

# Ananth Grama

Professor of Computer Sciences,  
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## Education

- Ph.D., Computer Science, University of Minnesota, Minneapolis, MN, May 1996.
- M.S., Computer Engineering, Wayne State University, Detroit, MI, July 1990.
- B. Engg., Computer Science, Indian Institute of Technology (IIT), Roorkee, India, July 1989.

## Research Interests

- Parallel and Distributed Computing: Algorithms, Software, and Infrastructure.
- Large Scale Data Handling and Analysis.
- Scientific Computing: Computational Biology and Bioinformatics, Molecular Dynamics, and Continuum Modeling (solvers, eigenvalue problems).

## Employment History

- Director, Computational Science and Engineering and Computational Life Sciences Programs, Purdue University, W. Lafayette, IN, June 2012 - 16.
- Associate Director, Center for Science of Information, 2010 - , a Science and Technology Center of the National Science Foundation.
- Associate Director, Center for Prediction of Reliability, Integrity, and Survivability of Microsystems, a National Nuclear Security Administration/ Department of Energy Center, 2009 - 2014.
- Professor, Department of Computer Science, Purdue University, W. Lafayette, IN, Aug. 2006 - .
- University Faculty Scholar, Purdue University, W. Lafayette, IN, Aug 2002 - July 2007.
- Associate Professor, Department of Computer Science, Purdue University, W. Lafayette, IN, Aug. 2001 - July 2006.
- Assistant Professor, Department of Computer Science, Purdue University, W. Lafayette, IN, Aug. 1996 - July 2001.
- Assistant Professor, Department of Computer Science, University of Minnesota, Minneapolis, MN, June 1996 - Aug. 1996.
- Visiting Research Scientist, Hewlett Packard Labs, Palo Alto, CA, June 1994 to Nov 1994.

## **Awards and Honors**

- Distinguished Alumnus Award, Department of Computer Science, University of Minnesota, 2015.
- Fellow, American Association for Advancement of Sciences (AAAS), 2013.
- Purdue University Most Influential Professor in Computer Science, 2010.
- Purdue University Scholar, 2002.
- Purdue University School of Science Outstanding Teacher Award, 2002.
- National Science Foundation CAREER Award, 1998–2002.
- Purdue University School of Science Outstanding Assistant Professor, 1999.
- Doctoral Dissertation Fellowship, Graduate School of the University of Minnesota, 1995-96.
- Doctoral Dissertation Award, Department of Computer Science, University of Minnesota, 1994.
- Vice-Chancellors Gold Medal for best overall grades among all engineering majors at the Indian Institute of Technology, Roorkee, India, 1989.
- Vice-Chancellors Gold Medal for best engineering design project titled “Load Balancing in LANs”, Indian Institute of Technology, Roorkee, India, 1989.

## **Professional/ Scholarly Service**

- Chair, Biodata Management and Analysis (BDMA) Study Section, National Institutes of Health.
- Editorial Boards: Parallel Computing, IEEE Trans. Parallel and Distributed Computing, Journal of Parallel and Distributed Computing, IEEE Transactions on Big Data, IEEE Trans. Molecular, Biological, and Multiscale Communications, PLoS ONE.
- Member, American Association for Advancement of Sciences, Sigma Xi.
- Large number of Program Committees of Premier Conferences in High Performance Computing, Computational Biology and Bioinformatics, Scientific Computing, and Data Mining.

## **Postdoctoral Scholars and Students**

### **Current Ph.D. Students:**

Sudhir Kylasa, Victor Santos, Servio Palacios, Edgardo Barasillo, Chih Hao, Vikram Ravindra, Xuejiao Kang.

### **Graduated Ph.D. Students (last-known affiliation):**

Shahin Mohammadi (MIT), Karthik Khambatta (Cloudera Inc.), Naresh Rapolu (Google Inc.), Anmer Daskin (Istanbul Medeniyet University), Hasan Metin Aktulga (Michigan State University), Murat Manguoglu (Middle-East Technical University, Ankara), Asad Awan (Google Inc.), Ramanathan Muralikrishna (Indian Institute of Science, India), Ronaldo Ferreira (Federal University of Mato Grosso do Sul, Brasil), Mehmet Koyuturk (Case Western Reserve University), Ioannis Ioannidis (Qnective Inc., Switzerland), Bogdan Car-bunar (Florida International University).

### **Current Post-Doctoral Researchers:**

Dr. Abram Magner, Dr. Jithin Sreetharan.

## Past Post-Doctoral Researchers (last-known affiliation):

George Kollias (IBM Research), Sagar Pandit (University of South Florida), Mehmet Koyuturk (Case Western Reserve University), Eric Polizzi (University of Massachusetts, Amherst), Pucha Raghuram (Georgia Tech.).

## Publications

### Books

1. Ananth Grama, Anshul Gupta, George Karypis, and Vipin Kumar, *Introduction to Parallel Computing*, Addison Wesley, 2003 (ISBN: 0-201-64865-2) <http://www.aw.com/catalog/academic/product/1,4096,0201648652,00.html>. (Note: Chinese translation available through the China Machine Press. Southeast Asian Edition available through Pearson Education Asia, Chinese (english) Edition available through China Machine Press.)
2. Vipin Kumar, Ananth Grama, Anshul Gupta, and George Karypis, *Introduction to Parallel Computing: Design and Analysis of Algorithms*. Benjamin Cummings/ Addison Wesley (ISBN 0-8053-3170-0), 600 pp, Redwood City, 1994.

### Edited Volumes/ Proceedings

1. Mehmet Koyuturk, Shankar Subramaniam, and Ananth Grama (Editors), *Functional Coherence of Molecular Networks in Bioinformatics*, ISBN-13: 9781461403197 Springer, (2011).
2. Michael Berry, Kyle Gallivan, Efstratios Gallopoulos, Ananth Grama, Bernard Philippe, Yousef Saad, and Faisal Saied (Editors), *High Performance Scientific Computing: Algorithms and Applications*, DOI 10.1007/978-1-4471-2437-5, Springer, (2012).

### Journal Articles

1. Shahin Mohammadi, Vikram Ravindra, David Gleich, and Ananth Grama, DECODE-ing sparsity patterns in single-cell RNA-seq, *Nature Communications*, 2018.
2. Wojciech Szpankowski and Ananth Grama, Frontiers of Science of Information: Shannon Meets Turing, *IEEE Computer*, Cover Feature, Outlook Issue, 2018.
3. Naresh Rapolu, Srimat Chakradhar, Ananth Grama, VAYU: Accelerating stream processing applications through dynamic network-aware topology re-optimization, *J. Parallel Distrib. Comput.*, 111: 13-23, 2018.
4. Folker Meyer, Saurabh Bagchi, Somali Chaterji, Wolfgang Gerlach, Ananth Grama, Travis Harrison, Tobias Paczian, Will Trimble, Andreas Wilke, MG-RAST Version 4 – Lessons learned from a decade of low-budget ultra-high throughput metagenome analysis, *Briefings in Bioinformatics*, 2017 (to appear).
5. Somali Chaterji, Jinkyu Koo, Ninghui Li, Folker Meyer, Ananth Grama, and Saurabh Bagchi, Federation in Genomics Pipelines: Techniques and Challenges, *Briefings in Bioinformatics*, 2017 (to appear).
6. Shahin Mohammadi, David Gleich, Tamara Kolda, and Ananth Grama, Triangular Alignment (TAME): A Tensor-Based Approach for Higher Order Network Alignment, *IEEE/ACM Trans. Computational Biology and Bioinformatics*, 2017 (to appear).
7. Asish Ghoshal, Jinyi Zhang, Michael Roth, Kevin Xia, Ananth Grama, Saurabh Bagchi, and Somali Chaterji, A Distributed Kernel SVM Algorithm for Predicting Non-Canonical MicroRNA Targets and Verified Using TCGA-Derived Expression Data, *IEEE/ACM Trans. Computational Biology and Bioinformatics*, 2017 (to appear).

8. Shahin Mohammadi, Neta S. Zuckerman, Andrea Goldsmith, Ananth Grama: A Critical Survey of Deconvolution Methods for Separating Cell Types in Complex Tissues. *Proceedings of the IEEE* 105(2): 340-366 (2017).
9. Yao Zhu, David F. Gleich, Ananth Grama: Erasure Coding for Fault-Oblivious Linear System Solvers. *SIAM J. Scientific Computing* 39(1) (2017).
10. Sudhir B. Kylasa, Hasan Metin Aktulga, Ananth Y. Grama: Reactive Molecular Dynamics on Massively Parallel Heterogeneous Architectures. *IEEE Trans. Parallel Distrib. Syst.* 28(1): 202-214 (2017).
11. Seong Kim, Mrudul Harwani, Ananth Grama, and Somali Chaterji, EP-DNN: A Deep Neural Network-Based Global Enhancer Prediction Algorithm, *Nature Scientific Reports*, 6, Article number: 38433 (2016).
12. Abram Magner, Jaroslaw Duda, Wojciech Szpankowski, Ananth Grama: Fundamental Bounds for Sequence Reconstruction From Nanopore Sequencers. *IEEE Trans. Molecular, Biological, and Multi-scale Communication*, 2(1): 92-106 (2016).
13. Sudhir Kylasa, Giorgos Kollias, and Ananth Grama, Social ties and checkin sites: Connections and latent structures in Location Based Social Networks, *Social Network Analysis and Mining*, 6(1): 95:1-95:14, 2016.
14. Seong Gon Kim, Nawanol Theera-Ampornpant, Chih-Hao Fang, Mrudul Harwani, Ananth Grama, and Somali Chaterji, Opening up the blackbox: An interpretable deep neural network-based classifier for cell-type specific enhancer predictions, *BMC Systems Biology*, 10(2): 54, 2016.
15. Dan Savel, Tom LaFromboise, Ananth Grama, and Mehmet Koyuturk, Pluribus - Exploring the Limits of Error Correction Using a Suffix Tree, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, vol PP, issue 99, June 2016.
16. Adri van Duin, Thomas Senftle, Sungwook Hong, Md Islam, Yuanxia Zhang, Yun Shin, Chad Junkermeier, Roman Engel-Herbert, Michael Janik, Hasan Aktulga, Toon Verstraelen, and Ananth Grama, The ReaxFF Reactive Force-field: Development, Applications, and Future Directions, *Nature Partner Journals: Computational Materials*, 2: 15011, 2016.
17. Shahin Mohammadi and Ananth Grama, A convex optimization approach for identification of human tissue-specific interactomes, *Bioinformatics*, 32 (12): i243-i252, 2016.
18. Asish Ghoshal, Raghavendran Shankar, Saurabh Bagchi, Ananth Grama, and Somali Chaterji, MicroRNA target prediction using thermodynamic and sequence curves, *BMC Genomics* 16 (2015): 999. PMC. Web. 7 Feb. 2016.
19. Andreas Wilke, Jared Bischof, Wolfgang Gerlach, Elizabeth Glass, Travis Harrison, Kevin Keegan, Tobias Paczian, William Trimble, Saurabh Bagchi, Ananth Grama, Somali Chaterji, and Folker Meyer, The MG-RAST metagenomics database and portal in 2015, *Nucleic Acids Research*, 44: 590-594, 2016.
20. Shahin Mohammadi, Baharak Saberidokht, Shankar Subramaniam and Ananth Grama, Scope and limitations of yeast as a model organism for studying human tissue-specific pathways, *BMC Systems Biology*, 9:96, Dec. 2015.
21. Anmer Daskin, Ananth Grama, Sabre Kais, Quantum Random State Generation with Predefined Entanglement Constraint, *International Journal of Quantum Information*, 12(05), 2014.

22. Sungmin Kim, Douglas E Adams, Hoon Sohn, Gustavo Rodriguez-Rivera, Noah Myrent, Ray Bond, Jan Vitek, Scott Carr, Ananth Grama, Janette Jaques Meyer, Crack detection technique for operating wind turbine blades using Vibro-Acoustic Modulation, *Structural Health Monitoring*, vol. 13, 6: pp. 660-670, 2014.
23. Anmer Daskin, Ananth Grama, and Sabre Kais, Multiple Network Alignment on Quantum Computers, *Quantum Information Processing*, 13 (12), 2014.
24. Sudhir Kylasa, Hasan Metin Aktulga, and Ananth Grama, PuReMD-GPU: A Reactive Molecular Dynamic Simulation Package for GPUs, *Journal of Computational Physics*, 272: 343-359, 2014.
25. Giorgos Kollias, Madan Sathe, Olaf Schenk, and Ananth Grama, Fast Parallel Algorithms for Graph Similarity and Matching, *Journal of Parallel and Distributed Computing*, 74(5): 2400 - 2410, 2014.
26. Karthik Kambatla, Giorgos Kollias, Vipin Kumar, and Ananth Grama, Trends in Big-Data Analytics, *Journal of Parallel and Distributed Computing*, 74(7), 2561 - 2573, 2014.
27. Giorgos Kollias, Efstratios Gallopoulos, and Ananth Grama, Surfing the Network for Ranking by Multidamping, *IEEE Transactions on Knowledge and Data Engineering*, 26(9): 2323-2336 (2014).
28. Anmer Daskin, Sabre Kais, and Ananth Grama, A Universal Quantum Circuit Scheme For Finding Complex Eigenvalues, *Quantum Information Processing*, 13(2), pp 333-353, 2014.
29. Alex Verstak, Naren Ramakrishnan, Layne Watson, Jian He, Clifford Shaffer, and Ananth Grama, Using Hierarchical Data Mining to Characterize Performance of Wireless System Configurations, *Advances in Engineering Software*, 65, pp 66-77, Nov 2013.
30. Giorgos Kollias, Madan Sathe, Shahin Mohammadi and Ananth Grama, A Fast Approach to Global Alignment of Protein-Protein Interaction Networks, *BMC Research Notes*, 2013, 6:35, 2013.
31. Shahin Mohammadi, Shankar Subramaniam, and Ananth Grama, Inferring the Effective TOR-Dependent Network: A Computational Study in Yeast. *BMC Systems Biology* 7(1):84, 2013.
32. Tobias Berka, Giorgos Kollias, Helge Hagenauer, Marian Vajtersic, Ananth Grama, Concurrent programming constructs for parallel MPI applications - The MPI threads library, *The Journal of Supercomputing*, 63(2): 385-406, 2013.
33. Giorgos Kollias, Shahin Mohammadi, and Ananth Grama, Network Similarity Decomposition for Network Alignment, *IEEE Transactions on Knowledge and Data Engineering*, 24(12): 2232-2243, 2012.
34. Anmer Daskin, Ananth Grama, Giorgos Kollias, and Sabre Kais, Universal Programmable Quantum Circuit Schemes to Emulate an Operator, *Journal of Chemical Physics*, 137, 234112, 2012.
35. Hasan Aktulga, Joseph C. Fogarty, S. A. Pandit, Ananth Grama: Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques. *Parallel Computing*, 38(4-5): 245-259, 2012.
36. Hasan Aktulga, Sagar Pandit, Adri C. T. van Duin, Ananth Grama: Reactive Molecular Dynamics: Numerical Methods and Algorithmic Techniques. *SIAM J. Scientific Computing*, 34(1), 2012.
37. Tejaswini Narayanan, Merril Gersten, Shankar Subramaniam, Ananth Grama, Modularity detection in protein-protein interaction networks, *BMC Research Notes*, 4:569, 2011.
38. Murat Manguoglu, Faisal Saied, Ahmed Sameh, and Ananth Grama, Performance Models for the Spike Banded Linear System Solver, *Scientific Programming*, 19(1), 13-25, 2011.
39. Joseph Fogarty, Hasan Aktulga, Adri van Duin, Ananth Grama, Sagar Pandit, A Reactive Simulation of the Silica-Water Interface, *J Chem Phys.*, 132(17):174704, 2010.

40. Murat Manguoglu, Mehmet Koyuturk, Ahmed Sameh, and Ananth Grama, Weighted Matrix Ordering and Parallel Banded Preconditioners for Iterative Linear System Solvers, *SIAM Journal on Scientific Computing*, 32(3), pp.1201-1216, 2010.
41. Jayesh Pandey, Mehmet Koyuturk, Ananth Grama, Functional Characterization and Topological Modularity of Molecular Interaction Networks, *BMC Bioinformatics*, 11(Suppl 1):S35, 18 January 2010.
42. Yumi Park, Metin Atkulga, Ananth Grama, Alejandro Strachan, Strain Relaxation in Si/Ge/Si Nanoscale Bars from Molecular Dynamics Simulations, *Journal of Applied Physics*, 106, 1, 2009
43. Bogdan Carbutar, Murali Krishna Ramanathan, Mehmet Koyuturk, Suresh Jagannathan, Ananth Grama, Efficient tag detection in RFID systems. *Journal of Parallel Distributed Computing*, 69(2): 180-196, 2009.
44. Jayesh Pandey, Mehmet Koyuturk, Shankar Subramaniam, Ananth Grama, Functional coherence in domain interaction networks, *Bioinformatics*, 24(16):i28-i34, 2008.
45. Ronaldo A. Ferreira, Mehmet Koyuturk, Suresh Jagannathan, Ananth Grama, Semantic indexing in structured peer-to-peer networks, *Journal of Parallel Distributed Computing*, 68(1): 64-77 (2008).
46. Sagar Pandit, See-Wing Chiu, Eric Jakobsson, Ananth Grama, and H. L. Scott, Cholesterol Packing Around Lipids with Saturated and Unsaturated Chains: A Simulation Study, *Langmuir*, 24, 6858-6865, 2008.
47. Jayesh Pandey, Mehmet Koyuturk, Yojan Kim, Wojciech Szpankowski, Shankar Subramaniam, and Ananth Grama. Functional annotation of regulatory pathways. *Bioinformatics Suppl.* on ISMB/ECCB'07, 23(13), i377-i386, 2007.
48. Hassan Aktulga, Ioannis Kontoyiannis, Leszek Lyznik, Lukasz Szpankowski, Wojciech Szpankowski, Ananth Grama, Identifying Statistical Dependence in Genomic Sequences via Mutual Information, *Journal on Bioinformatics and Systems Biology*, 14741, 2007.
49. Priya Vashishta, Rajiv Kalia, Aiichiro Nakano, Eftimios Kaxiras, Ananth Grama, Gang Lu, Steve Eidenbenz, Arthur Voter, Randy Hood, John Moriarty and Lin Yang, Hierarchical petascale simulation framework for stress corrosion cracking, *Journal of Physics*, Volume 78, 2007 (SciDAC 2007 papers).
50. Ronaldo Ferreira, Murali Krishna Ramanathan, Suresh Jagannathan, and Ananth Grama, Randomized Protocols for Duplicate Elimination in Peer-to-Peer Storage Systems, *IEEE Trans. Parallel and Distributed Systems*, 18(5), pp 686-696, May 2007.
51. Muralikrishna Ramanathan, Ronaldo Ferreira, Suresh Jagannathan, Ananth Grama, and Wojciech Szpankowski, Randomized Leader Election, *Distributed Computing* 19(5-6), pp 403-418, 2007.
52. Mehmet Koyutürk, Wojciech Szpankowski, and Ananth Grama, Assessing Significance of Connectivity and Conservation in Protein Interaction Networks, *Journal of Computational Biology* 14(6), 747-764, 2007.
53. Sagar Pandit, George Khelashvili, Eric Jakobsson, Ananth Grama, and H. L. Scott Lateral Organization in Lipid-Cholesterol Mixed Bilayers, *Biophysical Journal* 27 October 2006, 10.1529/biophysj.106.093864.
54. Sagar Pandit, See-Wing Chiu, Eric Jakobsson, Ananth Grama, and H. L. Scott, Cholesterol Surrogates: A Comparison of Cholesterol and 16:0 Ceramide in POPC Bilayers, *Biophysical Journal* 27 October 2006, 10.1529/biophysj.106.093864.
55. Mehmet Koyuturk, Yohan Kim, Shankar Subramaniam, Wojciech Szpankowski, and Ananth Grama, "Detecting conserved interaction patterns in biological networks", *Journal of Computational Biology*, 13(7), 1299-1322, 2006.

56. Jie Chi, Mehmet Koyuturk, and Ananth Grama, Conquest: A Coarse-Grained Algorithm for Constructing Summaries of Distributed Discrete Datasets, *Algorithmica*, 45(3), 377-401, 2006.
57. Mehmet Koyuturk, Yohan Kim, Umut Topkara, Shankar Subramaniam, Wojciech Szpankowski, and Ananth Grama, Pairwise Alignment of Protein Interaction Networks, *Journal of Computational Biology*, 13(2), 182-199, 2006.
58. Yohan Kim, Mehmet Koyuturk, Umut Topkara, Ananth Grama, and Shankar Subramaniam, Inferring Functional Information from Domain Co-evolution, *Bioinformatics*, 22(1), pp. 40-49, 2006.
59. Ronaldo Ferreira, Suresh Jagannathan, and Ananth Grama. Locality in Structured Peer-to-Peer Networks, *Journal of Parallel and Distributed Computing*, 66(2), pp 257-273, February 2006.
60. Mehmet Koyuturk, Ananth Grama, and Naren Ramakrishnan, Non-orthogonal Decomposition of Binary Matrices for Bounded-Error Data Compression and Analysis, *ACM Transactions on Mathematical Software*, 32(1), 2006.
61. Asad Awan, Ronaldo A. Ferreira, Suresh Jagannathan, Ananth Grama. Unstructured Peer-to-Peer Networks for Sharing Processor Cycles. *Parallel Computing*, 32(2) , pp 115-135, 2006.
62. Bogdan Carbutar, Ananth Grama, Jan Vitek, Octavian Carbutar "Redundancy and Coverage Detection in Sensor Networks", *ACM Transactions on Sensor Networks*, 2(1), 2006.
63. Ioannis Ioannidis, Ananth Grama, and Mikhail Atallah, Adaptive Data Structures for IP Lookups, *ACM Journal of Experimental Algorithmics*, vol. 10, 2005.
64. Ioannis Ioannidis and Ananth Grama, Level Compressed DAGs for Lookup Tables, *Computer Networks*, 49(2), pp 147-160, 2005.
65. Mehmet Koyutürk, Ananth Grama, and Naren Ramakrishnan, Proximus: A Framework for Compression, Clustering and Pattern Discovery in Very High Dimensional Discrete-Attributed Datasets, *IEEE Transactions on Knowledge and Data Engineering*, 17(4), pp 447–462, 2005.
66. Mehmet Koyutürk, Ananth Grama, and Wojciech Szpankowski, An Efficient Algorithm for Detecting Frequent Subgraphs in Biological Networks, *Bioinformatics*, 20(1), pp i200-i207, 2004.
67. Sreekanth Sambavaram, Vivek Sarin, Ahmed Sameh and Ananth Grama, Multipole-Based Preconditioners for Large Sparse Linear Systems, *Parallel Computing*, 29(9), pp 1261-1273, 2003.
68. Marc Alzina, Wojciech Szpankowski, and Ananth Grama, 2D Pattern Matching Image and Video Compression: Theory, Algorithms, and Experiments, *IEEE Transactions on Image Processing*, 11(3), pp 318-332, 2002.
69. Naren Ramakrishnan, Benjamin Keller, Batul Mirza, Ananth Grama, and George Karypis, Privacy Risks in Recommender Systems, *IEEE Internet Computing*, 5(6), pp 54-62, 2001.
70. Dow-Yung Yang, Ananth Grama, Vivek Sarin, and Naren Ramakrishnan, Compression of Particle Data for Hierarchical Approximation Techniques, *ACM Transactions on Mathematical Software*, 27(3), 2001.
71. Naren Ramakrishnan and Ananth Grama, Mining Large Scale Scientific Datasets, *Advances in Computers*, 55, pp 119-169, 2001.
72. Ananth Grama, Vivek Sarin, and Ahmed Sameh, Improving Error Bounds for Multipole-Based Treecodes, *SIAM Journal on Scientific Computing*, 21(5), pp 1790–1803, 2000.
73. Naren Ramakrishnan and Ananth Grama, Data Mining: From Serendipity to Science, *IEEE Computer*, 32(8):34–37, 1999.

74. Ananth Grama and Vipin Kumar, State-of-the-Art in Parallel Search Techniques for Discrete Optimization Problems, *IEEE Transactions on Knowledge and Data Engineering*, 11(1):28–35, Jan/Feb 1999.
75. Ananth Grama, Vipin Kumar, and Ahmed Sameh, Parallel Hierarchical Solvers and Preconditioners for Boundary Element Methods, *SIAM Journal on Scientific Computing*, 20(1):337–358, 1998.
76. Ananth Grama, Vipin Kumar, and Ahmed Sameh, Scalable Parallel Formulations of the Barnes-Hut Method for n-Body Simulations, *Parallel Computing*, 24(5-6):797–822, 1998.
77. Ananth Grama and Vipin Kumar, Parallel Search Algorithms for Discrete Optimization Problems, *ORSA Journal of Computing*, 7(4):365–385, 1995.
78. Vipin Kumar, Ananth Grama, and V. Nageshwara Rao, Scalable Load Balancing Techniques for Parallel Computers, *Journal of Parallel and Distributed Computing*, 22(1):60–79, 1994.
79. Ananth Grama, Anshul Gupta, and Vipin Kumar, Isoefficiency Function: A Scalability Metric for Parallel Algorithms and Architectures, *IEEE Parallel and Distributed Technology, Special Issue on Parallel and Distributed Systems: From Theory to Practice*, 1(3):12–21, 1993.
80. Ananth Grama and Vipin Kumar, Parallel Algorithms for Discrete Optimization Problems, *Bulletin of the Mathematical Programming Society*, 21:8–12, 1992.

#### Conference Proceedings (Refereed)

1. Mustafa Coskun, Ananth Grama, and Mehmet Koyuturk, Indexed Fast Network Proximity Querying, Proceedings of the VLDB Endowment (PVLDB), 2018 (to appear).
2. Abram Magner, Jithin K Sreedharan, Ananth Grama, and Wojciech Szpankowski, TIMES: Temporal Information Maximally Extracted from Structures, *The Web Conference (WWW)*, 2018 (to appear).
3. Huda Nassar, Nate Veldt, Shahin Mohammadi, Ananth Grama, and David Gleich, Low rank spectral network alignment, *The Web Conference (WWW)*, 2018 (to appear).
4. Karthik Kambatla, Vamsee Yarlagadda, Inigo Goiri and Ananth Grama, Utilization-aware cluster scheduling, *International Parallel and Distributed Processing Symposium, (IPDPS)*, 2018 (to appear).
5. Ashraf Mahgoub, Paul Wood, Sachandhan Ganesh, Subrata Mitra, Wolfgang Gerlach, Travis Harrison, Folker Meyer, Ananth Grama, Saurabh Bagchi, and Somali Chaterji, Rafiki: A Middleware for Parameter Tuning of NoSQL Datastores for Dynamic Metagenomics Workloads, ACM/IFIP/USENIX Middleware Conference, pp. 1-13, Dec 11-15, 2017, Las Vegas, Nevada.
6. Xuejiao Kang, David F. Gleich, Ahmed Sameh, and Ananth Grama, Distributed Fault Tolerant Linear System Solvers based on Erasure Coding, *International Conference on Distributed Computing Systems (ICDCS)*, 2017.
7. Abram Magner, Jithin Sreedharan, Wojciech Szpankowski, and Ananth Grama, Recovery of Vertex Orderings in Dynamic Graphs, *International Symposium on Information Theory (ISIT)*, 2017 (to appear).
8. Abram Magner, Jaroslaw Duda, Wojciech Szpankowski and Ananth Grama, Fundamental Bounds for Sequence Reconstruction from Nanopore Sequencers *9th International Conference on Bioinformatics and Computational Biology (ICBCB)*, March 2017.
9. Shahin Mohammadi and Ananth Grama, DeNovo Identification of Cell-Type Hierarchy with Application to Compound Marker Detection, *ACM Bioinformatics and Computational Biology (BCB)*, September 2016.



10. Mustafa Coskun, Ananth Grama, and Mehmet Koyuturk, Efficient Processing of Network Proximity Queries via Chebyshev Acceleration, *ACM Special Interest Group on Knowledge Discovery in Databases (SIGKDD)*, pp 1515-1524, August 2016.
11. Shahin Mohammadi and Ananth Grama, A convex optimization approach for identification of human tissue-specific interactomes, *Intelligent Systems for Molecular Biology (ISMB)*, pp 243-252, July 2016.
12. Nawanol Theera-Ampornpunt, Seong Gon Kim, Asish Ghoshal, Saurabh Bagchi, Ananth Grama, Somali Chaterji, Fast training on large genomics data using distributed Support Vector Machines. *COM-SNETS*, pp 1-8, Jan 2016.
13. Seong Kim, Nawanol Ampornpunt, Ananth Grama, and Somali Chaterji, Interpretable Deep Neural Networks for Enhancer Prediction, *IEEE International Conference on Bioinformatics and Biomedicine*, pp 242-249, 2015.
14. Asish Ghoshal, Ananth Grama, Saurabh Bagchi and Somali Chaterji. An Ensemble SVM Model for the Accurate Prediction of Non-Canonical MicroRNA Targets, *ACM Bioinformatics and Computational Biology (ACM-BCB) Best Paper*, pp 403-412, Atlanta, 2015.
15. Sudhir Kylasa, Giorgos Kollias and Ananth Grama, Social ties and checkin sites: Connections and latent structures in Location Based Social Networks, *IEEE/ACM International Conference on Advances in Social Networks Analysis and Mining (ASONAM)*, 194-201, 2015.
16. S. Kim, D. Adams, H. Sohn, G. Rodriguez Rivera, J. Vitek, S. Carr, and A. Grama, Validation of Vibro-Acoustic Modulation of wind turbine blades for structural health monitoring using operational vibration as a pumping signal, *Proceedings of the 9th International Workshop on Structural Health Monitoring*, Palo Alto, CA, 2013.
17. Daniel Savel, Thomas Laframboise, Ananth Grama and Mehmet Koyuturk, Suffix-Tree Based Error Correction of NGS Reads Using Multiple Manifestations of an Error, *ACM International Conference on Bioinformatics, Computational Biology, and Biomedical Informatics (BCB)*, pp 351-359, 2013.
18. Naresh Rapolu, Srimat Chakradhar, and Ananth Grama, M-Lock: Accelerating Distributed Transactions on Key-Value Stores Through Dynamic Lock Localization, *IEEE CLOUD* (best student paper), pp 179-187, 2013.
19. Shahin Mohammadi, Giorgos Kollias, and Ananth Grama, Synthetic Genetic Interactions and Pathway Crosstalk, *Pacific Symposium on Biocomputing (PSB)*, pp 43-54, 2012.
20. Naresh Rapolu, Karthik Kambatla, Suresh Jagannathan, Ananth Grama, TransMR: Data-Centric Programming Beyond Data Parallelism, *3rd Workshop on Hot Topics in Cloud Computing (HotCloud)*, 2011.
21. Karthik Kambatla, Naresh Rapolu, Suresh Jagannathan, Ananth Grama, Asynchronous Algorithms in MapReduce, *IEEE International Conference on Cluster Computing*, pp 245-254, 2010.
22. Karthik Kambatla, Naresh Rapolu, Jalaja Padma, Patrick Eugster, Ananth Grama, Revisiting I/O middleware for the Cloud, *8th USENIX Conference on File and Storage Technologies (FAST)*, Work in Progress Report, 2010.
23. Murat Manguoglu, Faisal Saied, Ahmed Sameh, and Ananth Grama, Performance Models for the Spike Banded Linear System Solver, *International Symposium on Parallel and Distributed Computing*, pp 181-188, 2010.
24. Jayesh Pandey, Mehmet Koyuturk, Ananth Grama, Functional Characterization and Topological Modularity of Molecular Interaction Networks, *Asia-Pacific Bioinformatics Conference (APBC)*, pp 35-43 2010.

25. Asad Awan, Suresh Jagannathan, Ananth Grama, Scalable Data Collection in Sensor Networks, *High Performance Computing conference*, pp 415-426, 2008.
26. Jayesh Pandey, Mehmet Koyuturk, Wojciech Szpankowski, Ananth Grama, Annotating Pathways of Interaction Networks, *Pacific Symposium on Biocomputing*, pp 153-165, 2008.
27. Murali Krishna Ramanathan, Mehmet Koyuturk, Ananth Grama, Suresh Jagannathan, PHALANX: a graph-theoretic framework for test case prioritization, *ACM Symposium on Applied Computing*, pp 667-673, 2008.
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33. Murali Krishna Ramanathan, Ananth Grama, Suresh Jagannathan, Path-Sensitive Inference of Function Precedence Protocols, *International Conference on Software Engineering (ICSE)*, pp 240-250, Minneapolis, 2007.
34. Asad Awan, Ahmed Sameh, Suresh Jagannathan, and Ananth Grama, Building Verifiable Sensing Applications Through Temporal Logic Specifications, *International Conference on Computational Science (ICCS)*, pp 1205-1212, Beijing, China, May 2007.
35. Jayesh Pandey, Mehmet Koyuturk, Wojciech Szpankowski, and Ananth Grama, A statistical model for functional characterization of regulatory pathways, *Data Mining for Biomedical Informatics, SIAM Data Mining*, 2007.
36. Asad Awan, Suresh Jagannathan, and Ananth Grama, Macroprogramming Heterogeneous Sensor Networks Using COSMOS, *EuroSys*, pp 159-172, Lisbon, Portugal 2007.
37. Murali Krishna Ramanathan, Ananth Grama, Suresh Jagannathan, Sieve: A Tool for Automatically Detecting Variations Across Program Versions, *21st IEEE/ACM International Conference on Automated Software Engineering*, (ASE), pp 241-252, September 2006.
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41. Bogdan Carbutar, Murali Ramanathan, Mehmet Koyuturk, Christoph Hoffmann, and Ananth Grama, Redundant-Reader Elimination in RFID Systems, *IEEE Sensor and Ad Hoc Communications and Networks (SECON)*, 26-29 Sept., 2005.
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44. Mehmet Koyutürk, Ananth Grama and Wojciech Szpankowski, Pairwise Local Alignment of Protein Interaction Networks Guided by Models of Evolution, *International Conference on Research in Computational Molecular Biology (RECOMB)*, pp 48-65, 2005.
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50. Ronaldo Ferreira, Suresh Jagannathan, and Ananth Grama, Enhancing Locality in Peer-to-Peer Networks, *International Conference on Parallel and Distributed Systems*, pp 25 - 34, 2004.
51. M. Koyuturk, W. Szpankowski and A Grama, Biclustering Gene-Feature Matrices for Statistically Significant Dense Patterns, *IEEE Computational Systems Bioinformatics Conf. (CSB)*, pp 480 - 484, 2004.
52. A. Grama and V. Sarin, Impact of Far-Field Interactions on Performance of Multipole-Based Preconditioners for Sparse Linear Systems, *ACM International Conference on Supercomputing*, St. Malo, France, pp 41 - 47, 2004.
53. A. Antoulas, D. Sorensen, K. Gallivan, P. Van Dooren, A. Grama, C. Hoffmann, and A. Sameh, Model Reduction of Large-Scale Dynamical Systems, *Proceedings 4th International Conference on Computational Science - ICCS 2004*, Krakow, Poland, June 6-9, 2004, Part III, Lecture Notes in Computer Science, Vol. 3038, Bubak, M.; Albada, G.D.v.; Sloot, P.M.A.; Dongarra, J. (Eds.), pp. 740-747.
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57. Mehmet Koyutürk and Ananth Grama, Proximus: A Framework for Analyzing Very High Dimensional Discrete-Attributed Datasets, *ACM SIGKDD*, 147 - 156, 2003.
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59. Changrui Cheng, Ihtesham Choudhury, Xianfan Xu, Jayathi Murthy, Ananth Grama, and Xinwei Wang, Numerical Simulation of Femtosecond Laser Ablation of Copper – Comparison Between Molecular Dynamics and Finite Difference Calculations, *Heat Transfer*, 2003.
60. Mehmet Koyutürk, Ananth Grama, and Wojciech Szpankowski, Algorithms for Bounded-Error Correlation of High Dimensional Data in Microarray Experiments, *The Computational Systems Bioinformatics Conference (CSB)*, pp 575-580, 2003.
61. Mohamed Mokbel, Walid Aref, and Ananth Grama, Spectral LPM: An Optimal Locality-Preserving Mapping using the Spectral (not Fractal) Order, *Proceedings of the 19 International Conference of Data Engineering ICDE*, pp 699 - 701, 2003 (Poster Presentation).
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63. Ioannis Ioannidis and Ananth Grama, An Efficient Protocol for Yao's Millionaires' Problem, *Hawaii International Conference on Computer Systems*, 6 pp (IEEE Digital Library), 2003.
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66. Ioannis Ioannidis, Ananth Grama, and Mikhail Atallah, A Secure Protocol for Computing Dot Products in Clustered and Distributed Environments, *International Conference on Parallel Processing (ICPP)*, pp 379 - 384, 2002.
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69. Ananth Grama, Vipin Kumar, Sanjay Ranka, and Vineet Singh, Architecture Independent Analysis of Parallel Programs, In *International Conference on Computational Science*, pp 599-608, San Francisco, CA, May 28-30, 2001.
70. Dow-Yung Yang, Akshay Johar, Wojciech Szpankowski, and Ananth Grama, Summary Structures for Frequency Queries on Large Transaction Sets, In *Data Compression Conference*, pp 238–247, Snowbird, UT, March 2000.

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72. Marc Alzina, Wojciech Szpankowski, and Ananth Grama, 2D-Pattern Matching Image and Video Compression, In *Proceedings of the Data Compression Conference*, pp 424–433, Snowbird, UT, 1999, IEEE Computer Society Press.
73. Ananth Grama, Vivek Sarin, and Ahmed Sameh, Analyzing the Error Bounds of Multipole-Based Treecodes, In *Proceedings of the 11th Supercomputing Conference*, page 10 pp, Orlando, FL, 1998. Proceedings on CD or online at <http://www.supercomp.org/sc98/papers/index.html>, sponsored by ACM and IEEE Computer Society.
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76. Chen Wang and Ananth Grama, Fast Parallel Techniques for Discrete Hadamard Transformations, In *Proceedings of the 10th International Conference on Parallel and Distributed Computing Systems*, page 10 pp, New Orleans, LA, 1997.
77. Ananth Grama, Vipin Kumar, and Ahmed Sameh, Parallel Hierarchical Solvers and Preconditioners for Boundary Element Methods, In *Proceedings of the 9th Supercomputing Conference*, page 8 pp, Pittsburgh, PA, 1996. Proceedings on CD and online at <http://www.supercomp.org/sc96/proceedings/>. Sponsored by ACM and IEEE Computer Society.
78. Ananth Grama, Vipin Kumar, Sanjay Ranka, and Vineet Singh,  $A^3$ : A Simple and Asymptotically Accurate Model for Parallel Computation, In *Proceedings of the Sixth Conference on Frontiers of Massively Parallel Computing*, page 8 pp, Annapolis, MD, 1996.
79. Vipin Kumar, Ahmed Sameh, Ananth Grama, and George Karypis, Architectures, Algorithms and Applications for Future Generation Supercomputers, In *Proceedings of the Sixth Conference on Frontiers of Massively Parallel Computing*, page 8 pp, Annapolis, MD, 1996.
80. Ananth Grama, Vipin Kumar, and Ahmed Sameh, Parallel Matrix-Vector Product Using Approximate Hierarchical Methods, In *Proceedings of the 8th Supercomputing Conference*, page 8 pp, San Diego, CA, 1995. Sponsored by ACM and IEEE Computer Society.
81. Minesh Amin, Ananth Grama, and Vineet Singh, Fast Volume Rendering Using an Efficient, Scalable Parallel Formulation of the Shear-Warp Algorithm, In *Proceedings of the Parallel Rendering Symposium (PRS) at Visualization Conference*, Atlanta, GA, 1995, IEEE Computer Society.
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83. Ananth Grama and Vipin Kumar, Scalability Analysis of Partitioning Strategies for Finite Element Graphs, In *Proceedings of the 5th Supercomputing Conference*, page 8 pp, Minneapolis, MN, 1992.
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## Book Chapters

1. Shahin Mohammadi and Ananth Grama, Biological Network Alignment, in *Functional Coherence of Molecular Networks in Bioinformatics* (Mehmet Koyuturk, Shankar Subramaniam, and Ananth Grama, eds.), Springer, pp. 97-136, 2011.
2. Bogdan Carbutar, Murali Krishna Ramanathan, Mehmet Koyuturk, Suresh Jagannathan, Ananth Grama. Optimal Tag Coverage and Tag Report Elimination, in *RFID Systems: Research Trends and Challenges*, Wiley Series in Wireless Communications and Mobile Computing. Editors M. Bolic, D. Simplot-Ryl, I. Stojmenovic, 2010.
3. Ananth Grama, Joseph Fogarty, Hasan Aktulga, Sagar Pandit, N-Body Computations, *Encyclopedia of Parallel Computing*, 2010.
4. George Kolias, Zhiyuan Li, Ananth Grama, Asynchronous Algorithms, *Encyclopedia of Parallel Computing*, 2010.
5. Ananth Grama, Vipin Kumar, Load Balancing for Parallel Optimization Techniques, *Encyclopedia of Optimization*, pp 1905-1911, 2009.
6. Ananth Grama and Vipin Kumar, Scalability of Parallel Programs, in *Handbook of Parallel Computing*, Chapman Hall/CRC Press, Sanguthevar Rajasekaran, John Reif, eds., 2007.
7. Anastasios Antoulas, Dan Sorensen, Kyle Gallivan, Paul Van Dooren, Ananth Grama, Christoph Hoffmann, and Ahmed Sameh, Model Reduction and Real-time Control of Dynamic Data Driven Systems, *Dynamic Data Driven Application Systems*, Kluwer Academic Publishers, Amsterdam, F. Darema, Ed., 2005.
8. Sacha Zyto, Ananth Grama, and Wojciech Szpankowski, Semi-Discrete Matrix Transforms for Image and Video Compression, *Process Coordination and Ubiquitous Computing*, pp 249 - 260, CRC Press, 2003.
9. Ananth Grama and Naren Ramakrishnan, Data Mining Applications in Bioinformatics, In *Data Mining for Scientific and Engineering Applications*, Kluwer Academic Press, 21 pp, 2001.
10. Ananth Grama and Vipin Kumar, Load Balancing of Parallel Search Techniques, In *Encyclopedia of Optimization*, Kluwer Academic Press, pp 203-209, 2000.
11. Ananth Grama, Vipin Kumar, George Karypis, and Anshul Gupta, Scalability Analysis for Petaflop Scale Parallel Algorithms, In *Ultrascale Computing*, 2000.
12. Ananth Grama, Vipin Kumar, and Ahmed Sameh, Parallel Hierarchical Solvers and Preconditioners for Boundary Element Methods, In Thomas Campbell, Roy Nicolaidis, and Manuel Salas, editors, *Computational Electromagnetics and Its Applications*, volume 5, pages 212–229, Kluwer Academic Publishers, 1997. ICASE/LaRC Interdisciplinary Series in Science and Engineering.
13. Ananth Grama, Vipin Kumar, and Panos Pardalos, Parallel Processing of Discrete Optimization Problems, In *Encyclopedia of Microcomputers*, pages 129–149, Marcel Dekker Publishers, NY, 1992.

## Major Software Packages

- **PuReMD:** PuReMD (Purdue Reactive Molecular Dynamics) is a large software package for reactive molecular dynamics simulations. Unlike conventional molecular dynamics techniques where bond structure stays static, in reactive molecular dynamics, the bond structure is dynamic. This makes the modeling paradigm vastly more powerful, while also making it very sophisticated from an algorithms and software perspective. PuReMD uses the ReaxFF force field, along with powerful solvers, data

structures, and parallel optimizations. It is available for message passing parallel platforms, GPUs, and GPU clusters. It is currently in use by over 1000 labs worldwide. Its integration with Department of Energy's LAMMPS code is used by thousands of other researchers to simulate diverse systems such as oxidative stress on biomembranes, stress corrosion cracking, and other nanostructures.

- **NSD:** NSD (Network Similarity Decomposition) is a simple and powerful technique that scales network alignment to large graphs. It has been tested on graphs with millions of nodes and billions of edges. It is currently used by a large number of groups to align networks in systems biology, social networks, and other networks in information retrieval.
- **MaWISH:** MaWISH (Maximum Weight Induced Subgraph Alignment) was the first local alignment technique for networks. It included a novel cost measure and alignment heuristic that was shown to return highly accurate local alignments in protein interaction networks. This code has been downloaded over 600 times, and is widely acknowledged to be one of the first efforts in this now-popular problem domain.
- **PROXIMUS:** PROXIMUS was the first software to use a modified Semi-Discrete Decomposition of boolean matrices to decompose matrices into their pattern and presence matrices. It used an EM algorithm to approximate the underlying optimization problem (known to be NP Hard). PROXIMUS has a large number of downloads and has been reimplemented in Python and R by independent groups.

## Invited Lectures

1. Erasure Coded Computations, Keynote Lecture, Computational Science and Engineering, University of Illinois, April 2015.
2. Reactive Molecular Dynamics: Algorithms, Software, and Applications, MICDE Distinguished Lecture, University of Michigan, January 2014.
3. Algorithms and Statistical Models for Large-Scale Network Analytics, Bell Labs / CSol Research Workshop, Princeton, Sept 2013.
4. Systems Biology of Cellular Aging and Age-Related Degeneracies, BioKDD, Aug. 2013.
5. TransMR: Data-Centric Programming Beyond Data Parallelism, Penn State University, March 2013.
6. Systems Biology of Cellular Aging and Age-Related Degeneracies, University of Minnesota, February 2013.
7. Network Models in Life Sciences, Indian Institute of Science, July 2012.
8. TransMR: Data-Centric Programming Beyond Data Parallelism, Executive Seminar Series, IBM Research, Bangalore, India, July 2012.
9. Large-Scale Reactive Molecular Dynamics: Methods, Applications, and Challenges, University of Notre Dame, June 2012.
10. Analysis of Molecular Interaction Networks, Stanford University, May 2012.
11. Functional Characterization and Topological Modularity of Molecular Interaction Networks, New Jersey Institute of Technology, 2011.
12. PuReMD: A Reactive (ReaxFF) Molecular Dynamics Package, University of Southern California, 2011.
13. Algorithms and Software for Network Modeling in Systems Biology, National Center for Biological Sciences, Bangalore, India, 2010.
14. GQ: A Graph Toolkit for Multicore Environments, Intel Corp, Santa Clara, 2010.

15. Algorithms for Biochemical Interaction Networks, Distinguished Lecture, Bioengineering Department, University of California, San Diego, 2008.
16. Parallel Banded Preconditioners for Non-Symmetric Linear System Solvers, 5th International Workshop on Parallel Matrix Algorithms and Applications (PMAA), June 20, 2008, Neuchatel, Switzerland.
17. Computational Analysis of Biological Networks, 6th Pathways, Networks and Systems Medicine Conference, June 16, 2008, Chania, Greece.
18. Weighted bandwidth reduction and preconditioning sparse systems, International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications, July 9-12, 2007, Meteopole, Toulouse, France.
19. Comparative Analysis of Molecular Interaction Networks, Deans Distinguished Lecture, Clemson University, Feb 16, 2007.
20. Algorithms and Infrastructure for Molecular Dynamics Simulations, Distinguished Lecture, College of Computing, Georgia Tech., Nov 6, 2006.
21. Molecular Dynamics Simulations of Reactive Systems, 4th International Workshop on Parallel Matrix Algorithms and Applications (PMAA), Rennes, France, Sept 8, 2006.
22. Software Support for Advanced Computing Platforms, Army Research Labs., Adelphi, MD, June 9, 2006.
23. Algorithms and Numerical Techniques for Scalable Molecular Dynamics Simulations, ICCES, Chennai, India, Dec 1-4, 2005.
24. Multipole-Based Preconditioners for Sparse Linear Systems, International Workshops on Advances in Computational Mechanics, Tokyo, Japan, 2004.
25. On Unstructured Peer-to-Peer Networks, their Eigenvalues, and Distributed Estimation, Parallel Matrix Algorithms and Applications, Marseilles, France, 2004.
26. Impact of Far-Field Interactions on Performance of Multipole-Based Preconditioners for Sparse Linear Systems, ACM International Conference on Supercomputing, St. Malo, France, 2004.
27. Multipole-Based Preconditioners for Large Sparse Linear Systems, Parallel Matrix Algorithms and Applications, Neuchatel, Switzerland, 2003.
28. Computational Aspects of Multipole Methods, Center for Computational Electromagnetics, University of Illinois at Urbana-Champaign, Nov. 27, 2001.
29. Mining Scientific Datasets, First SIAM Conference on Computational Science and Engineering, Sept. 21-23, 2000, Washington D.C.
30. Proximus: A Methodology for Error Bounded Compression and Categorization of Discrete Attribute Vector Sets, Workshop on Scientific Data Mining, Army High Performance Computing Research Center at the University of Minnesota, July 21, 2000.
31. Data Mining Applications in Battlefield Visualization, Army Research Labs, Adelphi, MD, April 6, 2000.
32. Approximation Techniques for Large-Scale Data Handling, Army High Performance Computing Center, Minneapolis, MN, Sept. 10, 1999.
33. Fast Algorithms for n-Body Simulations and their Applications, National Center for Supercomputing Applications, University of Illinois, Urbana-Champaign, March 12, 1998.



34. Parallel Solution Methods using Hierarchical Dense Approximation, International Conference on Computational Engineering Science, Atlanta, GA, 1998.
35. Fast Parallel Algorithms for Surface and Volumetric Scattering, PetaFLOPS Algorithms Workshop, Williamsburg, VA, Apr. 15, 1997.
36. Hierarchical Architectures for 100 TeraFLOPS Class Computers in a Ten Year Timeframe, Sixth Symposium on the Frontiers of Massively Parallel Computing, Annapolis, MD, Oct. 30, 1996.
37. Parallel Hierarchical Solvers and Preconditioners for Boundary Element Methods, NASA ICASE/LaRC Workshop on Computational Electromagnetics and Applications, Newport News, VA, May 30, 1996.
38. Architecture, Algorithms and Applications for Future Generation Supercomputers, PetaFLOPS Architectures Workshop, Oxnard, CA, April 16, 1996.
39. Efficient Parallel Formulations of Hierarchical Methods and their Applications, The PetaFLOPS Forum, Bodega Bay, CA, Aug. 20, 1995.

### **Other Presented Papers (Invited Papers)**

1. Ananth Grama and Naren Ramakrishnan, Mining Scientific Datasets, In *First SIAM Conference on Computational Science and Engineering*, Workshop on Scientific Data Mining, Washington D.C., Sept 2000.
2. Ananth Grama and Vipin Kumar, Data Mining Applications in Battlefield Visualization, In *Workshop on Battlefield Visualization and Real-time Geographic Information Systems*, Army Research Laboratory, Adelphi, Maryland, April, 2000.
3. Ananth Grama, Vivek Sarin, and Ahmed Sameh, Parallel Solution Methods Using Hierarchical Dense Approximation, In *International Conference on Computational Engineering and Science*, Atlanta, GA, 1998.
4. Ananth Grama, Vivek Sarin, and Ahmed Sameh, Piece-Wise Multipoles for Dense Iterative Solvers, In *Copper Mountain Conference on Iterative Methods*, Copper Mountain, CO, 1998.
5. Ananth Grama, Vivek Sarin, and Ahmed Sameh, Parallel Solution of Dense Linear Systems in Computational Electromagnetics, In *SIAM Workshop on Computational Electromagnetics*, Toronto, Canada, July 1998.
6. Ananth Grama and Vipin Kumar, Fast Parallel Algorithms for Surface and Volumetric Scattering, In *PetaFLOPS Algorithms Workshop*, Williamsburg, VA, April 15, 1997.
7. Vipin Kumar, George Karypis, and Ananth Grama, Role of Message-Passing in Performance Oriented Parallel Programming, In *Proceedings of the Eighth SIAM Conference on Parallel Processing for Scientific Computing*, San Antonio, TX, 1997.
8. Ananth Grama and Vipin Kumar, Parallel Algorithms for Discrete Optimization Problems, In *Symposium on Parallel Computing for Solving Large Scale and Irregular Applications*, Sophia-Antipolis, France, July, 1996.
9. Ananth Grama, Vipin Kumar, and Ahmed Sameh, On n-body Simulations Using Message Passing Parallel Computers, In *Proceedings of the SIAM Conference on Parallel Processing*, San Francisco, CA, Feb, 1995.

## Grants and Contracts

### Current Grants

1. Ananth Grama, Saurabh Bagchi, Somali Chaterji, and Folker Meyer, Continued Development and Maintenance of the MG-RAST Metagenomics Pipeline, NIH, \$3.8M, 10/15 - 9/20.
2. Douglas Lacount and Ananth Grama, Emerging virus-host cell protein interaction networks, NIH, \$3.2M, 4/15 - 4/20.
3. Mehmet Koyuturk, Ananth Grama, Wojciech Szpankowski, and Shankar Subramaniam, Theoretical Foundations and Software Infrastructure for Biological Network Databases, NIH, \$960K, 6/15 - 6/19.
4. David Gleich, Ahmed Sameh, and Ananth Grama, Fault Oblivious Computations, DOE, \$750K, 8/15 - 8/18.
5. Ananth Grama, XPS: EXPL: SDA: Scalable Concurrency Control Techniques for Distributed Systems, NSF, \$300K, 9/15 - 9/18.
6. Graham Cooks, Ananth Grama, David Thompson, Zoltan Nagi, and Eric Barker, Analytic-Directed Multi-scale Synthesis System, DARPA, \$8.3M, 1/16 - 12/19.
7. David Gleich, Ananth Grama, and Jennifer Neville, BIGDATA: F: Models, Algorithms, and Software for Spatial-Relational Networks, NSF, 900K, 9/15 - 8/19.
8. Ananth Grama, Software Infrastructure for Online Analytics, NSF, \$469K, 8/14 - 7/17.
9. Ananth Grama and Markus Lill, Network Analysis Aided Drug Re-purposing for Degenerative Diseases, OVPR Incentive Grant, Purdue University, \$398K, 1/14 - 5/16.
10. Wojciech Szpankowski, Ananth Grama (and others), Center for Science of Information, NSF Science and Technology Center, \$25M, 9/15 - 8/21.
11. Priya Vashistha, Rajiv Kalia, Aiichiro Nakano, and Ananth Grama, Probing Complex Dynamics of Small Interfering RNA (siRNA) Transfection by Petascale Simulations and Network Analysis, NSF, \$1.9M, 9/11 - 8/16.
12. Jan Vitek, Ananth Grama, Douglas Adams, and Suresh Jagannathan, Robust Distributed Wind Power Engineering, NSF, \$1.6M, 9/11 - 8/16.
13. Suresh Jagannathan and Ananth Grama, Profile-Guided Speculation for Multicore Architectures, Intel Corp., \$80K, 9/06 - 12/35.
14. Anthony Hosking, Suresh Jagannathan, Jan Vitek, and Ananth Grama, Language and Runtime Support for Safe and Scalable Programs, Microsoft, \$329K, 08 - .

### Past Grants

1. Wojciech Szpankowski, Ananth Grama, and Daisuke Kihara, Information Transfer in Biological Systems, NSF, \$480K, 7/08 - 6/15.
2. Wojciech Szpankowski, Ananth Grama (and others), Center for Science of Information, NSF Science and Technology Center, \$25M, 9/10 - 9/15.
3. Eric Jacobsson, Shankar Subramaniam, and Ananth Grama, Hierarchical Modularity in Evolution and Function, NSF, \$480K (Purdue's Budget), 10/08 - 9/14.

4. Jayathi Murthi, Ananth Grama, Anil Bajaj, Weinong Chen, PRISM: NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems, Department of Energy, \$21M, 4/08 - 4/14.
5. Priya Vashishtha, Rajiv Kalia, Aiichiro Nakano, and Ananth Grama, Petascale Simulations of DNA Dynamics and Self-Assembly, NSF, \$150K (Purdue's Budget), 9/08 - 8/13.
6. Ananth Grama, Cracking Under Stress: Developing a petascale simulation framework for stress corrosion cracking, Department of Energy, \$400K. (the total budget for the project is \$1.1M/year, with PI Priya Vashishtha at USC, and other participants being Gang Lu, Efthimios Kaxiras, Stephan Eidenbenz, Arthur F. Voter, Randy Q. Hood, John A. Moriarty, Lin H. Yang, Rajiv K. Kalia, and Aiichiro Nakano.), 9/06 - 8/12.
7. Zhiyuan Li and Ananth Grama, Compiler and Software Solutions for the Memory Bottleneck on Multi-core Processors, NSF, \$300K, 8/08 - 7/12.
8. Suresh Jagannathan and Ananth Grama, Eager Maps and Lazy Folds for Graph-Structured Applications, NSF, \$450K, 1/09 - 12/12.
9. Ananth Grama and Shankar Subramaniam, Biochemical Pathways Workbench, NSF, \$298K (Purdue's Budget), 11/07 - 10/11.
10. Ananth Grama, ITR-ASE-SIM: Collaborative Research: DeNovo Hierarchical Simulations of Stress Corrosion Cracking in Materials, NSF, \$361K (Purdue's Budget), 9/04-8/10. This is a collaborative proposal with University of Southern California and CalTech.
11. Ahmed Sameh, Ananth Grama, and Eric Polizzi, Developing a Robust Parallel Hybrid Solver, NSF, \$463K, 09/15/06 - 08/31/10.
12. Wojciech Szpankowski and Ananth Grama, Algebraic, Combinatorial and Probabilistic Methods for Biological Sequences, National Institute of Health, 5/15/03-4/30/08, \$924,865.
13. Zhiyuan Li, Ananth Grama, and Ahmed Sameh, AAD: Software Tools for Asynchronous-Algorithm Development, National Science Foundation, 1/1/05-12/31/07, \$650,000.
14. Ahmed Sameh and Ananth Grama, Evaluating Sparse Linear System Solvers on Scalable Parallel Architectures, AFRL, 08/24/06 - 08/23/07, \$149,999.
15. Ahmed Sameh, Ananth Grama, and Christoph Hoffmann, ITR/AP: Collaborative Research on Model Reduction of Dynamical Systems for Real-time Control, National Science Foundation, 9/1/03-8/31/07, \$958,502.
16. Suresh Jagannathan and Ananth Grama, Plethora: A Wide-Area Read-Write Object Repository for the Internet, National Science Foundation, 9/15/03-8/31/07, \$549,635.
17. Mete Sozen, George Chiu, Ananth Grama, Ahmed Sameh, and Christoph Hoffmann, Towards Real-Time Sensing and Control of Active Structures, National Science Foundation, 8/1/04-7/31/07, \$200,000.
18. Suresh Jagannathan, Jan Vitek, Tony Hosking, and Ananth Grama, A Computational Infrastructure for Experimentation on Relaxed Concurrency Abstracts, National Science Foundation, 3/1/06-2/28/08, \$99,979.
19. Ananth Grama, Biochemical Pathways Workbench, Purdue Research Foundation, 8/1/06 - 7/31/07, \$40,000.
20. Ahmed Sameh, Ananth Grama, and Gene Golub, Network for Computational Nanotechnology, NSF, 9/02 - 9/06, \$1.3M.

21. Greg Frederickson, Susanne Hambruch, and Ananth Grama, GAANN Fellowship Program, Department of Education, 8/03 - 7/06, \$650K.
22. Zhiyuan Li and Ahmed Sameh, Dynamic Compilation and Scheduling Techniques for Complex Simulations, NSF, 8/00 - 3/05, \$280K.
23. Bruce Craig and Ananth Grama, Calibrating the Two Antimicrobial Susceptibility Tests, NIH, 7/01 - 6/04, \$161K.
24. Ananth Grama and five other PIs, System Support, Appl. Dev., Benchmarking, and Instructional Infrastructure Using McKinley Servers, HP, 9/02 - , \$350K.
25. Christoph Hoffmann, Ananth Grama, Ahmed Sameh, David Ebert, Voicu Popescu, MRI: Acquisition of Equipment for Purdue Envision Center for Data Perceptualization, NSF, 9/02 - , \$900K.
26. Susanne Hambruch, Ananth Grama, and Jens Palsberg, Department of Education Fellowships in Areas of National Need, 8/00 - 8/03, \$425K.
27. Ananth Grama, Fast Methods for Particle Dynamics and their Applications, NSF, 02/99 - 01/04, \$235K.
28. Ananth Grama and Paul Ruth, Los Alamos National Lab Fellowship for PhD Research in High Performance Computing, Department of Energy, 8/00 - 8/03, \$100K.
29. Ahmed Sameh and Ananth Grama, Innovative Algorithms and Techniques for Large Scale Simulations, NSF, 6/99 - 5/03, \$309K.
30. Ananth Grama, Analytical and Computational Framework for n-Body Simulations, NSF, 12/98 - 11/03, \$188K.
31. Ananth Grama, Kihong Park, and David Yau, ISAC: Integrated System Support for Adaptive Communication and Computation Control in Clustered Environments, NSF, 08/98-08/02, \$584K.
32. Ananth Grama (and four other PIs), A Distributed Infrastructure for High Performance Computing and Networking, Intel, 6/98 - , \$998K.
33. Ananth Grama, Dominant and Deviant Pattern Detection in Event Traces for Intrusion Detection, Lilly/CERIAS, 6/00 - 12/01, \$50K.
34. Ahmed Sameh and Ananth Grama, Computational Methods in VLSI Design, NSF, 07/98 - 07/01, \$66K.
35. Ahmed Sameh, Ananth Grama, Zhiyuan Li, and Vivek Sarin, Development of Research Infrastructure for Scientific Computing and Computer Science, NSF, 7/98 - 7/01, \$800K.
36. Ahmed Sameh and Ananth Grama, Performance Evaluation and Optimization for Scientific Kernels, SGI, 7/98 - 7/01, \$25K.
37. Ananth Grama, n-Body Methods and their Applications in Dense Linear Solvers, Purdue Research Foundation, 07/98 - 07/00, \$22K.