSF IGERT funded visitor in the Polymers Division
Mentor: Jack Douglas

2004, **Clark University**, Worcester, MA
Visitor in the Department of Physics
Helped write *An Introduction to Computer Simulation Methods*, 3rd ed.
Mentor: Harvey Gould

2001–2002, **Green Hills Software**, Santa Barbara, CA
Software engineer, compiler development and back-end optimization

1999–2000, **Los Alamos National Laboratory**
Student researcher in the Physics Division, algorithms for confocal microscopy
Mentor: John George

Service

Executive committee member for the Center for Nonlinear Studies (2015–Present)
LANL LDRD review panel (2017, 2018, 2021, 2022)
NSF review panel (2020)
BES review panel (2020)

Awards

Graduate Book Prize, 2009, Boston University
GSNP Student Speaker Award, $1000 prize, 2009, APS March Meeting
NSF IGERT Fellowship, 2006–2008, Center for Computational Science,
Boston University
Chairman's Book Prize, 2007, Boston University
Dean's Fellow, 2005–2006, Boston University
Presidential Scholarship, 1997–2001, Carnegie Mellon University

Computational Skills	Algorithm design, numerical analysis, machine learning, high performance and GPU computing.
Open Source Code Contributions	**Sunny**, A general-purpose library for performing generalized SU(N) classical spin simulations.. `https://github.com/SunnySuite/Sunny.jl/`
	ElPhDynamics, Linear-scaling simulations for quantum models of electron-phonon interactions. `https://github.com/cohensbw/ElPhDynamics/`
	FastKPM, Linear-scaling electronic structure solver, GPU accelerated and MPI distributed. `https://github.com/kbarros/FastKPM`
	Kondo, Code to enable large-scale simulations of the Kondo lattice model. `https://github.com/kbarros/Kondo`
	ExMatEx project, Proxy-apps for multi-scale simulation on future exascale computers. `http://www.exmatex.org/`
	QUDA, Widely used GPU-based lattice quantum chromodynamics accelerator. `http://lattice.github.com/quda/`
	STP project, Interactive simulations to teach statistical and thermal physics. `http://stp.clarku.edu/simulations`
Project leadership	PI, *Data science driven quantum chemistry for reactive chemistry controlled by stimuli*, BES, DE-FOA-0002474, **$800k/year** (2022, 2023, 2024).
	Co-PI, *Artificial intelligence and data science enabled predictive modeling of collective phenomena in strongly correlated quantum materials* , BES, DE-FOA-0002474, **$700k/year** (2022, 2023, 2024).
	PI, *Sampling the unknown: Robust modeling of atomic potentials*, LDRD-20200209ER, **$309k/year** (2020, 2021, 2022).
	Machine learning lead, *Enabling Predictive Scale-Bridging Simulations through Active Learning*, LDRD-20190005DR, **$1.6M/year** (2019, 2020, 2021).
	Co-PI, *Critical Stress in Earth Crust*, LDRD-20170004DR, **$1.6M/year** (2017, 2018, 2019).
	PI, *Quantum Molecular Dynamics of Strongly Correlated Materials*, LDRD-20170450ER, **$320k/year** (2017, 2018, 2019).
	PI, *Efficient Method for Large Scale Simulations of Fermionic Gases Interacting with Classical Fields*, LDRD-20140458ER, **$320k/year** (2014, 2015, 2016).
Co-organized workshops	**Los Alamos–Arizona Days**, Los Alamos, NM, May 16–17 (2022).
	Machine Learning in Chemical and Materials Sciences, Virtual, May 23–26 (2022).
	2nd Machine Learning in Solid Earth Geoscience, Santa Fe, NM, Mar. 18–22 (2019).

Machine Learning and Informatics for Chemistry and Materials, Telluride, CO, Oct. 1–5 (2018).

Machine Learning in Solid Earth Geoscience, Santa Fe, NM, Feb. 20–22 (2018).

2nd Physics Informed Machine Learning, Santa Fe, NM, Jan. 21–25 (2018).

State of Stress in the Earth, Santa Fe, NM, Oct. 19–21 (2016).

Physics Informed Machine Learning, Santa Fe, NM, Jan. 19–22 (2016).

Manuscripts

63. N. Fedik, R. Zubatyuk, M. Kulichenko, N. Lubbers, J. S. Smith, B. Nebgen, R. Messerly, Y. W. Li, A. I. Boldyrev, K. Barros, O. Isayev, S. Tretiak, *Machine Learning for Molecular Properties: Going Beyond Interatomic Potentials* (submitted to Nature Rev. Chem.).
62. B. Cohen-Stead, O. Bradley, C. Miles, G. Batrouni, R. Scalettar, K. Barros, *Fast and scalable quantum Monte Carlo simulations of electron-phonon models* (submitted to PRE) [arXiv:2203.01291].
61. C. Miles, B. Cohen-Stead, O. Bradley, S. Johnston, R. Scalettar, K. Barros, *Dynamical tuning of the chemical potential to achieve a target particle number in grand canonical Monte Carlo simulations* (submitted to PRE) [arXiv:2201.01296].
60. G. Zhou, N. Lubber, K. Barros, S. Tretiak, and B. Nebgen, *Deep Learning of Dynamically Responsive Chemical Hamiltonians with Semi-Empirical Quantum Mechanics* (submitted to PNAS).
59. D. Rosenberger, K. Barros, T. C. Germann, N. Lubbers, *Machine Learning of consistent thermodynamic models using automatic differentiation* Accepted to PRE [arXiv:2108.04904].
58. C. Miles, M. R. Carbone, E. J. Sturm, D. Lu, A. Weichselbaum, K. Barros, R. M. Konik, *Machine learning of Kondo physics using variational autoencoders and symbolic regression*, Phys. Rev. B **104**, 235111 (2021) [arXiv:2107.08013].
57. J. Finkelstein, J. Smith, S. M. Mniszewski, K. Barros, C. F. A. Negre, E. H. Rubensson, A. M. N. Niklasson, *Quantum-based Molecular Dynamics Simulations using Tensor Cores*, J. Chem. Theory Comput. **17**, 6180 (2021) [arXiv:2107.02737].
56. A. E. Sifain, L. Lystrom, R. A. Messerly, J. S. Smith, B. Nebgen, K. Barros, S. Tretiak, N. Lubbers, B. J. Gifford, *Predicting Phosphorescence Energies and Inferring Wavefunction Localization with Machine Learning*, Chem. Science (2021) [ChemRxiv:14099696].
55. M. Kulichenko, J. S. Smith, B. Nebgen, Y. W. Li, N. Fedik, A. Boldyrev, N. Lubbers, K. Barros, S. Tretiak *The Rise of Neural Networks for Materials and Chemical Dynamics*, J. Phys. Chem. Lett. **12**, 6227–6243 (2021)
54. T. Zubatyuk et al., *Machine Learned Hückel Theory: Interfacing Physics and Deep Neural Networks*, J. Chem. Phys. **154**, 244108 (2021) [arXiv:1909.12963].
53. J. Finkelstein, J. S. Smith, S. M. Mniszewski, K. Barros, C. F. A. Negre, E. H. Rubensson, A. M. N. Niklasson, *Mixed Precision Fermi-Operator Expansion on Tensor Cores From a Machine Learning Perspective*, J. Chem. Theory Comput. **17**, 2256-2265 (2021) [arXiv:2101.06385]
52. G. Paleari, F. Hébert, B. Cohen-Stead, K. Barros, R. T. Scalettar, G. G. Batrouni, *Quantum Monte Carlo study of an anharmonic Holstein model*, Phys. Rev. B, **103**, 195117 (2021) [arXiv:2101.08285].

51. M. Lupo Pasini, Y. W. Li, J. Yin, J. Zhang, K. Barros, M. Eisenbach, *Fast and stable deep-learning predictions of material properties for solid solution alloys*, J. Phys.: Condens. Matter **33**, 084005 (2021).

50. J. S. Smith et al., *Automated discovery of a robust interatomic potential for aluminum*, Nat. Commun. **12**, 1257 (2021) [arXiv:2003.04934].

49. M. Shahzad, K. Barros, S. H. Curnoe, *Phase Diagram of a Spin-ice Kondo Lattice Model in the Breathing Pyrochlore Lattice*, Phys. Rev. B **102**, 144436 (2020). [arXiv:2007.15577]

48. J. S. Smith, N. Lubbers, A. P. Thompson, K. Barros, *Simple and efficient algorithms for training machine learning potentials to force data*, Open access at arXiv, [arXiv:2006.05475]

47. G. Craven, N. Lubbers, K. Barros, Sergei Tretiak, *Machine learning approaches for structural and thermodynamic properties of a Lennard-Jones fluid*, J. Chem. Phys. **153**, 104502 (2020)

46. A. Diaw, K. Barros, J. Haack, et al., *Multiscale simulation of plasma flows using active learning*, Phys. Rev. B. **102**, 023310 (2020).

45. G. T. Craven, N. Lubbers, K. Barros, S. Tretiak, *Ex Machina Determination of Structural Correlation Functions*, J. Phys. Chem. Lett. **11**, 4372 (2020).

44. B. Cohen-Stead, K. Barros, Z. Y. Meng, C. Chen, R. T. Scalettar, G. G. Batrouni, *Langevin Simulations of the Half-Filled Cubic Holstein Model*, Phys. Rev. B **102**, 161108R (2020) [arXiv:2005.00918].

43. C. Devereux et al., *Extending the applicability of the ANI deep learning molecular potential to Sulfur and Halogens*, J. Chem. Theory Comput. **16**, 4192 (2020) [ChemRxiv:11819268].

42. J. Smith et al., *The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules*, Sci. Data **7**, 134 (2020) [ChemRxiv:10050737].

41. A. Samarakoon et al., *Machine Learning Assisted Insight to Spin Ice* $Dy_2Ti_2O_7$, Nat. Commun. **11** 892 (2020) [arXiv:1906.11275].

40. L. Hao et al., *Anomalous Magnetoresistance due to Longitudinal Spin Fluctuations in a* $J_{\text{eff}} = 1/2$ *Mott Semiconductor*, Nat. Commun. **10**, 5301 (2019) [arXiv:1910.13611].

39. J. S. Smith et al., *Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning*, Nat. Commun. **10**, 2903 (2019) [ChemRxiv:6744440].

38. H. Suwa, J. S. Smith, N. Lubbers, C. D. Batista, G.-W. Chern, and K. Barros, *Machine learning for molecular dynamics with strongly correlated electrons*, Phys. Rev. B **99**, 161107 (2019) [arXiv:1811.01914].

37. G.-W. Chern and K. Barros, *Nonequilibrium dynamics of superconductivity in the attractive Hubbard model*, Phys. Rev. B **99**, 035162 (2019) [arXiv:1803.04118].

36. N. Lubbers, D. C. Bolton, J. Mohd-Yusof, C. Marone, K. Barros, and P. A. Johnson, *Earthquake catalog-based machine learning identification of laboratory fault states and the effects of magnitude of completeness*, Geophys. Res. Lett. **45**, 13269 (2018) [arXiv:1810.11539].

35. N. Lubbers, J. S. Smith, and K. Barros, *Hierarchical modeling of molecular energies using a deep neural network*,
J. Chem. Phys. **148**, 241715 (2018) [arXiv:1710.00017].

34. B. Nebgen, N. Lubbers, J. S. Smith, A. Sifain, A. Lokhov, O. Isayev, A. Roitberg, K. Barros, and S. Tretiak, *Transferable dynamic molecular charge prediction using deep neural networks*,
J. Chem. Theory Comput. **14**, 4687 (2018) [arXiv:1803.04395].

33. Z. Wang, G.-W. Chern, C. D. Batista, and K. Barros, *Gradient-based stochastic estimation of the density matrix*,
J. Chem. Phys. **148**, 094107 (2018), *Editor's Pick* [arXiv:1711.10570].

32. G. W. Chern, K. Barros, Z. Wang, H. Suwa, and C. D. Batista, *Semiclassical dynamics of spin density waves*,
Phys. Rev. B **97** 035120 (2018), *Editors' Suggestion* [arXiv:1708.08050].

31. A. E. Sifain, N. Lubbers, B. T. Nebgen, J. S. Smith, A. Y. Lokhov, O. Isayev, A. E. Roitberg, K. Barros, and S. Tretiak *Discovering a Transferable Charge Assignment Model Using Machine Learning*,
J. Phys. Chem. Lett. **9**, 4495 (2018) [ChemRxiv:6638981].

30. N. Lubbers, T. Lookman, and K. Barros, *Inferring low-dimensional microstructure representations using convolutional neural networks*,
Phys. Rev. E **96**, 052111 (2017) [arXiv:1611.02764].

29. B. Rouet-Leduc, C. Hulbert, N. Lubbers, K. Barros, C. Humpheys, and P. A. Johnson, *Machine Learning Predicts Laboratory Earthquakes*,
Geophys. Res. Lett. **44**, 9276 (2017) [arXiv:1702.05774].

28. R. Ozawa, S. Hayami, K. Barros, and Y. Motome, *Shape of magnetic domain walls formed by coupling to mobile charges*,
Phys. Rev. B **96**, 094417 (2017) [arXiv:1609.07189].

27. B. Rouet-Leduc, C. Hulbert, K. Barros, T. Lookman, and C. J. Humphreys, *Automatized convergence of optoelectronic simulations using active machine learning*,
Appl. Phys. Lett. **111**, 043506 (2017).

26. G.-W. Chern, K. Barros, C. D. Batista, J. D. Kress, and G. Kotliar, *Mott transition in a metallic liquid – Gutzwiller molecular dynamics simulations*,
Phys. Rev. Lett. **118**, 226401 (2017) [arXiv:1509.05860].

25. J. Jenkins, G. Shipman, J. Moud-Yusof, K. Barros, P. Carns, and R. Ross, *A Case Study in Computational Caching Microservices for HPC*,
IEEE IPDPS 1309–1316 (2017)

24. G. Ferré, T. Haut, and K. Barros, *Learning molecular energies using localized graph kernels*,
J. Chem. Phys. **146**, 114107 (2017) [arXiv:1612.00193].

23. D. Wulferding et al., *Domain engineering of the metastable domains in the 4f-uniaxial-ferromagnet CeRu2Ga2B*,
Sci. Rep. **7**, 46296 (2017) [arXiv:1703.05228].

22. Z. Wang, K. Barros, G.-W. Chern, D. Maslov, and C. D. Batista, *Resistivity Minimum in Highly Frustrated Itinerant Magnets*,
Phys. Rev. Lett. **117**, 206601 (2016) [arXiv:1604.03620].

21. R. Ozawa, S. Hayami, K. Barros, G.-W. Chern, Y. Motome, and C. D. Batista, *Vortex Crystals with Chiral Stripes in Itinerant Magnets*,
J. Phys. Soc. Jpn. **85**, 103703 (2016) [arXiv:1510.06830].

20. B. Rouet-Leduc, K. Barros, T. Lookman, and C. J. Humphries, *Optimisation of GaN LEDs and the reduction of efficiency droop using active machine learning*, Sci. Rep. **6**, 24862 (2016)

19. T. Lookman, P.V. Balachandran, D. Xue, G. Pilania, T. Shearman, J. Theiler, J.E. Gubernatis, J. Hogden, K. Barros, E. Ben-Naim, and F.J. Alexander, *A perspective on materials informatics: state-of-the-art and challenges*, Information Science for Materials Discovery and Design, Springer (2016)

18. S. Taverniers, T. S. Haut, K. Barros, F. J. Alexander, and T. Lookman, *Physics-based statistical learning approach to mesoscopic model selection*, Phys. Rev. E **92**, 053301 (2015).

17. D. Roehm, R. S. Pavel, K. Barros, B. Rouet-Leduc, A. L. McPherson, T. C. Germann, and C. Junghans. *Distributed database Kriging for adaptive sampling*, Comput. Phys. Commun. **192**, 138-147 (2015).

16. Z. Gan, H. Wu, K. Barros, Z. Xu, and E. Luijten. *Comparison of efficient techniques for the simulation of dielectric objects in electrolytes*, J. Comp. Phys. **291**, 317–333 (2015).

15. K. Barros, J. W. F. Venderbos, G.-W. Chern, and C. D. Batista. *Exotic magnetic orderings in the Kagome Kondo-lattice model*, Phys. Rev. B **90**, 245119 (2014) [arXiv:1407.5369].

14. S.-Z. Lin, K. Barros, E. Mun, J.-W. Kim, M. Frontzek, S. Barilo, S. V. Shiryaev, V. S. Zapf, and C. D. Batista. *Magnetic-field-induced phases in anisotropic triangular antiferromagnets: Application to CuCrO2*, Phys. Rev. B **89**, 220405 (2014) [arXiv:1404.0991].

13. B. Rouet-Leduc, K. Barros, E. Cieren, V. Elango, C. Junghans, T. Lookman, J. Mohd-Yusof, R. S. Pavel, A. Y. Rivera, D. Roehm, A. L. McPherson, and T. C. Germann, *Spatial adaptive sampling in multiscale simulation*, Comput. Phys. Commun. **185**, 1857–1864 (2014).

12. K. Barros and E. Luijten., *Dielectric effects in the self-assembly of binary colloidal aggregates*, Phys. Rev. Lett. **113**, 017801 (2014) [arXiv:1406.1854].

11. K. Barros, D. Sinkovits, and E. Luijten, *Efficient and accurate simulation of dynamic dielectric objects*, J. Chem. Phys. **140**, 06490 (2014) [arXiv:1401.1522].

10. K. Barros and W. Klein, *Liquid to solid nucleation via onion structure droplets*, J. Chem. Phys. **139**, 174505 (2013), [arXiv:1308.5244], *"A recent theoretical tour de force"*—L. Gránásy and G. Tóth, Nature Physics News & Views, **10**, 12–13 (2014).

9. K. Barros and Y. Kato, *Efficient Langevin simulation of coupled classical fields and fermions*, Phys. Rev. B **88**, 235101 (2013) [arXiv: 1303.1101].

8. C. R. Berardi, K. Barros, J. F. Douglas and W. Losert, *Direct observation of string-like collective motion in a two-dimensional driven granular fluid*, Phys. Rev. E **81**, 041301 (2010).

7. M. A. Clark, R. Babich, K. Barros, R. C. Brower, and C. Rebbi, *Solving Lattice QCD systems of equations using mixed precision solvers on GPUs*, Comput. Phys. Commun. **181**, 1517 (2010) [arXiv:0911.3191].

6. K. Barros, P. Krapivsky, and S. Redner, *Freezing into stripe states in two- dimensional ferromagnets and crossing probabilities in critical percolation*, Phys. Rev. E **80**, 040101 (2009) [arXiv:0905.3521].

5. K. Barros, R. Babich, R. Brower, M. A. Clark, and C. Rebbi, *Blasting through lattice calculations using CUDA*,
PoS (Lattice 2008) 045 [arXiv:0810.5365].
4. R. Dominguez, K. Barros, and W. Klein, *Early time kinetics of systems with spatial symmetry breaking*,
Phys. Rev. E **79**, 41121 (2009) [arXiv:0812.3889].
3. K. Barros, R. Dominguez, and W. Klein, *Beyond Cahn-Hilliard-Cook: Early time behavior of symmetry breaking phase transition kinetics*,
Phys. Rev. E **79**, 042104 (2009) [arXiv:0810.3949].
2. H. Wang, K. Barros, H. Gould, and W. Klein, *Approaching equilibrium and the distribution of clusters*,
Phys. Rev. E **76**, 041116 (2007) [arXiv:0704.0938].
1. A. O. Schweiger, K. Barros, and W. Klein, *Transient nucleation near the mean-field spinodal*,
Phys. Rev. E **75**, 039902 (2007) [arXiv:0609406].

POSTDOC CO-MENTORSHIP

1. Nicholas Lubbers, CNLS PD Fellow (2016–2018). Now staff scientist in the CCS-3 group, Information Sciences, LANL. (2018–)
2. Bertrand Rouet-Leduc, Director's PD Fellow (2017–2019). Became staff scientist in the EES-17 group, Geophysics, LANL (2019–2022). Joined faculty of Kyoto University (2022–).
3. Justin S. Smith, Metropolis PD Fellow (2018–2020). Became a staff scientist in the T-1 group, Physics and Chemistry of Materials, LANL (2020–2022). Joined Nvidia as a Senior Developer Relations Manager (2022–). `https://twitter.com/gpusciguy`
4. Daniel Trugman, Feynman PD Fellow (2018–2020). Joined faculty of University of Texas Austin, Department of Geological Sciences (2020–). `https://www.jsg.utexas.edu/researcher/daniel_trugman`
5. Ryan Jadrich, Metropolis PD Fellow (2019–2021). Now staff scientist in the T-1 group, Physics and Chemistry of Materials, LANL (2021–).
6. Galen Craven, Director's PD Fellow (2019–2021). Now staff scientist in the T-1 group, Physics and Chemistry of Materials, LANL (2021–).
7. Adela Habib, Director's PD fellow (2021–).
8. Alice Allen, CNLS PD fellow (2022–).
9. Xinyang Li, LANL PD associate (2022–).
10. Mathew Wilson, LANL PD associate (2022–).

STUDENT CO-MENTORSHIP

1. Toby Shearman, U. Arizona (2014), Developed statistical description of microstructure samples as part of his PhD thesis.
2. Dominic Roehm, U. Stuttgart (2014), Developed database driven adaptive sampling for multiscale simulation as part of his PhD thesis.
3. Bertrand Rouet-Leduc, Cambridge University (2014–2015), ML techniques for accelerated design of LEDs.
4. Ryo Ozawa, U. Tokyo (2014–2015), KPM algorithms with applications to Skyrmion dynamics in magnetic systems
5. Soren Taverniers, U.C. San Diego (2014–2015), ML for phase field model discovery in nonequilibrium domain coarsening.

6. Zhentao Wang, Rice U. (2015), KPM algorithms for itinerant magnetism, and resistivity measurement.
7. Nicholas Lubbers, Boston U. (2016), ML models for compression of synthetic microstructure.
8. Gregoire Ferré, Ecole des Ponts ParisTech (2016), Graph-based molecular modeling.
9. Rashi Verma, Boston U. (2016–2017), ML models of nucleation in atomic systems.
10. Claudia Hulbert, École Polytechnique, Paris (2016–2018), ML to model earthquake physics.
11. Isaac Curtis, U. Idaho (2016), ML models for phase field model discovery for martensitic transformations.
12. Julien Roy, École Polytechnique de Montréal (2016), Deep learning for texture completion.
13. Kishan Supreet Alguri, U. Utah (2017), ML for earthquake modeling, AML summer school. `https://twitter.com/supreet_alguri`
14. Carter L. Johnson, U. C. Davis (2017), ML for earthquake modeling, AML summer school. `http://www.math.utah.edu/~caljohnson/`
15. Justin S. Smith, U. Florida (2017–2018), ML for modeling interatomic potentials.
16. Andrew Sifain, U. Southern California (2018), ML for inferring charge partitioning.
17. Roman Zubatiuk, Jackson State U. (2018–2019), ML for predicting excited state properties of molecules.
18. Austin Walsh, Wayne State University (2019–2020), Uncertainty quantification of ML models.
19. Benjamin Cohen-Stead, UC Davis (2019–2022), Recipient of prestigious UC Fee fellowship, developed QMC methods of electron-phonon coupling.
20. Maksim Kulichenko, Utah State (2020–2021), Developed active learning methodologies.
21. Aleksandra Pachalieva, T. U. Munich (2020–2021), Statistical coarse graining for lattice Boltzmann simulation.
22. David Sanchez, Rey Juan Carlos University, Madrid (2020–2021), Uncertainty quantification of ML models.
23. Cole Miles, Cornell U. (2020–2022), Recipient of prestigious CSGF fellowship, numerical methods for spin dynamics simulations.
24. David Dahlbohm (2021), Geometric integration methods for spin dynamics.
25. Nikita Fedik, Utah State U. (2021), Self-consistent Coulomb interactions for ML models.
26. Shubhang Goswami, U. Illinois (2021), Rational approximation for compact representation of spectral functions.
27. Sakib Matin, Boston U. (2021–), Training ML models to a mixture of simulated and experimental data.
28. Michael Chigaev, U. C. Berkeley (2021–), Covariant tensor extensions of the HIP-NN model.