

Hasan Metin Aktulga

CONTACT INFORMATION

Michigan State University
Department of Computer Science & Engineering
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<https://scholar.google.com/citations?user=CfLHDYgAAAAJ>

RESEARCH INTERESTS

High Performance Computing (HPC), Parallel Algorithms, Performance Modeling, HPC Applications, Scientific Computing, Big Data Analytics, (Sparse) Numerical Linear Algebra, Non-Volatile Memory Architectures.

RESEARCH SYNOPSIS

At the **Scalable Parallel Technologies and Algorithms (SParTA)** Lab at Michigan State University, we primarily work on the design and development of parallel algorithms, numerical methods, performance models and software systems to harness the full potential of state-of-the-art HPC platforms for challenging problems in large scale scientific computing and big-data analytics. A distinguishing aspect of the research in the SParTA Lab is the close collaborations that we have built with domain experts in a wide range of fields such as molecular modeling and simulation, materials science, computational electromagnetics, and nuclear physics.

EDUCATION

Purdue University, West Lafayette, Indiana, USA

Ph.D., Computer Science, *August 2010.*

Thesis Title: Algorithmic and Numerical Techniques for Atomistic Modeling

Advisor: Ananth Grama

M.S., Computer Science, *Dec 2009.*

Advisor: Ananth Grama

Bilkent University, Ankara, Turkey

B.S., Computer Science, *May 2004.*

Senior Project: Smart City Map for PDAs

Advisor: Ibrahim Korpeoglu

WORK EXPERIENCE

Dept. of Computer Science and Engineering, Michigan State University, East Lansing, MI

Assistant Professor (Tenure-track), *August 2014 - present*

Absolute Academy, Okemos, MI

Founder and Executive Director, *December 2017 - present*

Computational Research Division, Lawrence Berkeley National Lab, Berkeley, CA

Affiliated Researcher, Scalable Solvers Group, *August 2014 - present*

Postdoctoral Researcher, Scientific Computing Group, *September 2010 - July 2014*

Supervisor: Esmond G. Ng

CSRI, Sandia National Laboratory, Albuquerque, NM

Summer Intern, *May 2009 - August 2009*

Mentors: Aidan Thompson and Steve Plimpton

Department of Computer Science, Purdue University, West Lafayette, IN

Research Assistant, *May 2005 - August 2010*

Teaching Assistant, *August 2004 - May 2005*
Advisor: Ananth Grama

Math and Science Initiative, Purdue University, West Lafayette, IN
Computer Science Instructor for High School Students, *September 2004 - May 2006*

Department of Computer Science, Bilkent University, Ankara, Turkey
Summer Intern, *June 2003 - August 2003*
Supervisor: Ozgur Ulusoy

Satek Defense Technologies Inc., Ankara, Turkey
Summer Intern, *June 2002 - August 2002*

RESEARCH GRANTS

- ◇ *OAC Core: Small: Efficient and scalable tools for design and analysis of active matter systems*, co-PI (PI: T. Gao, Mechanical Engineering), NSF CISE Core Programs, \$500,000 (share: \$160,000), Jun 2020 – May 2023
- ◇ *REU Site: iCER ACRES: iCER Advanced Computational Research Experience for Students*, Senior Personnel, NSF REU Program, \$472,456, Apr 2020 – Mar 2023
- ◇ *R01: Modeling Transition Metal Ion Binding to Proteins*, co-PI (PI: K. M. Merz, Jr., Chemistry), NIH General Medicine, \$1,290,000 (share: \$520,000), Sep 2019 – Aug 2023
- ◇ *CAREER: Scalable Sparse Linear Algebra for Extreme-Scale Data Analytics and Scientific Computing*, PI, NSF CAREER Program, \$500,000, Feb 2019 – Jan 2024
- ◇ *RET Site: Multidisciplinary Computational Solutions to Smart Sensors and Sensing Systems*, Senior Personnel, NSF RET Program, \$ 534,088, Feb 2019 – Jan 2022
- ◇ *A Geometry and Architecture Agnostic Scalable Framework for N-body Problems with Oscillatory Potentials*, PI (co-PI: B. Shanker, ECE), NSF Scalable Parallelism in the Extreme (SPX) Program, \$675,000 (share: \$340,000), Oct 2018 – Oct 2021
- ◇ *ReaxFF2: Efficient and Scalable Methods for Long-time Reactive Molecular Dynamics Simulations*, PI (co-PI: A. C. T. van Duin, Penn State), NSF Computational and Data-Enabled Science and Engineering Program (CDS&E), \$450,818 (share: \$250,818), Sep 2018 – Sep 2021
- ◇ *Nuclear Computational Low Energy Initiative (NUCLEI)*, MSU ASCR PI (Lead PI: J. Carlson, LANL), DOE Scientific Development through Advanced Computing Program, Phase 4 (SciDAC4), \$10M (share: \$244,000), Sep 2017 – Sep 2022
- ◇ *Highly Efficient Parallel MLFMA for Computational Electromagnetics*, co-PI (PI: B. Shanker, ECE), Air Force Research Lab RaDIEM Program, \$90,162 (share: \$45,000), Feb 2017 – Feb 2018
- ◇ *De Novo Computational Methods for Simulating Energy Materials*, co-PI (PI: Y. Qi, CHEMS), MSU Foundation Strategic Partnership Grant (SPG), \$480,000, (share: \$120,000), July 2016 – July 2019
- ◇ *Algorithms and Tools to Facilitate the Development of High Fidelity Reactive Molecular Dynamics Models*, PI, NSF Career Research Initiation Initiative Program (CRII), \$175,000, June 2016 – June 2019
- ◇ *SciDAC3: Nuclear Computational Low-Energy Initiative (NUCLEI)*, Research Staff (LBNL PI: E. G. Ng), DOE Scientific Discovery through Advanced Computing Program, Phase 3 (SciDAC3), \$850,000 (LBNL share), Aug 2012 – Jul 2017

JOURNAL ARTICLES *Italics* denote student/postdoc who has worked under direct mentorship of H. M. Aktulga.

1. A. Rahnamoun, M. C. Kaymak, M. Manathunga, A. W. Goetz, A. C.T. van Duin, K. M. Merz, Jr., *H. M. Aktulga*, “A ReaxFF/AMBER Tool for Reactive Molecular Dynamics Simulations with AMBER”, *Journal of Computational and Theoretical Chemistry*, *to appear*
2. K. A. O’Hearn, M. W. Swift, J. Liu, I. Magoulas, P. Piecuch, A. C.T. van Duin, *H. M. Aktulga*, Y. Qi, “Optimization of the Reax Force Field for Lithium Dioxide using a High Fidelity Charge Model”, *Journal of Chemical Physics*, 153 (8), 084107, 2020
3. S. Hughey, A. Alsnayyan, *H. M. Aktulga*, T. Gao, B. Shanker, “Fast and scalable evaluation of pairwise potentials”, *Computer Physics Communications*, 255, 107248, 2020
4. K. A. O’Hearn, A. Alperen, *H. M. Aktulga*, “Fast Scalable Solvers for Charge Distribution Models on Shared Memory Platforms”, *SIAM Journal on Scientific Computing* 42 (1), C1-C22, 2020
5. N. Michel, *H. M. Aktulga*, Y. Jaganathan, “Towards Scalable Weakly-Bound and Resonant Nuclear Structure Calculations using the Gamow Shell Model”, *Computer Physics Communications*, 247, 106978, 2020
6. B. Schuetrumpf, G. Martinez-Pinedo, *M. Afibuzzaman*, *H. M. Aktulga*, “Survey of nuclear pasta in the intermediate-density regime: Shapes and energies,” *Physical Review C*, 100, 045806, 2019 [[Editor’s Suggestion](#)]
7. S. Hughey, *H. M. Aktulga*, V. Melapudi, M. Lu, B. Shanker, E. Michielssen, “Parallel Wideband MLFMA for Analysis of Electrically Large, Non-Uniform, Multiscale Structures”, *IEEE Transactions on Antennas and Propagation (IEEE TAP)*, 67 (2), 1094-1107, 2019
8. *H. M. Aktulga*, C. Knight, P. Coffman, K. O’Hearn, T. R. Shan, W. Jiang, “Optimizing the Performance of Reactive Molecular Dynamics Simulations for Many-core Architectures,” *International Journal on High Performance Computing Applications*, 1094342017746221, 2018
9. *M. Afibuzzaman*, B. Schuetrumpf, *H. M. Aktulga*, “Scalable Nuclear Density Functional Theory with Sky3D”, *Computer Physics Communications*, 223, 34-44, 2018
10. M. Shao, *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, J. P. Vary, “Accelerating Nuclear Configuration Interaction Calculations through a Preconditioned Block Iterative Eigensolver”, *Computer Physics Communications*, 222, 1-13, 2018
11. *H. M. Aktulga*, *M. Afibuzzaman*, S. Williams, A. Buluç, M. Shao, C. Yang, E. G. Ng, P. Maris, J. P. Vary, “A High Performance Block Eigensolver for Nuclear Configuration Interaction Calculations,” *IEEE Transactions on Parallel and Distributed Systems*, 28 (6), 1550-1563, 2017
12. S. B. Kylasa, *H. M. Aktulga*, A. Y. Grama, “Reactive Molecular Dynamics on Massively Parallel Heterogeneous Architectures,” *IEEE Transactions on Parallel and Distributed Systems*, 28 (1), 202-214, 2017
13. T. P. Senftle, S. Hong, M. M. Islam, S. B. Kylasa, Y. Zheng, Y. K. Shin, C. Junkermeier, R. Engel-Herbert, M. J. Janik, T. Verstraelen, H. M. Aktulga, A. Grama, Adri C. T. van Duin, “The ReaxFF Reactive Force-field: Development, Applications, and Future Directions,” *Nature PJ Computational Materials*, 2, 15011, 2016
14. M. Dittner, J. Müller, *H. M. Aktulga*, B. Hartke, “Efficient global optimization of ReaxFF parameters,” *Journal of Computational Chemistry*, 36 (20), 1550-1561, 2015
15. D. Oryspayev, *H. M. Aktulga*, M. Sosonkina, P. Maris, J. P. Vary, “Performance analysis of distributed symmetric sparse matrix vector multiplication algorithm for multi-core architectures,” *Concurrency and Computation: Practice and Experience (CP&E)*, 27 (17), 5019-5036, 2015
16. M. Jung, E. H. Wilson III, W. Choi, J. Shalf, *H. M. Aktulga*, C. Yang, E. Saule, Ü. V. Çatalyürek, M. Kandemir, “Exploring the future of out-of-core computing with compute-local non-volatile memory,” *Scientific Programming* 22 (2), pp. 125-139, 2014

17. S. B. Kylasa, *H. M. Aktulga*, and A. Y. Grama, “PuReMD-GPU: A reactive molecular dynamics simulation package for GPUs,” *Journal of Computational Physics*, vol. 272, pp. 343–359, 2014
18. *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, J. P. Vary, “Improving the scalability of a symmetric iterative eigensolver for multi-core platforms,” *Concurrency and Computation: Practice and Experience (CP&E)*, vol. 26, no. 16, pp. 2631-2651, 2014
19. *H. M. Aktulga*, L. Lin, C. Haine, E. G. Ng, C. Yang, “Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method,” *Parallel Computing, Special Issue on Parallel Matrix Algorithms and Applications*, 2013
20. *H. M. Aktulga*, J. C. Fogarty, S. A. Pandit, A. Y. Grama, “Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques,” *Parallel Computing*, vol. 38, no. 4-5, pp. 245–259, 2012 [**Most Cited Article in the Parallel Computing Journal since 2012**]
21. *H. M. Aktulga*, S. A. Pandit, A. C. van Duin, A. Y. Grama, “Reactive molecular dynamics: Numerical methods and algorithmic techniques,” *SIAM Journal on Scientific Computing*, vol. 34, no. 1, pp. 1–23, 2012 [**Top 10 Most Downloaded Article in 2013-2015, Nanoscience and Nanotechnology Commons**]
22. J. C. Fogarty, *H. M. Aktulga*, A. Y. Grama, A. C. Van Duin, S. A. Pandit, “A reactive molecular dynamics simulation of the silica-water interface,” *The Journal of Chemical Physics*, vol. 132, p. 174704, 2010
23. Y. Park, *H. M. Aktulga*, A. Grama, A. Strachan, “Strain relaxation in si/ge/si nanoscale bars from molecular dynamics simulations,” *Journal of Applied Physics*, vol. 106, no. 3, pp. 034 304–034 304, 2009
24. *H. M. Aktulga*, I. Kontoyiannis, L. A. Lyznik, L. Szpankowski, A. Y. Grama, W. Szpankowski, “Identifying statistical dependence in genomic sequences via mutual information estimates,” *EURASIP Journal on Bioinformatics and Systems Biology*, vol. 2007, p. 3, 2007

Under review:

- ◇ *M. Lingg*, *S. Hughey*, *H. M. Aktulga*, B. Shanker, “High Performance Evaluation of Helmholtz Potentials using the Multi-Level Fast Multipole Algorithm”, *ACM Transactions on Parallel Computing (ACM TOPC)*, *under review*

PEER-REVIEWED
CONFERENCES,
WORKSHOPS &
PROCEEDINGS

Italics denote students/postdocs who worked under direct mentorship of H. M. Aktulga.

1. *M. Lingg*, *S. Hughey*, *D. Dikbayir*, *H. M. Aktulga*, B. Shanker, “Exploring Task Parallelism for the Multilevel Fast Multipole Algorithm”, *Proceedings of the 27th IEEE International Conference on High Performance Computing, Data, and Analytics (HiPC 2020)*, *accepted for publication*
2. *M. Afibuzzaman*, *M. F. Rabbi*, M. Y. Ozkaya, U. V. Catalyurek, *H. M. Aktulga*, “DeepSparse: A Task-parallel Framework for Sparse Solvers on Deep Memory Architectures”, *Proceedings of the 26th IEEE International Conference on High Performance Computing, Data, and Analytics (HiPC 2019)*, Hyderabad, India, Dec 2019
3. *M. F. Rabbi*, C. S. Daley, *H. M. Aktulga*, N. J. Wright, “Evaluation of Directive-based GPU Programming Models on a Block Eigensolver with Consideration of Large Sparse Matrices,” *Sixth Workshop on Accelerator Programming Using Directives (WACCPD 2019)*, *Proceedings of the Supercomputing 2019 Workshops (SC19 Workshops)*, Denver, CO, Nov 2019
4. *A. Alperen*, *K. A. O’Hearn*, *H. M. Aktulga*, “Performance Optimization of Reactive Molecular Dynamics Simulations With Dynamic Charge Distribution Models on Distributed Memory Platforms”, *Proceedings of the 2019 International Conference on Supercomputing (ICS 2019)*, Phoenix, AR, Jun 2019

5. *M. C. Kaymak*, R. Fox, S. Liddick, *H. M. Aktulga*, “Data Analysis for Atomic Shapes in Nuclear Science”, Proceedings of the 2019 International Conference on Computational Science (ICCS 2019), Faro, Algarve, Portugal, Jun 2019
6. *M. Lingg*, *S. Hughey*, *H. M. Aktulga* “Optimization of the Spherical Harmonics Transform based Tree Traversals in the Helmholtz FMM Algorithm”, Proceedings of the 47th International Conference on Parallel Processing (ICPP 2018), Eugene, OR, Aug 2018
7. *S. Hughey*, *H. M. Aktulga*, V. Melapudi, M. Lu, E. Michielssen, B. Shanker, “Parallel Non-Uniform MLFMA for Multiscale Electromagnetic Simulation”, Proceedings of the 2018 IEEE International Symposium on Antennas and Propagation and USNC/URSI National Radio Science Meeting, Boston, MA, July 2018
8. S. Salin, M. Manguoglu, *H. M. Aktulga*, “Learning the Domain of Sparse Matrices”, 2016 International Conference on Machine Learning Applications (ICMLA 2016), Anaheim, CA, Dec 2016
9. *K. A. O’Hearn*, *H. M. Aktulga*, “Towards Fast and Scalable Solvers for Charge Equilibration in Molecular Dynamics Applications,” ScalA16: Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems, Proceedings of the Supercomputing 2016 Workshops (SC16 Workshops), Salt Lake City, UT, Nov 2016
10. J. P. Vary, R. Basili, W. Du, M. Lockner, P. Maris, D. Oryspayev, S. Pal, S. Sarker, *H. M. Aktulga*, E. Ng , M. Shao, C. Yang, “*Ab initio* No Core Shell Model with Leadership-Class Supercomputers,” Proceedings of The International Conference on Nuclear Theory in the Supercomputing Era 2016 (NTSE 2016), Khabarovsk, Russia, Sep 2016
11. *S. Hughey*, B. Shanker, *H. M. Aktulga*, “Scalability Analysis of Parallel Wideband ACE-FMM”, Proceedings of the 2016 IEEE International Symposium on Antennas and Propagation (APSURSI), Fajardo, Puerto Rico, June 2016
12. J. P. Vary, P. Maris, H. Potter, M. Caprio, R. Smith, S. Binder, A. Calci, J. Langhammerd, R. Roth, *H. M. Aktulga*, E. Ng , C. Yang , D. Oryspayev, M. Sosonkina, U. CATALYUREK, “*Ab initio* no core shell model: Recent results and further prospects,” Proceedings of The International Conference on Nuclear Theory in the Supercomputing Era 2014 (NTSE 2014), Khabarovsk, Russia, June 2014
13. *H. M. Aktulga*, A. Buluç, S. Williams, C. Yang, “Performance optimization of block eigensolvers for nuclear configuration interaction calculations,” 28th IEEE International Parallel & Distributed Processing Symposium (IPDPS 2014), Phoenix, AZ, USA, May 2014
14. M. Jung, E. H. Wilson III, W. Choi, J. Shalf, *H. M. Aktulga*, C. Yang, E. Saule, Ü. V. Çatalyürek, M. Kandemir, “Exploring the future of out-of-core computing with compute-local non-volatile memory,” Proceedings of The International Conference for High Performance Computing Networking, Storage, and Analysis 2013 (SC13), Denver, CO, USA, Nov 2013 **Best Paper Finalist**
15. C. Yang, *H. M. Aktulga*, P. Maris, E. Ng, J. Vary, “Recent Advances in MFDn,” Proceedings of The International Conference on Nuclear Theory in the Supercomputing Era 2013 (NTSE 2013), Ames, IA, USA, May 13–17, 2013
16. P. Maris, *H. M. Aktulga*, S. Binder, A. Calci, Ü. V. Çatalyürek, J. Langhammer, E. Ng, E. Saule, R. Roth, J. P. Vary, C. Yang, “No core CI calculations for light nuclei with chiral 2- and 3-body forces,” Journal of Physics: Conference Series, vol. 454, no. 1, p. 012063, 2013
17. P. Maris, *H. M. Aktulga*, M. A. Caprio, Ü. V. Çatalyürek, E. G. Ng, D. Oryspayev, H. Potter, E. Saule, M. Sosonkina, J. P. Vary *et al.*, “Large-scale *ab initio* configuration interaction calculations for light nuclei,” Journal of Physics: Conference Series, vol. 403, no. 1, p. 012019, 2012

18. Z. Zhou, E. Saule, *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, J. P. Vary, Ü. V. Çatalyürek, “An out-of-core eigensolver on SSD-equipped clusters,” Proceedings of 2012 IEEE International Conference on Cluster Computing (CLUSTER 2012), pp. 248–256, Beijing, China, Sep 2012
19. Z. Zhou, E. Saule, *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, J. P. Vary, Ü. V. Çatalyürek, “An out-of-core dataflow middleware to reduce the cost of large scale iterative solvers,” Proceedings of 2012 41st International Conference on Parallel Processing Workshops (ICPPW 2012), pp. 71–80, Pittsburgh, PA, USA, Sep 2012
20. *H. M. Aktulga*, C. Yang, E. Ng, P. Maris, J. Vary, “Topology-aware mappings for large-scale eigenvalue problems,” in Proceedings of Euro-Par 2012 Parallel Processing, Lecture Notes in Computer Science (LNCS), vol. 7484, pp. 830–842, Rhodes, Greece, Aug 2012
21. *H. M. Aktulga*, C. Yang, Ü. Çatalyürek, P. Maris, J. Vary, E. Ng, “On reducing I/O overheads in large-scale invariant subspace projections,” Proceedings of Euro-Par 2011: Parallel Processing Workshops, Lecture Notes in Computer Science (LNCS), vol. 7155, pp. 305–314, Bordeaux, France, Aug 2011
22. *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, J. P. Vary, “Large-scale parallel null space calculation for nuclear configuration interaction,” in 2011 International Conference on High Performance Computing and Simulation (HPCS 2011), IEEE, pp. 176–185, Istanbul, Turkey, Jul 2011 **Best Paper Finalist**
23. E. Ng, J. Sarich, S. Wild, T. Munson, *H. M. Aktulga*, C. Yang, P. Maris, J. Vary, N. Schunck, M. Bertolli, M. Kortelainen, W. Nazarewicz, T. Papenbrock, M. V. Stoitsov, “Advancing nuclear physics through TOPS solvers and tools,” Proceedings of SciDAC Conference, Denver, CO, USA, Jul 2011
24. *H. M. Aktulga*, A. Y. Grama, S. Plimpton, A. Thompson, “A fast ILU preconditioning-based solver for the charge equilibration problem,” CSRI Summer Proceedings 2009, p. 50, Albuquerque, NM, USA, Aug 2009
25. *H. M. Aktulga*, I. Kontoyiannis, L. A. Lyznik, L. Szpankowski, A. Y. Grama, W. Szpankowski, “Statistical dependence in biological sequences,” 2007 IEEE International Symposium on Information Theory (ISIT 2007), pp. 2676–2680, Nice, France, Jun 2007

Under review and in preparation:

- ◇ *M. Afibuzzaman*, P. Maris, T. Groves, D. Oryspayev, B. Cook, C. Yang, *H. M. Aktulga*, “Evaluation of the Communication Motif for a Distributed Eigensolver using the SST Network Simulation Tool”, 11th IEEE International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems, *under review*

BOOK CHAPTERS & THESIS

1. E. Saule, *H. M. Aktulga*, C. Yang, E. G. Ng, Ü. V. Çatalyürek, “An Out-of-Core Task-based Middleware for Data-Intensive Scientific Computing,” *Handbook on Data Centers*, pp. 647–667, Springer-Verlag New York, Feb 2015, ISBN: 978-1-4939-2091-4
2. A. Y. Grama, J. C. Fogarty, *H. M. Aktulga*, S. A. Pandit, “N-Body computational methods,” *Encyclopedia of Parallel Computing 2011*, pp. 1259–1268.
3. *H. M. Aktulga*, “Algorithmic and numerical techniques for atomistic modeling”, *Ph.D. dissertation*, Purdue University, West Lafayette, IN, USA. (Jul 2010)

TEACHING

CSE 415 - Introduction to Parallel Computing, Michigan State University
Fall 2015, Spring 2017, Spring 2018, Spring 2019, Spring 2020

CMSE/CSE 822 - Parallel Computing, Michigan State University
Fall 2014, Fall 2017, Fall 2019

CSE 820 - Advanced Computer Architecture, Michigan State University

Spring 2015, Fall 2016, Fall 2018, Fall 2020

INVITED TALKS,
SEMINARS AND
COLLOQUIA

Accelerating N-body Computations: Reactive Molecular Dynamics Simulations, Nuclear Structure Calculations, and Oscillatory Wave Potentials

Seminar, Computational Science and Research Institute, Sandia National Labs, Albuquerque, NM, Jan 2020

Towards Fast, Scalable and High Fidelity Reactive Molecular Dynamics Simulations

Colloquium, MICDE Seminar Series, University of Michigan, Ann Arbor, MI, Sep 2019
Colloquium, Department of Computer Science, Old Dominion University, Norfolk, VA, Oct 2018

High Performance Data Analytics: Why and How?

Data in the D Meeting, Title Source, Detroit, MI, Sep 2015

Careers in Computer Science & Engineering

Michigan Math & Science Academy, Center Line, MI, Feb 2015

Parallel Algorithms and Software Systems for Data-intensive Scientific Computing

Nuclear Theory Seminar, MSU/NSCL, East Lansing, MI, Oct 2014
Electrical Engineering and Computer Science Division, UC Merced, CA, Apr 2014
Computer Science & Engineering Dept., Michigan State University, East Lansing, MI, Mar 2014
Electrical and Computer Engineering Department., Iowa State University, Ames, IA, Mar 2014
Computer Science Department, University of Georgia, Athens, GA, Feb 2014

Eigensolvers for Modern High Performance Computing Platforms

Computer, Electrical and Mathematical Sci. & Eng., KAUST, Thuwal, Saudi Arabia, Apr 2013
Computer Science and Engineering Department, SUNY Buffalo, Buffalo, NY, Apr 2013
Computer and Information Science Department, IUPUI, Indianapolis, IN, Feb 2013
Department of Mathematics, Southern Methodist University, Dallas, TX, Feb 2013

Scalable Eigensolvers For Large-scale Sparse Matrices

Computer Engineering Department, Middle East Technical University, Ankara, Turkey, Sep 2012

ReaxC for the Knowledge-base of Interatomic Models

KIM Content Carnival Meeting, Mar 2012, Minneapolis, MN

Performance Evaluation of the USER-REAXC Package

LAMMPS Users Workshop, Albuquerque, NM, Aug 2011

High-Performance Computing and Its Applications

Dept. of Computer Engineering, Meliksah University, Kayseri, Turkey, Jul 2012
Dept. of Computer Engineering, Hacettepe University, Ankara, Turkey, Jul 2012
Dept. of Computer Engineering, Bilkent University, Ankara, Turkey, Jul 2012

Sparse Linear Algebra on an SSD-equipped Testbed

CRD All-Hands Meeting, LBNL, Apr 2012

POSTERS &
ABSTRACTS

1. C. Tyler, K. O'Hearn, M. C. Kaymak, H. M. Aktulga, "Machine Learning Based Prediction of Initial Guesses for Charge Solvers in Molecular Dynamics Applications", MSU Engineering NSF-RET Summer Projects Poster Session, Kellogg Center, MSU (July 2019)
2. M. F. Rabbi, M. Afibuzzaman, H. M. Aktulga, "DeepSparse: Reducing Data Movement in Sparse Solver Computations on Deep Memory Architectures", Engineering Graduate Re-

search Symposium, Breslin Center, MSU (March 2019)

3. M. C. Kaymak, H. M. Aktulga, Sean N. Liddick, "Data Analysis for Atomic Shapes in Nuclear Science", Engineering Graduate Research Symposium, Breslin Center, MSU (March 2019)
4. K. A. O'Hearn, A. Alperen, H. M. Aktulga, "Efficient, Scalable Techniques for Charge Assignment in Polarizable Molecular Dynamics Applications", Engineering Graduate Research Symposium, Breslin Center, MSU (March 2018)
5. F. Rabbi, M. Afibuzzaman, H. M. Aktulga, "Towards an Efficient Data Dependency Driven Parallel Task-based Sparse Linear Algebra Framework for Extreme-scale Scientific Computing", Engineering Graduate Research Symposium, Breslin Center, MSU (March 2018)
6. S. Hughey, H. M. Aktulga, B. Shanker, "Efficient Parallelization of MLFMA with a Hybrid Global Interpolation/Anterpolation Scheme", 2017 IEEE International Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting, San Diego, CA (July 2017)
7. S. Hughey, H. M. Aktulga, B. Shanker, "Algorithms for Adaptive Trees Within a Parallel MLFMA", 2017 IEEE AP-S Symposium on Antennas and Propagation and USNC-URSI Radio Science Meeting, San Diego, CA (July 2017)
8. H. M. Aktulga, K. A. O'Hearn, "Fast Charge Equilibration Solvers for Polarizable Force Fields", 2017 SIAM Computational Science and Engineering Conference, Atlanta, GA (March 2017)
9. S. Hughey, H. M. Aktulga, B. Shanker, "Parallel Adaptive Fast Multipole Method for Electromagnetics", MSU College of Engineering Graduate Research Symposium (March 2017)
10. S. Hughey, B. Shanker, H. M. Aktulga "Parallel Wideband ACE-FMM for Large-Scale Distributed-Memory Clusters", 2016 FEM Workshop, Rome, Italy, May 2016
11. A. C. T. van Duin, H. M. Aktulga, "Development of the ReaxFF force field for complex materials and interfaces", 2016 TMS Annual Meeting & Exhibition, Nashville, TN (Feb 2016)
12. M. E. Ozturk, M. Thavappiragasam, H. M. Aktulga, "Accelerating Molecular Dynamics Simulations", 2015 Engineering Summer Undergraduate Research Experience (EnSURE 2015) Posters Session, East Lansing, MI (July 2015)
13. M. E. Ozturk, M. Thavappiragasam, H. M. Aktulga, "Accelerating Molecular Dynamics Simulations", 2015 Internship in Global Engineering & Advanced Research (inGEAR 2015) Posters Session, East Lansing, MI (July 2015)
14. R. S. Brayfield II, H. M. Aktulga, A. Y. Grama, and A. L. Garner, "Molecular Dynamics Simulation of Plasma Reactive Species with Lipid Bilayers", 2015 Annual Meeting of the Bioelectromagnetics Society and the European BioElectromagnetics Association, Monterey, CA (June 2015)
15. H. M. Aktulga, A. C. T. van Duin, "Towards a Fully Automated Framework for Optimization of Empirical Potentials", 2015 TMS Annual Meeting & Exhibition, Orlando, FL (Mar 2015)
16. R. S. Brayfield II, H. M. Aktulga, A. Y. Grama, and A. L. Garner, "Molecular dynamics simulations for assessing plasma reactive species interactions with lipid bilayers", 11th International Bioelectrics Symposium, Columbia, MO, p. 25 (Oct 2014)
17. F. Farzad, E. G. Ng, H. M. Aktulga, "A Study of Variations on the Conjugate Gradient Algorithm", IISME-CSEE Summer Program Posters Day, Berkeley, CA, USA (Aug 2012)
18. H. M. Aktulga, J. C. Fogarty, S. A. Pandit, A. Y. Grama, "Parallel Reactive Molecular Dynamics: Algorithmic Techniques and Numerical Methods", Conference on Materials Genome: Simulations, Synthesis, Characterization and Manufacturing, Palos Verdes, CA, USA (Apr 2012)
19. H. M. Aktulga, J. C. Fogarty, S. A. Pandit, A. Y. Grama, "PuReMD: Purdue Reactive Molecular Dynamics Program", Conference on Emerging Trends in Materials Simulations and Experiments, Palos Verdes, CA, USA (Mar 2010)

20. H. M. Aktulga, S. A. Pandit, A. Y. Grama, "PurdueReax: A Molecular Dynamics Tool for Simulating Reactive Systems", Joint Indo-US Workshop on Scalable Nanomaterials for Enhanced Energy Transport, Conversion and Efficiency, JNCASR, Bangalore, India (Aug 2008)

TALKS &
PRESENTATIONS

1. "DeepSparse: A Task-parallel Framework for Efficiently Executing Sparse Solvers on Deep Memory Architectures", 2019 NUCLEI Meeting, Santa Fe, NM, May 2019
2. "Machine Learning based Prediction of Charges in Polarizable Molecular Dynamics Models", MSU Engineering NSF-RET Summer Projects, 2019 Kick-off Meeting, East Lansing, MI, May 2019
3. "ReaxFF/AMBER: A Hybrid Force Field to Facilitate the Study of Metalloproteins", 2019 AMBER Developers Meeting, Tampa, FL, Apr 2019
4. "Performance Optimization of Reactive Molecular Dynamics Simulations with Dynamic Charge Models on Distributed Memory Platforms", 2019 SIAM Conference on Computational Science and Engineering, Spokane, WA, Feb 2019
5. "Optimization of the Spherical Harmonics Transform based Tree Traversals in the Helmholtz FMM Algorithm", 2018 International Conference on Parallel Processing (ICPP 2018), Eugene, OR, Aug 2018
6. "Performance Optimization of Sky3D and Gamow Shell Model Codes", 2018 NUCLEI Meeting, Knoxville, TN, June 2018
7. "De Novo Computational Methods for Simulating Energy Materials", MSU Foundation SPG Projects Meeting, Michigan State University, East Lansing, MI, May 2018 (co-author)
8. "Parallel Wideband Non-uniform MLFMA for Multiscale EM Simulations", Air Force Research Laboratory Project Closing Meeting, Dayton, OH, December 2017 (co-presenter)
9. "Scalable nuclear density functional theory based on the code Sky3D", 2017 NUCLEI Meeting, Santa Fe, NM, June 2017 (co-author)
10. "De Novo Computational Methods for Simulating Energy Materials", MSU Foundation SPG Projects Meeting, Michigan State University, East Lansing, MI, May 2017 (co-author)
11. "Efficient and Accurate Parallel MLFMA for Computational Electromagnetics", Air Force Research Laboratory Project Kickoff Meeting, Dayton, OH, April 2017 (co-presenter)
12. "Scalable Algorithms and Implementations for Molecular Dynamics, Charge Equilibration and Force Field Optimization", SPG Kickoff Workshop, Michigan State University, East Lansing, MI, August 2016
13. "A High Performance Block Eigensolver for Nuclear Configuration Interaction Calculations", NUCLEI Annual Meeting, Argonne National Laboratory, Lemont, IL, June 2016
14. "Challenges and Opportunities in/through Molecular Modeling & Simulation", GrandEng 2015 Conference, Northwestern University, Evanston, IL, May 2015
15. "Optimizing Sparse Matrix-Multiple Vectors Multiplication (SpMM) for Nuclear Structure Calculations", 28th IEEE International Parallel & Distributed Processing Symposium (IPDPS 2014), Phoenix, AZ, May 2014 (conference presentation)
16. "Performance Optimization of a Parallel Block Eigensolver for Nuclear Structure Computations", SIAM Parallel Processing Conference (SIAM PP 2014), Portland, OR, Feb 2014 (conference presentation)
17. "Recent Progress in MFDn v14", NUCLEI Collaboration Meeting, Bloomington, IN, Jun 2013 (project meeting)
18. "An Efficient and Scalable Lanczos-based Eigensolver for Multi-core Systems", SIAM Computational Science & Engineering Conference (SIAM CSE 2013), Boston, MA, Feb 2013 (conference presentation)

19. “Improving the Scalability of MFDn”, NUCLEI Kick-off Meeting, Institute for Nuclear Theory, Seattle, WA, Jan 2013
20. “Topology-aware Mappings for Large-scale Eigenvalue Problems”, 2012 International European Conference on Parallel and Distributed Computing (Euro-Par 2012), Rhodes Island, Greece, Aug 2012 (conference presentation)
21. “Solving Large-scale Eigenvalue problems in Nuclear Structure Calculations”, 12th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, Mar 2012 (conference presentation)
22. “On Reducing I/O Overheads in Large-Scale Invariant Subspace Projections”, 2011 High Performance Scientific Software Workshop (HPSS 2011), Bordeaux, France, Aug 2011 (conference talk)
23. “Large-scale Parallel Null Space Calculation for Nuclear Configuration Interaction”, H. M. Aktulga, 2011 High Performance Computing and Simulation Conference (HPCS 2011), Istanbul, Turkey, Jul 2011 (conference talk)
24. “Accelerating Total-J Calculations”, UNEDF 2011 Meeting, East Lansing, MI, Jun 2011 (project meeting)

HONORS, AWARDS &
SCHOLARSHIPS

- ◇ NSF CAREER Award, 2019
- ◇ 2014 AcademicKeys Who’s Who in Engineering Higher Education (WWEHE)
- ◇ SC13 – Best Paper Finalist, SC 2013, Denver, CO
- ◇ ParCo12 – Top 25 Hottest Article in 2012 & 2013, Parallel Computing Journal
- ◇ SISC12 – Top 10 Hottest Article of 2013, Nanoscience and Nanotechnology Commons
- ◇ HPCS11 – Best Paper Finalist, HPCS 2011, Istanbul, Turkey
- ◇ Startup Allocation on XSEDE Gordon Supercomputer, “Distributed Out-of-core Linear Algebra Framework for SSD-equipped Clusters”, 100,000 CPU hours, June 2013-June 2014
- ◇ USC Travel Grant award to attend the Conference on Materials Genome: Simulations, Synthesis, Characterization and Manufacturing, Rachos Palos Verdes, CA, April 2012
- ◇ USC Travel Grant award to attend the Conference on Emerging Trends in Materials Simulations and Experiments, Rachos Palos Verdes, CA, April 2010
- ◇ Discovery Park Travel Grant award to attend Joint Indo-US Workshop on Scalable Nanomaterials for Enhanced Energy Transport, Conversion and Efficiency, Bangalore, India, August 2008
- ◇ Full financial support (tuition, fees, monthly stipend) throughout the Ph.D. studies, Computer Science Department, Purdue University, 2004-2010
- ◇ Full Undergraduate Scholarship, Bilkent University, 2000-2004
- ◇ Ranked among top 1000 out of 1,000,000+ students in National University Entrance Exams
- ◇ Represented Turkey in International Olympiad in Informatics (IOI), Beijing, China, 2000
- ◇ Gold Medal in International Mathematics Project Olympiads, Almaty, Kazakhstan, 1999
- ◇ Bronze Medals in National Informatics Olympiads, Ankara, Turkey, 1998 and 1999
- ◇ Full High School Scholarship, Yamanlar Science High School, 1997-2000
- ◇ Ranked among top 200 out of 130,000+ students in National High School Entrance Exams
- ◇ National Merit Scholarship for Secondary School Education, 1993-1997
- ◇ Ranked among top 200 out of 100,000+ students in National Secondary School Entrance Exams

Committees

Review Panel Member for NSF (4) and DOE (2), Aug 2015 - present
Colloquium Committee, MSU Dept. of Computer Science and Engineering, Aug 2015 - May 2018, August 2019 - Present
Faculty Search Committee, MSU Dept. of Computational Mathematics, Science and Engineering, Fall 2016 - Spring 2017
Graduate Studies and Research Committee, MSU Dept. of Computer Science and Engineering, Aug 2016 - May 2017
Curriculum Committee, MSU Dept. of Computer Science and Engineering, Aug 2014 - Aug 2015
Faculty Search Committee, MSU Dept. of Mechanical Engineering & Computational Mathematics, Science and Engineering, Fall 2014 - Spring 2015

Conference Program Committees

SC18 - 30th International Conference for High Performance Computing, Networking, Storage and Analysis
SC16 - 28th International Conference for High Performance Computing, Networking, Storage and Analysis
IPDPS 2016 - 30th IEEE International Parallel & Distributed Processing Symposium
SC15 - 27th International Conference for High Performance Computing, Networking, Storage and Analysis
Basarim 2015 - 4th Turkish National High Performance Computing Conference
CCGrid 2015 - 15th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing
CCGrid 2014 - 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing
ICIT 2014 - 2nd ScienceOne International Conference on Information Technology
ADVCOMP 2013 - 7th Intl Conf on Advanced Engineering Comp. and Applications in Sciences

Journal Reviewer

Parallel Computing (ParCo), SIAM Scientific Computing (SISC), ACM Transactions on Parallel Computing (ACM TOPC), IEEE Transactions on Parallel and Distributed Systems (IEEE TPDS), IEEE Transactions on Cloud Computing (IEEE TCC), IEEE Transactions on Computational Biology and Bioinformatics (IEEE TCBBI), IEEE Transactions on Antennas and Propagation (IEEE TAP), Concurrency and Computation: Practice and Experience Journal (CPE), Journal of Computational Science, Numerical Linear Algebra with Applications (NLAA), Journal of Computational Chemistry, Journal of Chemical Physics, Computational Materials Science (CMS)

Conference Reviewer

Basarim 2012 - 3rd Turkish National High Performance Computing Conference
SC11 - Intl Conf for High Performance Computing, Networking, Storage and Analysis
Euro-Par 2011 - 17th European Conference on Parallel Processing
ECCB 2007 - 6th European Conference on Computational Biology

Student Organizations

College of Science Rep., Computer Science Graduate Student Board, Purdue University, 2006-07
Treasurer, Dialogue International, Purdue University, 2006-07
President, Math and Science Initiative, Purdue University, 2005-06