# XIAODONG YU

Assistant Computer Scientist

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Google scholar: scholar.google.com/citations?user=1sefeCkAAAAJ&hl=en

#### RESEARCH INTERESTS

My research interests broadly lie in parallel, distributed, and reconfigurable computing, computer systems, and computer architecture. Specifically, I am working on system design and optimization to support large-scale deep learning; performance benchmarking and modeling of next-generation AI hardware; parallel compressor design and optimization for exascale scientific data; accelerator-based (e.g., GPU) application acceleration; and performance optimization of collective communications in GPU-aware MPI.

#### **EDUCATION**

Doctor of Philosophy, Computer Science and Applications

Virginia Tech, Blacksburg, VA, USA

August 2019

Dissertation - Algorithms and Frameworks for Accelerating Security Applications on HPC Platforms
Thesis committee: Prof. Danfeng (Daphne) Yao (Chair), Prof. Michela Becchi (NCSU), Prof. Ali Butt,
Prof. Matthew Hicks, Prof. Xinming (Simon) Ou (USF)

Master of Science, Electrical Engineering

University of Missouri, Columbia, MO, USA

August 2013

Thesis - Deep Packet Inspection on Large Datasets: Algorithmic and Parallelization Techniques for Accelerating Regular Expression Matching on Many-Core Processors

Thesis Advisor: Prof. Michela Becchi

Bachelor of Science, Mathematics and Applied Mathematics China University of Mining and Technology (CUMT), China

June 2008

### PROFESSIONAL APPOINTMENTS

Argonne National Laboratory, Lemont, IL Assistant Computer Scientist Postdoctoral Appointee

June 2022 - Current

September 2019 - May 2022

- Designing benchmark suite for next-generation AI hardware (LDRD and FAIR-SBI).
- Optimizing data loading for large-scale surrogate training (FAIR-SBI).
- Designing and implementing fast GPU-based lossy compressors for scientific data (VeloC/SZ).
- Designing and implementing MPI collective communications with compression (Exascale MPI).
- Designing and implementing multi-GPU-based ptychographic image reconstruction (RAVEN).

The University of Chicago Consortium for Advanced Science and Engineering, Chicago, IL

Scientist-at-Large

November 2022 - Current

AMD, Austin, TX

Co-op Software Engineer

May 2017 - Aug. 2017

• Developing GPU Deep learning library (MIOpen).

Virginia Tech, Blacksburg, VA Graduate Research Assistant Graduate Teaching Assistant

August 2013 - August 2019 August 2013 - May 2017

- Designing and implementing GPU-assisted program analysis for vetting Android apps.
- Studying vulnerability of the systems to cache side-channel attacks.

- Designing and implementing programming framework for Micron's Automata Processor.
- Designing and implementing GPU-based CT image reconstruction.
- Teaching assistant of undergraduate courses: CS2505 and CS2506.

University of Missouri, Columbia, MO

Graduate Research Assistant

May 2011 - August 2013

Designing and implementing GPU-based automata processing.

#### **GRANTS**

• PI: LDRD Advanced Computing Expedition, "Scalability Study of AI-based Surrogate for Ptychographic Image Reconstruction on Graphcore."

Award Amount: \$50K

Award Period: 07/01/2022 - 09/30/2022

• Host and Primary collaborator: NSF EPSCoR RII Track-4 Program, "Massively Parallel Graph Processing on Next-Generation Multi-GPU Supercomputers." (PI: Prof. Da Yan)

Award Amount: \$275K

Award Period: 02/01/2023 - 01/31/2025

## **PROJECT LEADERSHIP**

• LDRD Advanced Computing Expedition: Scalability Study of AI-based Surrogate for Ptychographic Image Reconstruction on Graphcore.

My Role: PI

Period: 07/01/2022 - 09/30/2022

• DOE ASCR: FAIR-SBI: Surrogate Benchmarks Supporting AI and Simulation Research.

My Role: Senior Personnel and Technical Lead

Period: 03/01/2021 - Current

Supervision and Mentoring: Baixi Sun (Ph.D. student, August 2021 - Current), Chengming Zhang (Ph.D. student, September 2022 - Current)

• DOE ECP: VeloC/SZ: VEry-Low Overhead Checkpointing System and Error-bounded Lossy Compression for Scientific HPC Datasets.

My Role: Senior Personnel and Technical Lead

Period: 01/01/2021 - Current

Supervision and Mentoring: Milan Shah (Ph.D. student, May 2022 - Current)

Co-Mentoring: Jiannan Tian (Ph.D. student, January 2021 - Current), Cody Rivera (Undergraduate student, May 2021 - August 2021)

• DOE ECP: Exascale MPI / MPICH.

My Role: Senior Personnel Period: 10/01/2021 – Current

Co-Mentoring: Jiajun Huang (Ph.D. student, October 2022 - Current)

## **PUBLICATIONS**

#### Refereed Journal Articles

- [Scientific Reports] Xiaodong Yu, Viktor Nikitin, Daniel J Ching, Selin Aslan, Doga Gursoy, and Tekin Bicer, "Scalable and Accurate Multi-GPU-Based Image Reconstruction of Large-Scale Ptychography Data." Scientific Reports 12.1 (2022): 1-16. (2022 impact factor=4.996)
- [JSPS] Xiaodong Yu, Hao Wang, Wu-chun Feng, Hao Gong, and Guohua Cao, "GPU-Based Iterative Medical CT Image Reconstructions." *Journal of Signal Processing Systems* 91.3 (2019): 321-338. (2022 impact factor=1.813)
- 3. [JSAC] Xiaodong Yu, Bill Lin, and Michela Becchi, "Revisiting State Blow-up: Automatically Building Augmented-FA while Preserving Functional Equivalence." *IEEE Journal on Selected Areas in Communications* 32.10 (2014): 1822-1833. (2022 impact factor=13.081)

### Peer-Reviewed Conference Papers (with my student protégés underlined)

- 1. [HPDC'22] Xiaodong Yu, Sheng Di, Kai Zhao, <u>Jiannan Tian</u>, Dingwen Tao, Xin Liang, and Franck Cappello, "Ultrafast Error-Bounded Lossy Compression for Scientific Datasets." In *Proceedings of the 31st ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC 2022)*, Minneapolis, MN, June 27-29, 2022. (acceptance rate=19.4%)
- [IPDPS'22] Cody Rivera, Sheng Di, Jiannan Tian, Xiaodong Yu, Dingwen Tao, and Franck Cappello, "Optimizing Huffman Decoding for Error-Bounded Lossy Compression on GPUs." In Proceedings of IEEE International Parallel and Distributed Processing Symposium (IPDPS), Lyon, France, May 30-June 3, 2022. (acceptance rate=27%)
- 3. [SSSDU'21] Guo, Yanfei, Ken Raffenetti, Hui Zhou, Travis Koehring, Sudheer Chunduri, Xiaodong Yu, and Rajeev Thakur, "Automated Validation and Verification for Scientific Software." In *Proceedings of the 2022 Workshop on the Science of Scientific-Software Development and Use*, virtual, December 13-15, 2021. (position paper)
- 4. [SMC'21] Tekin Bicer, Xiaodong Yu, Daniel Ching, Ryan Chard, Mathew Cherukara, Bogdan Nicolae, Rajkumar Kettimuthu, and Ian T Foster, "High-Performance Ptychographic Reconstruction with Federated Facilities." In Proceedings of the 2021 Smoky Mountains Computational Sciences and Engineering Conference, pages 173-189, Oak Ridge, TN, October 18-20, 2021.
- 5. [CLUSTER'21] Xiaodong Yu, Sheng Di, Ali Murat Gok, Dingwen Tao, and Franck Cappello, "cuZ-Checker: A GPU-Based Ultra-Fast Assessment System for Lossy Compressions." In *Proceedings of IEEE International Conference on Cluster Computing (CLUSTER)*, pages 307-319, Portland, OR, September 7-10, 2021. (acceptance rate=29%)
- 6. [CLUSTER'21] <u>Jiannan Tian</u>, Sheng Di, Xiaodong Yu, <u>Cody Rivera</u>, Kai Zhao, Sian Jin, Yunhe Feng, Xin Liang, Dingwen Tao, and Franck Cappello, "Optimizing Error-Bounded Lossy Compression for Scientific Data on GPUs." In *Proceedings of IEEE International Conference on Cluster Computing* (CLUSTER), pages 283-293, Portland, OR, September 7-10, 2021. (acceptance rate=29%)
- [ICS'21] Xiaodong Yu, Tekin Bicer, Rajkumar Kettimuthu, and Ian Foster, "Topology-Aware Optimizations for Multi-GPU Ptychographic Image Reconstruction." In *Proceedings of the ACM International Conference on Supercomputing (ICS)*, pages 354-366, Worldwide online event, June 14-18, 2021. (acceptance rate=24.2%)
- 8. [IPDPS'20] Xiaodong Yu, Fengguo Wei, Xinming Ou, Michela Becchi, Tekin Bicer, and Danfeng Yao, "GPU-Based Static Data-Flow Analysis for Fast and Scalable Android App Vetting." In *Proceedings* of IEEE International Parallel and Distributed Processing Symposium (IPDPS), pages 274-284, New Orleans, LA, May 18-22, 2020. (acceptance rate=24.7%)
- 9. [CSET'19] Xiaodong Yu, Ya Xiao, Kirk Cameron, and Danfeng (Daphne) Yao, "Comparative Measurement of Cache Configurations' Impacts on Cache Timing Side-Channel Attacks." In *Proceedings of the 12th USENIX Conference on Cyber Security Experimentation and Test (CSET 19)*, Santa Clara, CA, August 12, 2019. (acceptance rate=31%)
- 10. [SoutheastCon'18] Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Jon Bernard, Bo Li, Xiaodong Yu, Li Xu, Godmar Back, Ali R. Butt, Kirk W. Cameron, Yili Hong, Danfeng Yao, "Non-parametric Distribution Models for Predicting and Managing Computational Performance Variability." In Proceedings of IEEE Southeastcon 2018, pages 1-7, St. Petersburg, FL, April 19-22, 2018.
- 11. [ACMSE'18] Thomas C. H. Lux, Layne T. Watson, Tyler H. Chang, Jon Bernard, Bo Li, Xiaodong Yu, Li Xu, Godmar Back, Ali R. Butt, Kirk W. Cameron, Danfeng Yao, Yili Hong, "Novel Meshes for Multivariate Interpolation and Approximation." In *Proceedings of the ACMSE 2018 Conference*, pages 13:1-13:7, Richmond, KY, March 29-31, 2018.
- 12. [BigData'17] Xiaodong Yu, Kaixi Hou, Hao Wang, and Wu-chun Feng, "Robotomata: A Framework for Approximate Pattern Matching of Big Data on an Automata Processor." In *Proceedings of the IEEE International Conference on Big Data (IEEE BigData)*, pages 283–292, Boston, MA, December 11-14, 2017. (acceptance rate=17.9%)
- 13. [ICS'17] Marziyeh Nourian, Xiang Wang, Xiaodong Yu, Wu-chun Feng, and Michela Becchi, "De-

- mystifying Automata Processing: GPUs, FPGAs or Micron's AP?" In *Proceedings of the International Conference on Supercomputing (ICS)*, pages 1-11, Chicago, IL, June 14-16, 2017. (acceptance rate=15.8%)
- 14. [CF'17] Xiaodong Yu, Hao Wang, Wu-chun Feng, Hao Gong, and Guohua Cao, "An Enhanced Image Reconstruction Tool for Computed Tomography on GPUs." In *Proceedings of the ACM International Conference on Computing Frontiers (CF)*, pages 97-106, Siena, Italy, May 15-17, 2017. (acceptance rate=35.5%)
- 15. [CCGrid'16] Xiaodong Yu, Hao Wang, Wu-chun Feng, Hao Gong, and Guohua Cao, "cuART: Fine-Grained Algebraic Reconstruction Technique for Computed Tomography Images on GPUs." In *Proceedings of 16th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid)*, pages 165-168, Cartagena, Colombia, May 16-19, 2016. (short) (acceptance rate=25%)
- 16. [ANCS'16] Xiaodong Yu, Wu-chun Feng, Danfeng Yao, and Michela Becchi, "O3FA: A Scalable Finite Automata-based Pattern-Matching Engine for Out-of-Order Deep Packet Inspection." In Proceedings of the ACM/IEEE Symposium on Architectures for Networking and Communications Systems (ANCS), pages 1-11, Santa Clara, CA, March 17-18, 2016. (acceptance rate=20.7%)
- 17. [CF'13] Xiaodong Yu, and Michela Becchi, "GPU Acceleration of Regular Expression Matching for Large Datasets: Exploring the Implementation Space." In *Proceedings of the ACM International Conference on Computing Frontiers (CF)*, pages 1-10, Ischia, Italy, May 14-16, 2013.

## **Pending Conference Papers**

- 1. <u>Baixi Sun</u>, **Xiaodong Yu**, <u>Chengming Zhang</u>, <u>Jiannan Tian</u>, Sian Jin, Kamil A. Iskra, Tao Zhou, Tekin Bicer, Pete Beckman, and <u>Dingwen Tao</u>, "SOLAR: A Highly Optimized Data Loading Framework for Distributed Training of CNN-based Scientific Surrogates." Under review in *49th International Conference on Very Large Data Bases (VLDB)*, Vancouver, Canada, August 28-September 1, 2023.
- Milan Shah, Xiaodong Yu, Sheng Di, Danylo Lykov, Yuri Alexeev, Michela Becchi, and Franck Cappello, "GPU-Accelerated Error-Bounded Compression Framework for Quantum Circuit Simulations."
   Under review in IEEE International Parallel and Distributed Processing Symposium (IPDPS), St. Petersburg, FL, May 15-19, 2023.
- 3. Boyuan Zhang, <u>Jiannan Tian</u>, Sheng Di, **Xiaodong Yu**, Dingwen Tao, and Franck Cappello, "Fast GPU Lossy Compressor for Scientific Computing Applications." Under review in *IEEE International Parallel and Distributed Processing Symposium (IPDPS)*, St. Petersburg, FL, May 15-19, 2023.
- 4. Boyuan Zhang, Jiannan Tian, Sheng Di, Xiaodong Yu, Lizhi Xiang, Dingwen Tao, and Franck Cappello, "gpuLZ: Optimizing LZSS for Scientific Lossy Compression on Modern GPUs." Under review in the 28th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP), Montreal, Canada, February 25-March 1, 2023.

## Peer-Reviewed Posters/Extended Abstracts

- 1. [SC'22] <u>Baixi Sun</u>, Xiaodong Yu, Kamil Iskra, and Dingwen Tao, "Surrogate Train: Drastically Improving Performance of Data Loading for Training Scientific Surrogate Models." In *Proceedings of the 2022 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), Dallas, TX, November 13-18, 2022. (ACM Student Research Competition track)*
- 2. [SC'22] Milan Shah, Xiaodong Yu, Sheng Di, Franck Cappello, and Michela Becchi, "Compressing Quantum Circuit Simulation Tensor Data." In *Proceedings of the 2022 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC)*, Dallas, TX, November 13-18, 2022. (ACM Student Research Competition track)
- 3. [ECPAM'22] Yanfei Guo, Kenneth Raffenetti, Rob Latham, Marc Snir, Hui Zhou, Travis Koehring, Sudheer Chunduri, Xiaodong Yu, and Rajeev Thakur, "2.3.1.07 Exascale MPI (MPICH)." In Proceedings of the 2022 Exascale Computing Project Annual Meeting, virtual, May 2-6, 2022.
- 4. [SC'18] Xiaodong Yu, Michela Becchi, and Danfeng (Daphne) Yao, "The Algorithm and Framework Designs and Optimizations for Scalable Automata Processing on HPC Platforms." In *Proceedings of the 2018 International Conference for High Performance Computing, Networking, Storage, and Analysis*

- (SC), Dallas, TX, November 11-16, 2018. (Doctoral Showcase track)
- 5. [IISWC'17] Xiaodong Yu, Kaixi Hou, Hao Wang, and Wu-chun Feng, "A Framework for Fast and Fair Evaluation of Automata Processing Hardware." In *Proceedings of IEEE International Symposium on Workload Characterization (IISWC)*, pages 120-121, Seattle, WA, October 1-3, 2017.
- 6. [PPoPP'13] Xiaodong Yu, and Michela Becchi, "Exploring Different Automata Representations for Efficient Regular Expression Matching on GPUs." In Proceedings of the 18th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP), pages 287-288, Shenzhen China, February 23-27, 2013.

#### Theses

- 1. [Doctoral Dissertation] Xiaodong Yu, "Algorithms and Frameworks for Accelerating Security Applications on HPC Platforms." Virginia Tech, 2019.
- [Master Thesis] Xiaodong Yu, "Deep Packet Inspection on Large Datasets: Algorithmic and Parallelization Techniques for Accelerating Regular Expression Matching on Many-Core Processors." University of Missouri-Columbia, 2013.

#### SELECTED CONFERENCE PRESENTATIONS

- ACM HPDC: Ultrafast Error-Bounded Lossy Compression for Scientific Datasets, June 2022.
- IEEE CLUSTER: cuZ-Checker: A GPU-Based Ultra-Fast Assessment System for Lossy Compressions, September 2021.
- ACM ICS: Topology-Aware Optimizations for Multi-GPU Ptychographic Image Reconstruction, June 2021.
- IEEE IPDPS: GPU-Based Static Data-Flow Analysis for Fast and Scalable Android App Vetting, May 2020.
- USENIX CSET: comparative Measurement of Cache Configurations' Impacts on Cache Timing Side-Channel Attacks, August 2019.
- IEEE BigData: Robotomata: A Framework for Approximate Pattern Matching of Big Data on an Automata Processor, December 2017.
- ACM/IEEE ANCS: O3FA: A Scalable Finite Automata-based Pattern-Matching Engine for Out-of-Order Deep Packet Inspection, March 2016.

## SUPERVISION/MENTORING EXPERIENCE

## Postdoc Mentoring

• Yixuan Sun – Postdoctoral Appointee in ANL MCS, November 2022 - Current.

#### Student Supervision and Mentoring

- Baixi Sun (Ph.D. student in Intelligent Systems Engineering Department at Indiana University) Visiting Student–Subcontractor in ANL MCS, August 2021 Current.
- Milan Shah (Ph.D. student in Electrical and Computer Engineering Department at North Carolina State University) Visiting Student–Subcontractor in ANL MCS, May 2022 Current.
- Chengming Zhang (Ph.D. student in Intelligent Systems Engineering Department at Indiana University)
   Visiting Student-Subcontractor in ANL MCS, September 2022 Current.

## Student Co-Mentoring

- Jiannan Tian (Ph.D. student in Intelligent Systems Engineering Department at Indiana University) Visiting Student–Subcontractor in ANL MCS, January 2021 Current.
- Jiajun Huang (Ph.D. student in Computer Science and Engineering Department at the University of California, Riverside) Visiting Student–Subcontractor in ANL MCS, October 2022 Current.
- Cody Rivera (Undergraduate student in the Computer Science Department at the University of Alabama) – Science Undergraduate Laboratory Internship (SULI) Program Intern in ANL MCS, May 2021 - August 2021.

Boyuan Zhang (Ph.D. student in Intelligent Systems Engineering Department at Indiana University),
 May 2022 - Current.

## **PROFESSIONAL SERVICES**

### Conference Organizing Committee

- Finance Chair IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS), 2023.
- Publicity Co-Chair IEEE International Workshop on Signal Processing Systems (SiPS), 2022.

#### Journal Editorial Board

 Review Board Member – IEEE Transactions on Parallel and Distributed Systems (TPDS), 2022 -Current.

## Conference Technical Program Committee (TPC)

- **TPC Member** The Third International Workshop on Big Data Reduction (**IWBDR-3**) in conjunction with 2022 IEEE International Conference on Big Data (IEEE BigData), 2022.
- **TPC Member** The 24th IEEE International Conferences on High Performance Computing and Communications (**HPCC**), 2022.
- **TPC Member** 9th IEEE/ACM International Conference on Big Data Computing, Applications and Technologies (**BDCAT**), 2022.
- TPC Member IEEE International Workshop on Signal Processing Systems (SiPS), 2022.
- Posters Committee Member IEEE International Symposium on Performance Analysis of Systems and Software (ISPASS), 2022.
- **TPC Member** The 23rd IEEE International Conferences on High Performance Computing and Communications (**HPCC**), 2021.
- AD/AE Committee Member The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), 2021.
- TPC Member IEEE Hot Interconnects symposium (HotI), 2021.
- **TPC Member** The 22nd IEEE International Conferences on High Performance Computing and Communications (**HPCC**), 2020.

#### Journal Referee

- ACM Transactions on Storage (**TOS**), 2022.
- $\bullet$  Future Generation Computer Systems (FGCS) Elsevier, 2022
- IEEE Transactions on Parallel and Distributed Systems (TPDS), 2020 2022.
- Journal of Parallel and Distributed Computing (JPDC) Elsevier, 2019 2022.
- Journal of Systems Architecture (JSA) Elsevier, 2019, 2022.
- Software: Practice and Experience (SPE) Wiley, 2021.
- Journal of Computer Virology and Hacking Techniques (JICV) Springer Nature, 2021.
- IEEE Access, 2017 2021.
- IEEE Transactions on Dependable and Secure Computing (TDSC), 2018 2020.
- Computer Communications (COMCOM) Elsevier, 2018, 2020.
- Computer Networks (**COMNET**) Elsevier, 2019.
- Australasian Physical & Engineering Sciences in Medicine (APES) Springer Nature, 2019.
- $\bullet$  Journal of Systems and Software (JSS) Elsevier, 2015 2017.
- IEEE Journal on Selected Areas in Communications (JSAC), 2014.

#### Conference External Reviewer

- The ACM Symposium on Access Control Models and Technologies (SACMAT), 2022.
- 36th IEEE International Parallel & Distributed Processing Symposium (IPDPS), 2022.

- 26th International Workshop on High-Level Parallel Programming Models and Supportive Environments (**HIPS**) held in conjunction with IPDPS, 2021.
- The 27th International Conference on Computer Communications and Networks (ICCCN), 2018.
- IEEE Global Communications Conference (GLOBECOM), 2018.
- IEEE 88th Vehicular Technology Conference (VTC), 2018.

#### **ANL Internal Services**

- Co-Organizer CS seminar series hosted by the Mathematics and Computer Science (MCS) Division,
   2022 current.
- Interviewer two MCS postdoc hires, 2022.
- TPC Member Argonne Postdoctoral Research and Career Symposium, 2022.

#### Other Services

- Mentor SC22 Mentor-Protégé Program, 2022.
- Judge SIGHPC Computational and Data Science Fellowship, 2022.
- Executive Committee Member IEEE Fox Valley Subsection, 2019 2020.
- Student Volunteer The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC), 2018.

### **MAJOR SOFTWARE**

• SZx: an ultra-fast error-bounded lossy compressors.

Repository: https://github.com/szcompressor/SZx

My role: principal designer, developer, and maintainer of the GPU version

• **cuZ-Checker**: a GPU-based library to characterize the data and check the compression results of lossy compressors.

Repository: https://github.com/CODARcode/cuZ-checker

My role: principal designer, developer, and maintainer

• cuSZ: a CUDA-based error-bounded lossy compressor for scientific data.

Repository: https://github.com/szcompressor/cuSZ

My role: core developer and maintainer of the HIP version

• Tike: a toolbox for tomographic reconstruction of 3D objects from ptychography data.

Repository: https://github.com/tomography/tike

My role: principal designer, developer, and maintainer of the HPC part

• SOLAR: a data loading framework for training CNN-based scientific surrogates.

Repository: https://github.com/ANL-FAIR-SBI/SOLAR

My role: principal designer and architect

• MPICH: a high-performance and widely portable implementation of the MPI-3.1 standard.

Repository: https://github.com/pmodels/mpich

My role: developer and maintainer of the GPU-related part

## **HONORS AND AWARDS**

- Second place in ACM Student Research Competition Graduate Students at ACM/IEEE SC'22 (as the co-advisor of Milan Shah), 2022.
- Selected to present at ACM/IEEE SC'18 Doctoral Showcase (Selection Rate = 16/27), 2018.
- Outstanding Graduate Teaching Assistant Award, Computer Science Department at Virginia Tech, 2016.
- Learning Progress Scholarship, China University of Mining and Technology (CUMT), 2006 2007.

## **REFERENCES**

Danfeng (Daphne) Yao Professor, Elizabeth and James E. Turner Jr. '56 Faculty Fellow, and CACI Faculty Fellow Virginia Tech, Blacksburg, VA danfeng@vt.edu Michela Becchi Associate Professor North Carolina State University, Raleigh, NC mbecchi@ncsu.edu

Dingwen Tao Associate Professor Indiana University, Bloomington, IN ditao@iu.edu Pete Beckman
Co-Director, Northwestern Argonne Institute of Science
and Engineering and Argonne Distinguished Fellow
Argonne National Laboratory, Lemont, IL
beckman@mcs.anl.gov