## Hasan Metin Aktulga


CONTACT INFORMATION

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RESEARCH INTERESTS

Parallel Computing, High Performance Computing, Data Intensive Computing, Big Data Analytics, Scientific Computing, Algorithms, Numerical Linear Algebra, Non-Volatile Memory Architectures, Runtime Systems.

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.
*Overall GPA:* 3.75/4.0

M.S., Computer Science, *Dec 2009*.
*Advisor:* Ananth Grama.
*Overall GPA:* 3.70/4.0

**Bilkent University**, Ankara, Turkey

B.S., Computer Science, *May 2004*.
*Senior Project:* Smart City Map for PDAs
*Advisor:* Ibrahim Korpeoglu
*Overall GPA:* 3.86/4.0

WORK EXPERIENCE

**Lawrence Berkeley National Lab**, Berkeley, CA

Postdoctoral Researcher, *September 2010 - present*.
Scientific Computing Group

**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*.

**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*.

**Satek Defense Technologies Inc.**, Ankara, Turkey

Summer Intern, *June 2002 - August 2002*.

## JOURNAL ARTICLES

1. *H. M. Aktulga*, L. Lin, C. Haine, E. G.Ng, and C. Yang, "Parallel eigenvalue calculation based on multiple shift-invert Lanczos and contour integral based spectral projection method," *Parallel Computing*, to appear in the Special Issue on Parallel Matrix Algorithms and Applications (2013) [ParCo13]
2. *H. M. Aktulga*, C. Yang, E. G. Ng, P. Maris, and J. P. Vary, "Improving the scalability of a symmetric iterative eigensolver for multi-core platforms," *Concurrency and Computation: Practice and Experience (CCP&E)*, published online, Sep 2013, DOI: 10.1002/cpe.3129 (2013) [CPE13]
3. *H. M. Aktulga*, J. C. Fogarty, S. A. Pandit, and A. Y. Grama, "Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques," *Parallel Computing*, vol. 38, no. 4-5, pp. 245–259, 2012. [ParCo12] **Top 10 Hottest Article of 2012 in Parallel Computing Journal by ScienceDirect**
4. *H. M. Aktulga*, S. A. Pandit, A. C. van Duin, and A. Y. Grama, "Reactive molecular dynamics: Numerical methods and algorithmic techniques," *SIAM Journal on Scientific Computing*, vol. 34, no. 1, pp. 1–23, 2012. [SISC12] **Top 10 Most Downloaded Article of 2013 in Nanoscience and Nanotechnology Commons**
5. J. C. Fogarty, *H. M. Aktulga*, A. Y. Grama, A. C. Van Duin, and S. A. Pandit, "A reactive molecular dynamics simulation of the silica-water interface," *The Journal of Chemical Physics*, vol. 132, p. 174704, 2010. [JCP10]
6. Y. Park, *H. M. Aktulga*, A. Grama, and 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. [JAP09]
7. *H. M. Aktulga*, I. Kontoyiannis, L. A. Lyznik, L. Szpankowski, A. Y. Grama, and W. Szpankowski, "Identifying statistical dependence in genomic sequences via mutual information estimates," *EURASIP Journal on Bioinformatics and Systems Biology*, vol. 2007, p. 3, 2007. [EURASIP07]

- S. B. Kylasa, *H. M. Aktulga*, and A. Y. Grama, "PuReMD-GPU: A reactive molecular dynamics simulation package for GPUs," *submitted to the Journal of Computational Physics*, under review. [JCP13]

## PEER-REVIEWED CONFERENCES & PROCEEDINGS

1. *H. M. Aktulga*, A. Buluç, S. Williams, and C. Yang, "Performance optimization of block eigensolvers for nuclear configuration interaction calculations," *28th IEEE International Parallel & Distributed Processing Symposium (IPDPS 2014)*, to appear. [IPDPS14]
2. 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", in *Proceedings of SC'13*, Denver, CO. (Nov 2013) [SC13] **Best Paper Finalist**
3. P. Maris, H. M. Aktulga, S. Binder, A. Calci, Ü. V. Çatalyürek, J. Langhammer, E. Ng, E. Saule, R. Roth, J. P. Vary, and 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. [JPCS13]
4. 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. [JPCS12]
5. Z. Zhou, E. Saule, H. M. Aktulga, C. Yang, E. G. Ng, P. Maris, J. P. Vary, and Ü. V. Çatalyürek, "An out-of-core eigensolver on SSD-equipped clusters," in *Proceedings of 2012 IEEE International Conference on Cluster Computing (CLUSTER 2012)*, pp. 248–256, Beijing, China (Sep 2012). [CLUSTER12]

6. Z. Zhou, E. Saule, H. M. Aktulga, C. Yang, E. G. Ng, P. Maris, J. P. Vary, and Ü. V. Çatalyürek, "An out-of-core dataflow middleware to reduce the cost of large scale iterative solvers," in *Proceedings of 2012 41st International Conference on Parallel Processing Workshops (ICPPW 2012)*, pp. 71–80, Pittsburgh, PA, USA (Sep 2012). [ICPPW12]
7. H. M. Aktulga, C. Yang, E. Ng, P. Maris, and 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). [EuroPar12]
8. H. M. Aktulga, C. Yang, Ü. Çatalyürek, P. Maris, J. Vary, and E. Ng, "On reducing I/O overheads in large-scale invariant subspace projections," in *Proceedings of Euro-Par 2011: Parallel Processing Workshops*, Lecture Notes in Computer Science (LNCS), vol. 7155, pp. 305-314, Bordeaux, France (Aug 2011) [EuroParW11]
9. H. M. Aktulga, C. Yang, E. G. Ng, P. Maris, and J. P. Vary, "Large-scale parallel null space calculation for nuclear configuration interaction," in *High Performance Computing and Simulation (HPCS), 2011 International Conference on*, IEEE, pp. 176–185, Istanbul, Turkey (Jul 2011) [HPCS11] **Best Paper Finalist**
10. 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," in *Proceedings of SciDAC Conference*, Denver, CO, USA (Jul 2011) [SciDAC11]
11. H. M. Aktulga, A. Y. Grama, S. Plimpton, and A. Thompson, "A fast ILU preconditioning-based solver for the charge equilibration problem," *CSRI Summer Proceedings 2009*, p. 50, Albuquerque, NM, USA (Aug 2009) [CSRI09].
12. H. M. Aktulga, I. Kontoyiannis, L. A. Lyznik, L. Szpankowski, A. Y. Grama, and W. Szpankowski, "Statistical dependence in biological sequences," in *Information Theory 2007 (ISIT 2007), IEEE International Symposium on*, pp. 2676–2680, Nice, France (Jun 2007) [ISIT07]

## Book Chapters & Thesis

1. A. Y. Grama, J. C. Fogarty, H. M. Aktulga, S. A. Pandit, "N-Body computational methods", *Encyclopedia of Parallel Computing 2011*, pp. 1259-1268. [EPC11]
2. H. M. Aktulga, "Algorithmic and numerical techniques for atomistic modeling", *Ph.D. dissertation*, Purdue University, West Lafayette, IN, USA. (Jul 2010)
3. 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", *to appear in the Handbook on Data Centers*, Springer, invited book chapter.

## Under Preparation

- S. B. Kylasa, *H. M. Aktulga*, and A. Y. Grama, "PG-PuReMD: A parallel-GPU reactive molecular dynamics package," *under submission*.
- D. Oryspayev, *H. M. Aktulga*, "Memory-efficient Symmetric Sparse Matrix Vector Multiplication Algorithms for Distributed Memory Multi-core Architectures", *under preparation*.

## Grant Writing Experience

◇ Helped with "Nuclear Computational Low-Energy Initiative (NUCLEI)", Scientific Discovery through Advanced Computing Program, Advanced Scientific Computing Research and Nuclear Physics, Office of Science, US Department of Energy, Contract no. DE-AC02-05CH11231.
Role: Research Staff, LBNL PI: Esmond Ng
Secured Funding: $850,000 for over 5 years (LBNL portion).
Funding Term: Aug 2012 – Jul 2017.

## HONORS, AWARDS & SCHOLARSHIPS

* ParCo12 – Top 10 Hottest Article of 2012 in Parallel Computing Journal by ScienceDirect
* SISC12 – Top 10 Hottest Article of 2013 Nanoscience and Nanotechnology Commons
* SC13 – Best Paper Finalist, SC 2013, Denver, CO
* 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 Undergradute 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

## RESEARCH PROJECTS

**Postdoctoral Researcher, Lawrence Berkeley National Lab** (September 2010-Present)

**Data Intensive Graph and Matrix Analytics on Non-Volatile Memory Architectures**
Worked on the design and development of iterative linear solvers and eigensolvers for clusters equipped with fast non-volatile memory (NVM) storages, such as SSDs. Solvers are built on top of the Distributed Out-of-Core Linear Algebra Framework, a task-based data-flow middleware. Demonstrated a scalable and efficient execution in production environments [CLUSTER12, ICPPW12]. Explored the implications of future NVM computer architectures on software design and application performance. Demonstrated that an application managed, compute-node local NVM can boost performance significantly [SC13]. Future work is to extend our framework to a general purpose data-analysis framework with graph analytics and sparse linear algebra support. Working on NSF and DOE proposals for funding.

**Fully Automated Force Field Generation for Materials Simulation & Design**
A high quality force field parametrization can have a huge impact in the design and simulation of advanced materials. However, generation and tuning of force field parameters is a labor-intensive task, but more importantly, it requires deep expert knowledge. Working on the preliminary phases for the design and development of a software infrastructure to fully automate the generation and tuning of classical and reactive molecular dynamics force field parameters. Machine learning and data mining techniques are required to identify a reference data set based on density-functional theory (DFT) simulations. Sensitivity analysis and numerical optimization techniques are needed for fitting large force field parameter sets to the reference data set. High-throughput simulation

infrastructure will be used for running massively parallel DFT and classical/reactive MD simulations. Establishing a collaboration with the Materials Project and the Electrolyte Genome groups at LBL, which are large DOE funded projects under the Materials Genome Initiative. Working on a DOE proposal for funding.

**Eigensolvers for Quantum Molecular Dynamics Simulations**
Designed and developed a fast and scalable shift-invert Lanczos based eigensolver (SHINES) for massively parallel distributed memory machines. SHINES is currently used in computing a fraction of the spectrum for large sparse symmetric matrices which arise in density-functional theory (DFT) calculations. The target application is the simulation of the interface dynamics in Lithium Ion batteries, which is funded by the DOE SciDAC program as part of the Materials Genome Initiative. While existing methods fail to scale in this situation, we exploit the massive parallelism available in today's supercomputers with SHINES by partitioning the spectrum into small intervals based on inertial counts and assigning each interval to a small set of processors. Developed a performance model to determine the processor group size and the number of eigenpairs per interval for best performance [ParCo13]. Currently working on resolving issues with special cases such as clustered eigenpairs and multiple eigenvalues.

**Optimization of Sparse Matrix Computations on Emerging Multi/Many-core Architectures**
Two important trends in high performance computing is (i) increasing number of cores per node, (ii) decreasing memory space available per core. These trends pose significant challenges for data-intensive applications. Currently exploring various algorithms on emerging multi-core and many-core systems to enable memory-efficient sparse matrix computations, which constitutes the main kernel of iterative linear solvers and eigensolvers. Working on a model to explain the performance characteristics and bottlenecks of the algorithms investigated. Working on a new algorithm to overcome the identified bottlenecks for better performance.

**Eigensolvers for Large-Scale Symmetric Sparse Matrices**
Developed a new algorithm for a highly scalable implementation of iterative eigensolvers on multi-core platforms for computing the lowest eigenpairs of large symmetric unstructured sparse matrices. In this algorithm, communication overheads are significantly reduced through a topology-aware mapping of the processes to physical processors [EuroPar12]. Using hybrid MPI/OpenMP parallelism on multi-core systems and a 1D hierarchical decomposition of basis vectors during orthogonalization, further reductions in communication overheads are achieved. Developed a novel strategy to overlap the expensive collective communication operations with symmetric sparse matrix vector (SpMV) computations [CPE13]. The resulting Lanczos-based eigensolver is now used in MFDn, a computational physics code for nuclear structure calculations. The new eigensolver achieves up to 6x speedup compared to an earlier version on 18,000 cores and exhibits almost perfect scaling to 260,000 cores [JPCS12].

**Reactive Molecular Dynamics on GPUs**
Supervised the design and development of the GPU version of the highly successful reactive molecular dynamics code, PuReMD. On a typical GPU-equipped workstation, obtained over 15x improvement in runtime compared to the highly optimized CPU-only PuReMD code. Work is underway to enable the execution of the PuReMD-GPU code on large GPU clusters, such as GaTech/Keeneland and ORNL/Titan machines.

**PhD Student, Purdue University** (August 2004-August 2010)

**Reactive Molecular Dynamics on Massively Parallel Architectures**
Lead software architect and developer for the open-source PuReMD code, a highly efficient and scalable reactive molecular dynamics code based on the ReaxFF force field. With PuReMD, we extend current spatio-temporal simulation capability for reactive atomistic systems by over an order of magnitude. This is made possible by incorporating efficient dynamic data structures, algorithmic optimizations, and effective iterative linear solvers to deliver low per-time-step simu-

lation time, with a small memory footprint [ParCo12, SISC12]. PuReMD has been used to model diverse systems, ranging from strain relaxation in Si–Ge nanobars [JAP09], water–silica surface interaction [JCP10], and oxidative stress in lipid bilayers (bio-membranes). PuReMD is currently available in LAMMPS, a widely popular MD simulation suite, and is being used by hundreds of researchers worldwide.

**Identifying Statistical Dependence in Genomic Sequences via Mutual Information** Demonstrated the use of information–theoretic tools for the task of identifying segments of biomolecules (DNA or RNA) that are statistically correlated. Developed a precise and reliable methodology, based on the notion of mutual information, for finding and extracting statistical as well as structural dependencies. A simple threshold function is defined, and its use in quantifying the level of significance of dependencies between biological segments is explored. These tools are used in two specific applications. First, they are used for the identification of correlations between different parts of the maize zmSRp32 gene. There, we find significant dependencies between the 5 untranslated regions in zmSRp32 and its alternatively spliced exons. This observation may indicate the presence of as-yet unknown alternative splicing mechanisms or structural scaffolds. Second, using data from the FBIs combined DNA index system (CODIS), we demonstrate that our approach is particularly well suited for the problem of discovering short tandem repeatsan application of importance in genetic profiling [ISIT07, EURASIP07].

## POSTER PRESENTATIONS

- 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)
- 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)
- 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)
- 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

- ◇ "Recent Progress in MFDn v14", NUCLEI Collaboration Meeting, Bloomington, IN, Jun 2013 (project meeting)
- ◇ "Scalable and Efficient Eigensolvers for Modern Supercomputers", Computer, Electrical and Mathematical Sciences and Engineering Seminars, KAUST, Thuwal, Saudi Arabia, Apr 2013 (invited talk)
- ◇ "Eigensolvers for Modern High Performance Computing Platforms", Computer Science and Engineering Seminars, Buffalo, NY, Apr 2013 (invited talk)
- ◇ "Eigensolvers for Modern High Performance Computing Platforms", Computer Science and Engineering Seminars, Buffalo, NY, Apr 2013 (invited talk)
- ◇ "An Efficient and Scalable Lanczos-based Eigensolver for Multi-core Systems", SIAM Computational Science & Engineering Conference (SIAM CSE 2013), Boston, MA, Feb 2013 (project meeting)
- ◇ "Eigensolvers for Modern High Performance Computing Platforms", Computer and Information Science Seminars, Indianapolis, IN, Feb 2013 (invited talk)
- ◇ "Scalable and Efficient Eigensolvers for Modern Supercomputers", Mathematics Seminars, Dallas, TX, Feb 2013 (invited talk)

- ◇ "Improving the Scalability of MFDn", NUCLEI Kick-off Meeting, Institue for Nuclear Theory, Seatlle, WA, Jan 2013 (project meeting)
- ◇ "Scalable Eigensolver For Large-scale Sparse Matrices", Computer Engineering Seminars, Middle East Technical University, Ankara, Turkey, Sep 2012 (invited talk)
- ◇ "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 talk)
- ◇ "Sparse Linear Algebra on an SSD-equipped Testbed", CRD All-Hands Meeting, LBNL, Apr 2012 (departmental presentation)
- ◇ "Solving Large-scale Eigenvalue problems in Nuclear Structure Calculations", 12th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, Mar 2012 (conference talk)
- ◇ "ReaxC for the Knowledge-base of Interatomic Models", KIM Content Carnival Meeting, Mar 2012, Minneapolis, MN (project meeting)
- ◇ "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)
- ◇ "Performance Evaluation of USER-REAXC Package", LAMMPS Users Workshop, Albuquerque, NM, Aug 2011 (invited talk)
- ◇ "High-Performance Computing and Applications", Computer Engineering Seminars, Meliksah University, Kayseri, Turkey, Jul 2012 (invited talk)
- ◇ "High-Performance Computing and Applications", Computer Engineering Seminars, Hacettepe University, Ankara, Turkey, Jul 2012 (invited talk)
- ◇ "High-Performance Computing and Applications", Computer Engineering Seminars, Bilkent University, Ankara, Turkey, Jul 2012 (invited talk)
- ◇ "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)
- ◇ "Accelerating Total-J Calculations", UNEDF 2011 Meeting, East Lansing, MI, Jun 2011 (project meeting)

SOFTWARE

**SHINES (SHift-INvert based Eigen-Solver)**
Main author. A fast and scalable shift-invert Lanczos based parallel eigensolver developed for multi-core platforms. Used to compute a large fraction of the spectrum for sparse symmetric matrices which arise in density-functional theory (DFT) calculations. Built using numerical libraries MUMPS and ARPACK. Developed in Fortran/MPI, porting to C++ is underway. Under active development, will be released as an open-source project. 3000-5000 lines of code.

**MFDn (Many Fermion Dynamics - nuclear)**
Developer. MFDn is used to compute structures of light nuclei using the Configuration Interaction model, which is a first principles quantum mechanical model. This requires the solution of extremely large-scale sparse eigenvalue problems, where few extremal eigenpairs are of interest. OpenMP/MPI hybrid programming model and Fortran is used for code development. Developed load-balancing and communication overhead minimization techniques to achieve scaling to tens of thousands of processors on modern multi-core supercomputers. Open-source code developed in Fortran, using MPI/OpenMP parallelism. Contributed about 5000-6000 lines of code.

**Total-J**
Developer. Built on top of the MFDn code. Total-J is especially useful when all eigenvalues associated with a particular state of a nucleus is needed. This requires the computation of the basis

space of interest, projection of the extremely large Hamiltonian matrix into this basis space and the solution of the eigenvalue problem in this subspace. Developed load-balancing and I/O overhead minimization techniques to achieve scaling to thousands of processors on modern supercomputers. Open-source code developed using Fortran/MPI. Contributed around 7000-8000 lines of code.

**PuReMD (Purdue Reactive Molecular Dynamics)**
Main author. A parallel reactive molecular dynamics code based on the Reax force field. PuReMD exhibits excellent performance and scalability. It extends the spatio-temporal capabilities of existing parallel ReaxFF implementations by over an order of magnitude. Developed using C/MPI, open-source code, distributed freely with GPL. Around 15000 lines of code.

**USER-REAXC**
Main author. Integration of the PuReMD software into the widely used LAMMPS platform as a package. Still responsible for maintaining the code for bug fixes and adding additional features as requested by users. Distributed freely with LAMMPS software, used by hundreds of researchers worldwide. Developed using C++ and MPI parallelization. Contributed around 2000 lines of code.

**SerialReax**
Main author. Constitutes the heart of PuReMD. Uses various algorithmic, numerical analysis and numerical linear algebra techniques to achieve an excellent CPU performance. Features a fully dynamic and adaptive memory manager to make efficient use of the memory resources. Open-source code, distributed freely with GPL. Implemented in C, around 15000 lines of code.

## SERVICES & LEADERSHIP

### Program Committees

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

### Reviewer

Concurrency and Computation: Practice and Experience Journal
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

### Service

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

## COMPUTER SKILLS

### Programming Languages

C, C++, Java, Fortran, MATLAB, Awk.

### Parallel Programming

MPI, OpenMP, POSIX Threads.

### Libraries

BLAS, LAPACK, ScaLAPACK, ARPACK, MUMPS.

REFERENCES

**Prof. Ananth Grama**
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