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Curriculum Vitae

Russ Miller

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Hauptman-Woodward Medical Research Institute, 700 Ellicott Street, Buffalo, New York 14203; (716) 898-8600 (office); (716) 852-8660 (FAX); miller@buffalo.edu; <http://www.hwi.buffalo.edu/>

Degrees:

- Ph.D., Department of Mathematical Sciences, State University of New York at Binghamton, 1985.
Dissertation: *Pyramid Computer Algorithms*
Advisor: Quentin F. Stout
- M.A., Department of Mathematical Sciences, State University of New York at Binghamton, 1982.
- B.S. in Computer Science – Mathematics, Department of Mathematical Sciences, State University of New York at Binghamton, 1980.

Employment:

- 2002-present UB Distinguished Professor, State University of New York at Buffalo.
- 1992-present Senior Research Scientist, Department of Molecular Biophysics, Hauptman-Woodward Medical Research Institute (formerly The Medical Foundation of Buffalo Research Institute), Buffalo, NY.
- 2001-present Adjunct Professor, Department of Structural Biology, State University of New York at Buffalo.
- 1998-present Adjunct Professor, Department of Electrical Engineering, State University of New York at Buffalo.
- 2006-2007 Founding Executive Director and Member of the Governing Board, Cyberinfrastructure Initiative in the State of New York.
- 1998-2006 Founding Director, Center for Computational Research, State University of New York at Buffalo.
- 1995-2002 Professor, Department of Computer Science (and Engineering), State University of New York at Buffalo.
- 1991-1996 Consultant, Thinking Machines Corporation, Cambridge, Mass.
- 1990-1995 Associate Professor, Department of Computer Science, State University of New York at Buffalo.
- 1985-1990 Assistant Professor, Department of Computer Science, State University of New York at Buffalo.
- 1985 Adjunct Lecturer, Department of Mathematical Sciences, State University of New York at Binghamton.

Research Interests:

Cyberinfrastructure, Grid Computing, High-Performance Computing, Parallel Algorithms and Architectures, Computational Crystallography, Computational Geometry, Combinatorial Optimization

Honors:

- Fellow of the IEEE, 2012.
- Elected Senior Member of the IEEE, 2006.
- Inducted into Amherst (NY) *Avenue of Athletes* for “outstanding contributions in the area of youth sports,” June, 2005.
- Certificate of Recognition, Career Services Office, SUNY-Buffalo, based on survey of Graduates of the Class of 2003, 2005.
- *SGI Innovator Award*, one of six in the inaugural class, 2003.
- Listed in *HPCwire 2003 Top People & Organizations to Watch*, <http://www.tgc.com/hpcwire/features/topwatch03.html>, March, 2003.
- *International Scientist of the Year*, International Biographical Centre, Cambridge, England, 2003.
- *Best Practices Award*, Bio-IT World, 2003.
- Michael Dell presented CCR with its first Dell Center in Research Excellence, September, 2002.
- Elected as member to the *European Academy of Sciences* (Computer Science) with the citation “for an outstanding and lasting contribution to parallel algorithms and computer science education,” August, 2002.
- Designated as *UB Distinguished Professor*, State University of New York at Buffalo, April, 2002.
- *Shake-and-Bake* was mentioned on the poster “The Top Ten Algorithms of the Century,” published in *Computing in Science & Engineering*, Nov/Dec, 2000, produced in cooperation with the IEEE and The Computer Museum History Center.
- *Best Presentation Award* for the 1987 International Conference on Parallel Processing, St. Charles, Illinois, August 17-21, 1987.
- Listed in dozens of *Who’s Who*.
- *Distinguished Dissertation Award in the Science, Mathematics, and Engineering Category*, State University of New York at Binghamton, 1985.
- Elected to *Phi Beta Kappa*, 1980.

Professional Associations:

- *infoTech Niagara*, Board of Directors, 2002-2005.
- American Association for the Advancement of Science (AAAS)
- American Crystallographic Association (ACA)
- Association for Computing Machinery (ACM), including the Special Interest Group on Computer Architecture.
- Institute of Electrical and Electronics Engineers (IEEE), including IEEE Computer Society, Technical Committees on Distributed Processing, Pattern Analysis and Machine Intelligence, and Parallel Processing, as well as the Special Interest Group on Automata and Computability Theory.
- Society for Industrial and Applied Mathematics (SIAM), including the Special Interest Group on Supercomputing.

Teaching Interests:

- Cyberinfrastructure
- Grid Computing
- Cluster Computing
- Parallel Algorithms
- Analysis of Algorithms
- Computational Geometry
- Data Structures

Funding:**External Individual Funding:**

2004:	Hewlett-Packard Company 'Sponsored Training Program for a Postdoctoral Academic Fellowship Program'	\$150,000
1995-1998:	National Science Foundation 'Scalable Parallel Algorithms for Image Processing and Computational Geometry'	\$239,994
1991-1994:	National Science Foundation 'Parallel Algorithms for Image Processing and Computational Geometry' Includes Research Experiences for Undergraduates (REU) Supplement	\$277,418
1988-1991:	National Science Foundation 'Parallel Algorithms for Image Analysis, Computational Geometry, and Graph Theory'	\$170,000
1986-1988:	National Science Foundation 'Algorithms for Parallel Computers'	\$44,000
1986:	Supercomputing Research Center Workshop on Supercomputing	\$3,000

Internal Individual Funding:

1993	NYS/UUP Faculty Development Award Program 'Support for TCPP Report'	\$750
1990-1991	NYS/UUP Experienced Faculty Travel Award 'Parallel Computing'	\$500
1987-1988:	NYS/UUP New Faculty Development Award 'Parallel Algorithms'	\$750
1985-1987:	State University of New York at Buffalo Research Development Fund Research Grant 'Parallel Algorithms and Languages'	\$7,500
1985-1987:	State University of New York at Buffalo New Faculty Program Research Development Fund 'Parallel Algorithms'	\$2,000

External Joint Funding:

2005-2009:	National Science Foundation 'CRI: A Western New York Computational and Data Science Grid' PIs are as follows: R. Miller (PD, CCR/CSE), M. Green (CCR), C.M. Weeks (HWI), M. McCourt (NU) and H. Farian (Geneseo)	\$801,925
2002-2009:	National Science Foundation 'ITR: Enhancing Crystal Structure Determination through Data mining, Collaborative Environments, and Grid Computing' Includes Research Experiences for Undergraduates (REU) Supplement PIs are as follows: R. Miller (PD, CSE/CCR), J. Anstey (Media), H.A. Hauptman (HWI), C.M. Weeks (HWI) and A. Zhang (CSE)	\$2,054,063
2002-2006:	National Imagery and Mapping Agency 'Management and Technology Development of the National Technology Alliance' Prime contract to Rosettex Technology and Ventures Group UB subcontracts led by: David Mark: Imagery and Motion Imagery Processing and Analysis, Geographic Information Systems (GIS), and Cartography Aidong Zhang: Processing, Analysis, and Management of Data, Information, and Knowledge Russ Miller: Digital Technology Infrastructure	
2002-2005:	Federal/State Appropriations, Foundations, Donations 'Center of Excellence in Bioinformatics' Major Enablers: B.A. Holm, J.E. Penksa, R. Miller, and E.D. Capaldi	\$200,000,000+
2001-2003:	National Science Foundation 'High Performance Network Connections for Science and Engineering Research - HPNC: High Performance Network Connections for Hauptman-Woodward Inst' PIs are as follows: C.M. Weeks (PD, HWI), W. Pangborn (HWI), E.B. Pitman (Math), G.T. DeTitta (HWI), and R. Miller (CCR)	\$150,000
2001-2006:	National Science Foundation 'MultiStore: A Research Infrastructure for Management, Analysis and Visualization of Large-Scale Multidimensional Data Sets' PIs are as follows: A. Zhang (PD, CSE), R. Acharya (CSE), A. Garg (CSE), D. Mark (Geog), and R. Miller (CSE)	\$1,003,088
2001:	New York State Office of Science, Technology and Academic Research 'Center for Disease Modeling and Therapy Discovery Section Leader of Bioinformatics Laboratory' (One of Thirty Senior Personnel Listed in Proposal) PIs are as follows: B.A. Holm (PD, UB), D.C. Hohn (RPCI), G.T. DeTitta (HWI), and J.E. Friedlander (Kaleida)	\$15,300,000

External Joint Funding (cont'd):

2001-2006:	National Institutes of Health 'New Methods of Biomolecular Structure Determination' H.A. Hauptman (PD/HWI), G.T. DeTitta (HWI), C.M. Weeks (HWI), Q. Shen (CHESS), J.F. Griffin (HWI), R.H. Blessing (HWI), S.A. Ealick (CHESS), W. Furey (Pitt), D. Guo (HWI), D.A. Langa (HWI), R. Miller (UB), S. Potter (HWI), G.D. Smith (HWI), W.D. Tolbert (CHESS), and H. Xu (HWI).	\$7,820,345
1999:	Sun Microsystems 'Development of a 64-Node Ultra 5 Linux/Beowulf Parallel Computing System' Russ Miller (PD) and Corky Brunskill (co-PI)	\$112,000
1998-1999:	IBM Shared University Research (SUR) Grant 'Determination of Molecular Structure of Large Proteins via <i>SnB</i> and Parallel Algorithms for Hidden Markov Modeling' R. Miller (PD), H.A. Hauptman (HWI), F. Sachs (Biophysics), and A. Auerbach (Biophysics)	\$1,200,000
1998-2001:	National Science Foundation 'Determining Molecular Structures over the Web via <i>SnB</i> ' Includes Research Experiences for Undergraduates (REU) Supplement R. Miller (PD) and C.M. Weeks (co-PI)	\$303,787
1998-2001:	National Science Foundation 'MRI: Structural Studies and Methodologies in Chemistry and Molecular Biology' Includes Research Experiences for Undergraduates (REU) Supplement R. Miller (PD/CS), P. Coppens (Chem), T.R. Furlani (Chem), J. Gao (Chem), and H.F. King (Chem)	\$310,500
1998:	Oishei Foundation 'Web-Based Computing with <i>SnB</i> ' H.A. Hauptman (PD/HWI), R. Miller (HWI), and C.M. Weeks (HWI).	\$200,000
1998:	W.M. Keck Foundation 'W.M. Keck Foundation Center for Computational Structural Biology' F. Sachs, A. Auerbach, F. Qin, and R. Miller (consultant).	\$1,000,000
1997-2000:	Department of Energy 'Supercomputer Solution of Massive Crystallographic and Microtomographic Structural Problems' I. Foster (PD/Argonne), K. Jones (Brookhaven), H. Hauptman (HWI), C. Kesselman (CalTech), I. McNulty (Argonne), R. Miller (UB/HWI), K. Moffat (U. Chicago), J. Nosedal (Northwestern), Z. Ren (U. Chicago), M. Rivers (U. Chicago), S. Sinha (PD/Argonne), R. Stevens (Argonne), E. Westbrook (Argonne), and S. Wright (Argonne).	Year 1: \$520,000
1996-2001:	National Institutes of Health 'New Methods of Biomolecular Structure Determination' H.A. Hauptman (PD/HWI), R. Blessing (HWI), C.-S. Chang (HWI), G.T. DeTitta (HWI), D.L. Dorset (HWI), S.E. Ealick (CHESS), J.F. Griffin (HWI), D. Guo (HWI), D.A. Langa (HWI), R. Miller (UB) G.D. Smith (HWI), and C.M. Weeks (HWI).	\$5,699,308

External Joint Funding (cont'd):

1993-1996:	National Institutes of Health 'Direct Methods of Phase Determination' (Supplement to 'New Methods of Biomolecular Structure Determination') H.A. Hauptman (PD/MFB), R. Blessing (MFB), G. DeTitta (MFB), R. Miller (MFB/UB)	\$187,437
1992-1996:	National Institutes of Health 'New Methods of Biomolecular Structure Determination' H.A. Hauptman (PD/MFB), D.L. Dorset (MFB), J.F. Griffin (MFB), D. Guo (MFB), D.A. Langs (MFB), R. Miller (UB), G.D. Smith (MFB), and C.M. Weeks (MFB).	\$3,009,370
1990-1991:	National Science Foundation 'Acquisition of a High Performance Parallel Computer' A. Auerbach, D. Faber, F. Sachs, and R. Miller (consultant)	\$270,000
1988-1989:	National Science Foundation 'Hypercube for Parallel Algorithms Research' R. Miller (PD/CS), P.J. Eberlein (CS) and S.N. Srihari (CS)	\$50,000
1987-1990:	National Science Foundation 'Parallel Algorithms on a Hypercube Multiprocessor' Includes Research Experiences for Undergraduates (REU) Supplement P.J. Eberlein (co-PD, Computer Science), T. Furlani (Calspan), T. George (Physics), H. King (Chemistry), J. Lordi (Calspan), J. McIver (co-PD, Chemistry), and R. Miller (Computer Science).	\$232,000

Individual Supercomputing Support:

1995-1996	Cornell Theory Center ' <i>SnB</i> : Direct Methods for Crystal Structure Determination' IBM SP2
1995-1996	NSF MetaCenter Allocations 'Crystal Structure Determination via Shake-and-Bake' Cray C90 (PSC), Cray T3D (PSC)
1994-1995	NSF MetaCenter Allocations 'Crystal Structure Determination via Shake-and-Bake' Cray C90 (PSC), Cray T3D (PSC), TMC CM-5 (NCSA)
1993-1994	NSF Supercomputing Center Advanced Computing Resources 'The Phase Problem of X-Ray Crystallography' TMC CM-5 (NCSA)
1991-1993	NSF Supercomputing Center Advanced Computing Resources 'Parallel Solutions to the Phase Problem in X-Ray Crystallography' TMC CM-2 (PSC)

Joint Supercomputing Support:

- 1995: Lawrence Livermore National Laboratory
‘Applications of Massively Parallel Computing Techniques to the
Direct Solution of Macromolecular Structures’
PI: Sean Parkin, LLNL
Cray T3D

Publications (h-index of 29, 5/2010)

Refereed Journal Papers:

1. R. Miller and Q.F. Stout, Geometric algorithms for digitized pictures on a mesh-connected computer, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, PAMI-7 (1985), pp. 216-228.
2. R. Miller and Q.F. Stout, Data movement techniques for the pyramid computer, *SIAM Journal on Computing*, vol. 16, no. 1, Feb. 1987, pp. 38-60.
3. R. Miller and Q.F. Stout, Simulating essential pyramids, *IEEE Transactions on Computers*, vol. 37, no. 12, Dec. 1988, pp. 1642-1647.
4. R. Miller and Q.F. Stout, Efficient parallel convex hull algorithms, *IEEE Transactions on Computers*, vol. 37, no. 12, Dec. 1988, pp. 1605-1619.
5. E. Cohen and R. Miller, Hypercube algorithms for the multiprocessor scheduling problem, *Supercomputer Journal* **27**, vol. V, no. 5, September, 1988, pp. 17-32.
6. R. Miller and Q.F. Stout, Mesh computer algorithms for computational geometry, *IEEE Transactions on Computers*, vol. 38, no. 3, March 1989, pp. 321-340.
7. L. Boxer and R. Miller, Parallel dynamic computational geometry, *The Journal of New Generation Computer Systems* **2** (1989) 3, pp. 227-246.
8. R. Miller and S.E. Miller, Convexity algorithms for digitized pictures on an Intel iPSC hypercube, *Supercomputer Journal* **31**, vol. VI, no. 3, May 1989, pp. 45-53.
9. L. Boxer and R. Miller, A parallel circle-cover minimization algorithm, *Information Processing Letters* **32**, July 1989, pp. 57-60.
10. L. Boxer and R. Miller, Dynamic computational geometry on meshes and hypercubes, *Journal of Supercomputing*, vol. 3, no. 3, September, 1989, pp. 161-192.
11. L. Boxer and R. Miller, Common intersections of polygons, *Information Processing Letters* **33**, February 1990, pp. 249-254.
12. R. Miller and Q.F. Stout, Seymour: A portable parallel programming language, *Structured Programming* (1990), vol. 11, no. 4, pp. 157-171.
13. R. Miller and Q.F. Stout, Computing convexity properties of images on a pyramid computer, *Algorithmica*, vol. 6, no. 5, 1991, pp. 658-684.
14. F. Dehne, R. Miller, and A. Rau-Chaplin, Optical clustering on a mesh-connected computer, *International Journal on Parallel Programming*, Vol. 20, No. 6, 1991, pp. 475-486.
15. E. Cohen, R. Miller, E. Sarraf, and Q.F. Stout, Efficient convexity and domination algorithms for fine- and medium-grain hypercube computers, *Algorithmica*, vol. 7, no. 1, 1992, pp. 51-75.
16. C.M. Weeks, G.T. DeTitta, R. Miller, and H.A. Hauptman, Applications of the minimal principle to peptide structures, *Acta Crystallographica* **D49**, 1993, pp. 179-181.
17. L. Boxer, C.-S. Chang, R. Miller, and A. Rau-Chaplin, Polygonal approximation by boundary reduction, *Pattern Recognition Letters* **14** (1993), pp. 111-119.
18. L. Boxer and R. Miller, Parallel algorithms for all maximal equally-spaced collinear sets and all maximal regular coplanar lattices, *Pattern Recognition Letters* **14** (1993), pp. 17-22.

19. R. Miller, G.T. DeTitta, R. Jones, D.A. Langs, C.M. Weeks, and H.A. Hauptman, On the application of the minimal principle to solve unknown structures, *Science*, vol. 259, March, 1993, pp. 1430-1433.
20. C.-S. Chang, G. DeTitta, H. Hauptman, R. Miller, P. Thuman, and C. Weeks, Using parallel computers to solve the phase problem of x-ray crystallography, *The International Journal of Supercomputer Applications*, vol. 7, no. 1, Spring 1993, pp. 25-49.
21. R. Miller, V.K. Prasanna Kumar, D. Reisis, and Q.F. Stout, Parallel computations on reconfigurable meshes, *IEEE Transactions on Computers*, vol. 42, no. 6, June 1993, pp. 678-692.
22. R. Miller, N.M. Galitsky, W.L. Duax, D.A. Langs, V.Z. Pletnev, and V.T. Ivanov, Molecular structures of two crystalline polymorphs of the cyclic heptapeptide antibiotic ternatin: cyclo [- β -OH-D-Leu-D-Ile-(NMe)Ala-(NMe)Leu-Leu-(NMe)Ala-D-(NMe)Ala-], *International Journal of Peptide & Protein Research* **42**, 1993, pp. 539-549.
23. M.J. Atallah, F. Dehne, R. Miller, A. Rau-Chaplin, and J.-J. Tsay, Multisearch techniques for implementing data structures on a mesh-connected computer, *Journal of Parallel and Distributed Computing* **20**, 1994, pp. 1-13.
24. S. Hambrusch, X. He, and R. Miller, Parallel algorithms for gray-scale digitized picture component labeling on a mesh-connected computer, *Journal of Parallel and Distributed Computing* **20**, 1994, pp. 56-68.
25. G.T. DeTitta, C.M. Weeks, P. Thuman, R. Miller, and H.A. Hauptman, Structure solution by minimal function phase refinement and Fourier filtering. I. Theoretical basis, *Acta Crystallographica* **A50**, 1994, pp. 203-210.
26. C.M. Weeks, G.T. DeTitta, H.A. Hauptman, P. Thuman, and R. Miller, Structure solution by minimal function phase refinement and Fourier filtering. II. Implementation and applications, *Acta Crystallographica* **A50**, 1994, pp. 210-220.
27. R. Miller, S.M. Gallo, H.G. Khalak, and C.M. Weeks, *SnB*: Crystal structure determination via Shake-and-Bake, *Journal of Applied Crystallography* **27**, 1994, pp. 613-621.
28. R. Miller, The status of parallel processing education, *Computer*, August, 1994, pp. 40-43.
29. S.L. Tanimoto and R. Miller, Mesh algorithms for finding repetitions and partial symmetries in arrays, *International Journal of Pattern Recognition and Artificial Intelligence*, Vol. 8, No. 2, 1994, pp. 465-483.
30. D.A. Langs, R. Miller, H.A. Hauptman, and G.W. Han, Use of the minimal function for partial structure development in direct methods, *Acta Crystallographica* **A51**, 1995, pp. 81-87.
31. C.M. Weeks, H.A. Hauptman, G.D. Smith, R.H. Blessing, M.M. Teeter, and R. Miller, Crambin: a direct solution for a 400 atom structure, *Acta Crystallographica* **D51**, 1995, pp. 33-38.
32. M.P. McCourt, N. Li, W.A. Pangborn, R. Miller, C.M. Weeks, and D.L. Dorset, Crystallography of linear molecule binary solids. X-ray structure of a cholesteryl myristate/cholesteryl pentadecanoate solid solution, *J. Phys. Chem.*, vol. 100, no. 23, 1996, pp. 9842-9847.
33. M.P. McCourt, K. Ashraf, R. Miller, C.M. Weeks, N. Li, W. Pangborn, and D.L. Dorset, X-ray crystal structure of cytotoxic, oxidized cholesterols: 7-ketocholesterol and 25-hydroxycholesterol, *Journal of Lipid Research*, vol. 38, 1997, pp. 1014-1021.
34. C.-S. Chang, C.M. Weeks, R. Miller, and H.A. Hauptman, Incorporating tangent refinement in the *Shake-and-Bake* formalism, *Acta Crystallographica* **A53**, 1997, pp. 436-444.

35. G.D. Smith, R.H. Blessing, S.E. Ealick, J.C. Fontecilla-Camps, H.A. Hauptman, D. Housset, D.A. Langs, and R. Miller, The *ab initio* structure determination and refinement of a scorpion protein toxin, *Acta Crystallographica* **D53**, 1997, pp. 551-557.
36. P.J. Loll, R. Miller, C.M. Weeks, and P.H. Axelsen, A ligand-mediated dimerization mode for vancomycin, *Chemistry and Biology* **5**, 1998, pp. 293-298.
37. A. Deacon, C.M. Weeks, R. Miller, and S.E. Ealick, The *Shake-and-Bake* structure determination of triclinic lysozyme, *Proceedings of the National Academy of Sciences, U.S.A.*, **95**, August 1998, pp. 9284-9289.
38. S.-H. Hu, M. Loughnan, R. Miller, C.M. Weeks, R.H. Blessing, P.F. Alewood, R.J. Lewis, and J.L. Martin, The 1.1Å Crystal Structure of [Tyr¹⁵]-EpI, A novel α -conotoxin from *Conus Episcopatus*, solved by direct methods, *Biochemistry* **37**, 1998, pp. 11425-11433.
39. L. Boxer, R. Miller, and A. Rau-Chaplin, Scalable parallel algorithms for lower envelope with applications, *Journal of Parallel and Distributed Computing* **53**, 1998, pp. 91-118.
40. C.M. Weeks and R. Miller, Optimizing *Shake-and-Bake* for proteins, *Acta Crystallographica* **D55**, 1999, pp. 492-500.
41. C.M. Weeks and R. Miller, The design and implementation of *SnB* v2.0, *Journal of Applied Crystallography* **32**, 1999, pp. 120-124.
42. L. Boxer, R. Miller, and A. Rau-Chaplin, Scalable parallel algorithms for geometric pattern recognition, *Journal for Parallel and Distributed Computing* **58**, 1999, pp. 466-486.
43. H.A. Hauptman, H. Xu, C.M. Weeks, and R. Miller, Exponential *Shake-and-Bake*: theoretical basis and applications, *Acta Crystallographica* **A55**, 1999, pp. 891-900.
44. M. Egli, V. Tereshko, M. Teplova, G. Minasov, A. Joachimiak, R. Sanishvilli, C.M. Weeks, R. Miller, M.A. Maier, H. An, P.D. Cook, and M. Manoharan, X-ray crystallographic analysis of the hydration of A- and B-form DNA at atomic resolution, *Biopolymers (Nucleic Acid Sciences)* **48**, 2000, pp. 234-252.
45. H. Xu, H.A. Hauptman, C.M. Weeks, and R. Miller, P1 *Shake-and-Bake*: Can success be guaranteed?, *Acta Crystallographica* **D56**, 2000, pp. 238-240.
46. H. Xu, C.M. Weeks, A.M. Deacon, R. Miller, and H.A. Hauptman, Ill-conditioned *Shake-and-Bake*: The trap of the false minimum, *Acta Crystallographica* **A56**, 2000, pp. 112-118.
47. L. Boxer and R. Miller, Efficient computation of the Euclidean distance transform, *Computer Vision and Image Understanding* **80**, 2000, pp. 379-383.
48. Y. Vekhter and R. Miller, An improved phase-extension procedure for isomorphous-replacement phases, *Acta Crystallographica* **D57**, 2001, pp. 1048-1051.
49. L. Boxer and R. Miller, A parallel algorithm for approximate regularity, *Information Processing Letters*, **80**, 2001, pp. 311-316.
50. J. Rappleye, M. Innus, C.M. Weeks, and R. Miller, *SnB* v2.2: An example of crystallographic multiprocessing, *Journal of Applied Crystallography* **35**, 2002, pp. 374-376.
51. C.M. Weeks, R.H. Blessing, R. Miller, R. Mungee, S.A. Potter, J. Rappleye, G.D. Smith, H. Xu, and W. Furey, Towards automated protein structure determination: *BnP*, the *SnB*-PHASES interface, *A. Kristallogr.* **217**, 2002, pp. 686-693.

52. M.L. Green and R. Miller, Grid computing in Buffalo, New York, *Annals of the European Academy of Sciences*, 2003, pp. 191-218.
53. M.L. Green and R. Miller, A client-server prototype for grid-enabling application template design, *Parallel Processing Letters*, Vol. 14, No. 2 (2004), pp. 241-253.
54. M.L. Green and R. Miller, Molecular structure determination on a computational & data grid, *Parallel Computing Journal* **30** (2004), pp. 1001-1017.
55. M.L. Green and R. Miller, Evolutionary molecular structure determination using grid-enabled data mining, *Parallel Computing Journal* **30** (2004), pp. 1057-1071.
56. L. Boxer and R. Miller, Coarse Grained Gather and Scatter Operations with Applications, *Journal of Parallel and Distributed Computing* **64** (2004), pp. 1297-1310.
57. M.M. Eshaghian-Wilner and R. Miller, The Systolic Reconfigurable Mesh, *Parallel Processing Letters*, Vol. 14, Nos. 3&4 (2004), pp. 335-350.
58. C.L. Ruby, M.L. Green, and R. Miller, The Operations Dashboard: A Collaborative Environment for Monitoring Virtual Organization-Specific Compute Element Operational Status, *Parallel Processing Letters*, Vol. 16, No. 4 (2006), pp. 485-500.
59. R. Miller, N. Shah, M. Green, W. Furey, and C. Weeks, *Shake-and-Bake* on the grid, *Journal of Applied Crystallography* **40**, 2007, pp. 938-944.
60. L. Boxer and R. Miller Efficient coarse-grained data distributions and string pattern matching, *International journal of Information and Systems Sciences*, vol. 6, no. 4, 2010, pp. 424-434.

Refereed Papers in Major Conferences (Complete Papers Published):

61. R. Miller and Q.F. Stout, The pyramid computer for image processing, *Proceedings of the 1984 IEEE International Conference on Pattern Recognition*, pp. 240-242.
62. Q.F. Stout and R. Miller, Mesh-connected computer algorithms for determining geometric properties of figures, *Proceedings of the 1984 IEEE International Conference on Pattern Recognition*, pp. 475-477.
63. R. Miller and Q.F. Stout, Computational geometry on a mesh-connected computer, *Proceedings of the 1984 IEEE International Conference on Parallel Processing*, pp. 66-73.
64. R. Miller and Q.F. Stout, Convexity algorithms for pyramid computers, *Proceedings of the 1984 IEEE International Conference on Parallel Processing*, pp. 177-184.
65. R. Miller and Q.F. Stout, Pyramid computer algorithms for determining geometric properties of images, *Proceedings of the ACM Symposium on Computational Geometry*, 1985, pp. 263-277.
66. R. Miller and Q.F. Stout, Varying diameter and problem size in mesh-connected computers, *Proceedings of the 1985 IEEE International Conference on Parallel Processing*, pp. 697-699.
67. R. Miller, Writing SIMD Algorithms, *Proceedings of the 1985 IEEE International Conference on Computer Design: VLSI in Computers*, pp. 122-125.
68. R. Miller and S.E. Miller, Using hypercube multiprocessors to determine geometric properties of digitized pictures, *Proceedings of the 1987 International Conference on Parallel Processing*, IEEE Computer Society Press, pp. 638-640.
69. R. Miller and Q.F. Stout, Mesh computer algorithms for line segments and simple polygons, *Proceedings of the 1987 International Conference on Parallel Processing*, IEEE Computer Society Press, pp. 282-285.

70. L. Boxer and R. Miller, Parallel algorithms for dynamic systems with known trajectories, *Proceedings of the 1987 IEEE Workshop on Computer Architecture for Pattern Analysis and Machine Intelligence*, pp. 37-43.
71. R. Miller, V.K. Prasanna Kumar, D. Reisis, and Q.F. Stout, Meshes with reconfigurable buses, *Advanced Research in VLSI: Proceedings of the Fifth MIT Conference*, The MIT Press, 1988, pp. 163-178.
72. R. Miller and Q.F. Stout, Simulating essential pyramids, *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 1988, pp. 912-917.
73. R. Miller and Q.F. Stout, Convexity algorithms for parallel machines, *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 1988, pp. 918-924.
74. R. Miller, V.K. Prasanna Kumar, D. Reisis, and Q.F. Stout, Image computations on reconfigurable VLSI arrays, *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 1988, pp. 925-930.
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- H. Xu, C.M. Weeks, R. Miller, and H.A. Hauptman, *Applications of an Exponential Minimal Function*, *Annual Meeting of the American Crystallographic Association*, 1998, p. 132.
- A.M. Deacon, C.M. Weeks, R. Miller, and S.E. Ealick, The *Shake-and-Bake* Structure Determination of Triclinic Lysozyme, *Annual Meeting of the American Crystallographic Association*, P162, 1998, p. 132.
- R. Miller and C.M. Weeks, An Introduction to *SnB* v2.0: A Cool Way to Solve Structures (or How to Beat the Heat in Washington, D.C.), *Annual Meeting of the American Crystallographic Association*, WK.02.03, 1998, pp. 33-34 (**invited**).
- C.M. Weeks, H. Xu, R. Miller, and H.A. Hauptman, *Shake-and-Bake* Summer '98 Update: Improving Limited Data with Magnitude Estimation, *Eighteenth European Crystallographic Meeting*, Prague, Czech Republic, August, 1998, E5-06, (**invited**).
- C.M. Weeks, R. Miller, H.A. Hauptman, R.H. Blessing, and A.M. Deacon, Solving Structures with *SnB*, Workshop WK02: Solving Structures with *SnB*, *Annual Meeting of the American Crystallographic Association*, 1999, WK.02.01, p. 23.
- R. Miller, A. Palumbo, and C.M. Weeks, *SnB* Version 2.0: Direct Methods for Both Conventional Applications and Large Substructures, *Annual Meeting of the American Crystallographic Association*, 1999, PT09, p. 107.
- H.A. Hauptman, H. Xu, C.M. Weeks, and R. Miller, Is 100% Success for Shake-and-Bake Possible?, *54th Pittsburgh Diffraction Conference*, Columbus, OH, October, 1999.
- H.A. Hauptman, H. Xu, C.M. Weeks, and R. Miller, Is 100% Success for Shake-and-Bake Possible?, *Annual Meeting of the American Crystallographic Association*, 1999, 03.01.10, p. 46.

- H. Xu, H.A. Hauptman, C.M. Weeks, and R. Miller, Exponential *Shake-and-Bake*: Can Success be Guaranteed?, *XVIII Congress and General Assembly of the International Union of Crystallography*, to appear.
- C.M. Weeks and R. Miller *SnB* Version 2.0: Direct Methods for Large Molecules and Large Substructures, *IUCr Crystallographic Computing School*, Cambridge, UK, August, 1999.
- C.M. Weeks, R. Miller, H.A. Hauptman, R.H. Blessing, and A.M. Deacon, Solving Structures with *SnB*, *XVIII Congress and General Assembly of the International Union of Crystallography*, to appear.
- C.M. Weeks, R. Miller, and A.M. Deacon, What role can *SnB* play in automated macromolecular crystallography?, *Workshop on Automation of Structure Determination*, Brookhaven National Laboratory, Upton, NY, June, 1999.
- R. Miller, The Center for Computational Science at SUNY-Buffalo, *New Trends in High Performance Computing*, 1999, p. 32 (**invited**).
- C.M. Weeks and R. Miller, Software development for crystal structure determination, Health Care Industries Association Regional Research Forum, Sept., 1999, Buffalo, NY.
- C.M. Weeks, P.L. Howell, A.M. Deacon, R.H. Blessing, G.D. Smith, R. Miller, S.E. Ealick, and H.A. Hauptman, Finding seleniums with *SnB*, M12.BB.005, *Eighteenth IUCR Congress and General Assembly*, Glasgow, Scotland, August, 1999 (**invited**).
- C.M. Weeks and R. Miller, *SnB* Version 2.0: Direct methods for large molecules and large substructures, *IUCR Crystallographic Computing School* on "Frontiers in Computational Crystallography," Cambridge, UK, August, 1999 (**invited**).
- W. Furey, C.M. Weeks, and R. Miller, Towards Automated Macromolecular Structure Determination: The *SnB*-PHASES Interface, Abstract P067, *Annual Meeting of the American Crystallographic Association*, St. Paul, MN, July, 2000, p. 84.
- R. Miller, M. Innus, J. Rappleye and C.M. Weeks, *SnB* v2.0: An Example of Crystallographic Multiprocessing, Abstract P140, *Annual Meeting of the American Crystallographic Association*, St. Paul, MN, July, 2000, p. 103.
- Weeks, Blessing, Miller, Mungee, Potter, Rappleye, Smith, Xu and Furey, Integrating Direct Methods into a Semi-Automated, Protein-Phasing Package, *XIX Congress and General Assembly of the International Union of Crystallography*, Geneva, Switzerland, 2002.
- C.M. Weeks, S.A. Potter, R. Miller and W. Furey, Automated Protein Structure Solution with *BnP*, *Annual Meeting of the American Crystallographic Association*, to appear.
- C.M. Weeks, S.A. Potter, R. Miller and W. Furey, Automated Protein Structure Determination with *BnP*, *21st European Crystallographic Association Meeting*, Durban, South Africa, August 24-29, 2003.
- W. Furey, L. Pasupulati, S. A. Potter, H. Xu, R. Miller, and C. M. Weeks, Automated Applications of *BnP*. I. Methodology, *Annual Meeting of the American Crystallographic Association*, 01.03.03, Chicago, IL, July, 2004.
- C. M. Weeks, S. A. Potter, H. Xu, R. Miller, L. Pasupulati, and W. Furey, Automated Applications of *BnP*. II. Test Results, *Annual Meeting of the American Crystallographic Association*, P258, Chicago, IL, July, 2004.
- R. Miller, M. L. Green, and C. M. Weeks, *BnP* on the Grid, *Annual Meeting of the American Crystallographic Association*, 06.03.01, Chicago, IL, July, 2004.

- W. Furey, L. Pasupulati, S.A. Potter, H. Xu, R. Miller, and C.W. Weeks, Recent Developments in the *BnP* Package for Automated Protein Structure Determination, *Annual Meeting of the American Crystallographic Association*, 01.03.07, W0324, Orlando, FL, May-June, 2005.
- A. Ghadersohi, D. Pape, C. Weeks, M. Green, and R. Miller, Shake-and-Bake Visualizer, *Annual Meeting of the American Crystallographic Association*, P088, W0094, Orlando, FL, May-June, 2005.
- C. M. Weeks, S. A. Potter, N. Shah, H. Xu, M. L. Green, R. Miller, L. Pasupulati, and W. Furey, Adapting BnP for Different Computing Environments, *Annual Meeting of the American Crystallographic Association*, 2006.

Unpublished Manuscripts:

- R. Miller, *The Status of Parallel Processing Education: 1993*. Available by anonymous ftp from ftp.cs.buffalo.edu in users/miller or as Technical Report #93-27.
- H.G. Khalak, S.M. Gallo, C.M. Weeks, and R. Miller, *SnB: A Structure Determination Package, User's Manual*, 1993.

Television Credits:

- MTV2's Video Mods presented five new animated videos that blend live action with motion capture and inject a unique video game environment, including characters from one or more video games, into music videos: November 21, 2005.
 - Avenged Sevenfold's "Bat Country" was animated with the gaming environment from *Everquest II*.
 - Weezer's "Beverly Hills" was animated with the gaming environment from *The Sims: Nightlife*.
 - TI's "Do Your Thang" was animated with the gaming environment from *Need for Speed: Most Wanted*.
 - Sum 41's "Fat Lip" was animated with the gaming environment from *Guitar Hero*.
 - Nelly/Fat Joe's "Get it Poppin'" was animated with the gaming environment from *True Crime: New York City*.
- MTV2's Video Mods presented four new animated videos that blend live action with motion capture and inject a unique video game environment, including characters from one or more video games, into music videos: October 28, 2005.
 - Foo Fighters's "DOA" was animated with the gaming environment from *Star Wars: Battlefront 2*.
 - All American Reject's "Dirty Little Secret" was animated with the gaming environment from *Sid Mier's Pirates*.
 - Jane's Addiction's "Mountain Song" was animated with the gaming environment from *Getting Up*.
 - Twista's "Hit the Floor" was animated with the gaming environment from *LA Rush*.
- MTV2's Video Mods presented four new animated videos that blend live action with motion capture and inject a unique video game environment, including characters from one or more video games, into music videos: September 30, 2005.
 - Unwritten Law's "Save Me" was animated with the gaming environment from *X-Men Legends 2 - Rise of the Apocalypse*.
 - Ciara's "1,2 Step" was animated with the gaming environment from *Dance, Dance Revolution*.
 - Hoobastank's "The Reason" was animated with the gaming environment from *Dungeon Lords*.
 - Jimmy Eat World's "Pain" was animated with the gaming environment from *Juiced*.
- MTV2's Video Mods presented four new and one previously aired animated videos that blends live action with motion capture and injects a unique video game environment, including characters from one or more video games, into music videos: August 26, 2005.
 - The Used's "Take It Away" was animated with the gaming environment from *SWAT 4*.
 - Taking Back Sunday's "This Photograph is Proof" was animated with the gaming environment from *Silent Hill 3 & 4*.
 - The Killers' "Mr. Brightside" was animated with the gaming environment from *Lineage 2*.
 - Queens of the Stone Age's "Little Sister" was animated with the gaming environment from *Indigo Prophecy*.
 - An encore of Franz Ferdinand's hit "Take Me Out" is animated with the *Star Wars: Episode III Revenge of the Sith* video game.

- Video Mods, an MTV2 show, presented three new and one previously aired animated MTV video that blends live action with motion capture and injects a unique video game environment, including characters from one or more video games, into the music videos: July 22, 2005.
 - The Beastie Boys “Oh Word” is inserted into an *NBA Street V3* environment.
 - The Blink 182 song “All the Small Things” is recreated with the *Spongebob Squarepants* characters.
 - The Yellowcard song “Only One” is recreated with *Medal of Honor:European Assault*.
 - My Chemical Romance’s “I’m Not Okay (I Promise)” is recreated with *Death Jr.* (replay from prior show).
- Video Mods (MTV2) presented four animated videos that blend live action with motion capture and inject a unique video game environment, including characters from one or more video games, into the music videos: June 24, 2005.
 - Franz Ferdinand’s hit “Take Me Out” is reconstructed with the *Star Wars: Episode III Revenge of the Sixth* video game.
 - Sum 41’s “Pieces” is overhauled with *Destroy All Humans!*.
 - Good Charlotte’s “Predictable” features *Darkwatch*.
 - My Chemical Romance’s “I’m Not Okay (I Promise)” is recreated with *Death Jr.*

Colloquia and Other Invited Presentations: ¹ ² ³

- *High Performance Computing* \Rightarrow *Discovery & Innovation*, Lehigh HPC Symposium 2011, Lehigh University, April, 2011.
- *Molecular Structure Determination, Cyberinfrastructure, Discovery & Innovation, Environmental Molecular Sciences Laboratory*, PNL, Richland, WA, July, 2009.
- *Enabling Discovery and Innovation via High-End Computing*, Alumni Symposium, Department of Computer Science and Engineering, University at Buffalo, April, 2009.
- *Discovery and Innovation via High-End Computational Resources*, Symposium on Computational Science, University of South Florida, Tampa, Florida, January, 2009.
- *The Cyberinfrastructure Laboratory, BioGrid'08*, a workshop of the 2008 HealthGrid Conference, Chicago, June, 2008.
- *Discovery & Innovation via Cyberinfrastructure*, University of Virginia, March 17, 2008.
- *Discovery via Cyberinfrastructure*, Clemson University, School of Computing, October 24, 2007
- *The Cyberinfrastructure Laboratory, NYS Grid, & NYSGrid.org*, University of Rochester, March 21, 2007.
- *The Cyberinfrastructure Laboratory: An Overview*, A Presentation to the NYSGrid.org Middleware Group, February 21, 2007.
- *A Status Report on NYSGrid*, New York State Workshop on Data-Driven Science and Cyberinfrastructure, Rochester, NY, January 23-24, 2007.
- *A Status Report on the Prototype NYS Grid*, New York State Workshop on Data-Driven Science and Cyberinfrastructure, Troy, NY, September 21-22, 2006.
- *Cyberinfrastructure and Molecular Structure Determination*, Department of Computer Science, University of Miami, September 27, 2006.
- *An Overview of CSNY, the Cyberinstitute of SuNY-buffalo*, New York State Workshop on Data-Driven Science and Cyberinfrastructure, Ithaca, NY, July 11-12, 2006.
- *Molecular Structure Determination, Grid Computing, and the Center for Computational Research*, Department of Computer Science and Engineering, The Ohio State University, March 16, 2006.
- *Molecular Structure Determination on the Grid*, Department of Computer Science, State University of New York at Albany, Albany, NY, December 8, 2005.
- *Grid Computing and Buffalo's Center for Computational Research*, Workshop on Conformal Computing, SUNY-Albany, October 14-15, 2005.
- *ACDC-Grid Monitoring: A Hand's-On Tutorial*, Workshop on Conformal Computing, SUNY-Albany, October 14-15, 2005.
- *Shake-and-Bake, Grid Computing, and Visualization*, University of Tennessee, Knoxville, TN, August 26, 2005.

¹Note: Invited presentations that resulted in a publication appear in earlier sections of this vita.

²Note: Colloquium talks given in the Department of Computer Science (and Engineering), SUNY-Buffalo, have been omitted.

³Note: Presentations at SUNY-Buffalo concerning the creation of the Center for Computational Research have been omitted.

- *High-Performance Computing and High-End Visualization in Buffalo*, Oak Ridge National Laboratory, August 25, 2005.
- *The Center for Computational Research: High-End Computation & Visualization and Grid Computing*, Ontario R&E Summit, Toronto, Canada, June 14, 2005.
- *Molecular Structure Determination and the ACDC Computational and Data Grid*, Brown University, Department of Computer Science, May 20, 2005.
- *High-Performance Computing in Buffalo*, San Diego Supercomputing Center, May 9, 2005.
- *Data Driven Computing*, Brown University, April 21, 2005.
- *The Center for Computational Research: Grid, Visualization, and BioMedical Computing*, AMDeC (Academic Medicine Development Company), Columbia University, September 29, 2004.
- *The Center for Computational Research & Grid Computing, CCR-SHARCNET Retreat*, Buffalo, September 22, 2004.
- *Computational and Data Grids*, SHARCNET Annual General Meeting 2004, Keynote Presentation, The University of Waterloo, Ontario, June 24, 2004.
- *The Center for Computational Research (CCR): An Overview*, IBM, Cambridge, MA, June 17, 2004.
- *An Overview of High-Performance Computing at the University at Buffalo*, Equality Club, WNY YMCA, Paddock Chevrolet Golf Dome, Tonawanda, NY, May 7, 2004.
- *The Center for Computational Research*, University Advancement, Center for Tomorrow, SUNY-Buffalo, March 5, 2004.
- *The Center for Computational Research*, Buffalo Niagara & Silicon Graphics, SUNY-Buffalo, February 26, 2004.
- *The Advanced CCR Data Center ACDC Grid*, NIH Program Project Presentation, The Hauptman-Woodward Medical Research Institute, January 15, 2004
- *The Center for Computational Research*, Power Computing with the SUNY-Buffalo, infoTech Niagara, December 1, 2003.
- *Grid-Enabled Shake-and-Bake*, Albany NanoTech School of NanoSciences & NanoEngineering, SUNY-Albany, September 25, 2003.
- *CCR: Now & the Future*, UB Alumni 50 Year Reunion Celebration, Buffalo, NY, June 20, 2003.
- *Enabling Collaborative Science Through Grid Technology*, Executive IT Life Science Forum, Boston, MA, June 4-5, 2003.
- *Supercomputing and Visualization*, Technical Societies Council of the Niagara Frontier, SUNY-Buffalo, March 8, 2003.
- *Center for Computational Research: FSEC Status Report*, University at Buffalo Faculty Senate Executive Committee Meeting, February 26, 2003.
- *Buffalo Center of Excellence in Bioinformatics*, Bioinformatics Grid Workshop, Southeastern Universities Research Association (SURA), January 29, 2003.
- *A Career in Computing*, Career Day, Williamsville East High School, January 10, 2003.

- *An Overview of the Center for Computational Research and the Center of Excellence in Bioinformatics*, SEAS Dean's Council, Center for Computational Research, October 24, 2002.
- *The Center for Computational Research: An Overview*, Irish Delegation, Center for Computational Research, October 7, 2002.
- *The Center of Excellence in Bioinformatics*, Delivering Technology Leadership for Life Sciences: Research Advances for Drug Discovery and Bioterrorism, Delaware Biotechnology Institute, October 3, 2002.
- *The Center for Computational Research: An Overview*, Presentation for Administration and Faculty, McMaster University, September 26, 2002.
- *Center for Computational Research*, IDC HPC User Forum on Earth and Space Science, Portland, ME, September 9-11, 2002.
- *Buffalo's Bioinformatics Initiative*, Central Park Men's Club, April, 2002.
- *Career Day*, Williamsville East High School, January 11, 2002.
- *Brief Overview of CCR*, Presentation for Sen. Schumer, December 10, 2001.
- *Computation and Applied Sciences*, SUNY-Albany, May 11, 2001.
- *Career Day*, Williamsville East High School, January 5, 2001.
- *Buffalo Byte Belt*, January 4, 2001.
- *RIT*, Administrative Personnel, October 5, 2000
- *Science Day 2000*, Capitol Hill, Washington D.C., July 12, 2000.
- *High-School Workshop on Computational Chemistry*, July 6, 2000.
- *Life Sciences Symposium*, SGI, Mt. View, CA, March 28-29, 2000.
- University of Rochester, Department of Computer Science, Jan 23, 2000.
- The Buffalo Sun Ultra5 Cluster, *HPC Consortium Meeting*, SC99, November 14, 1999, Portland, Oregon.
- Parallel Computing in Education Consortium, Ohio Supercomputer Center, Columbus, Ohio, October 8, 1999.
- JPC4-5 "Beowulf and Beyond", The Fifth Joint DOE/NASA PC Clustered Computing Conference, Oak Ridge, Tennessee, October 6-8, 1999.
- The Association of Old Crows, Niagara Frontier Chapter, September 23, 1999.
- HPCU99, SUNY Stony Brook, August 17-19, 1999.
- Campus2000, Columbia University, 1999.
- State University of New York at Geneseo, 1999.
- Campus2000, Boston University, 1999.
- Argonne National Laboratory, Mathematics and Computer Science Division, 1998.
- Country Parkway Elementary School, Career Day, 1998.

- Argonne National Laboratory, Mathematics and Computer Science Division, 1997.
- State University of New York at Buffalo, Department of Physiology and Biophysics, 1997.
- Science Alumni Association, State University of New York at Buffalo, 1997.
- Pennsylvania State University, Department of Computer Science and Engineering, 1997.
- Argonne National Laboratory, Crystallographic Software Workshop, August, 1996.
- Old Dominion University, Department of Computer Science, 1995.
- Brock University (St.Catharines, Ontario), Department of Computer Science, October, 1994.
- Calspan Advanced Technology Center, October, 1994.
- New Jersey Institute of Technology, Department of Computer and Information Science, September, 1994.
- 12th Annual Computer and Information Sciences Lecture, co-sponsored by Niagara University and the Niagara Frontier Chapter of the Association for Computing Machinery, Niagara University, 1993.
- *Symposium on Challenges for Direct Methods of Crystallography in the 21st Century*, Buffalo, New York, Oct. 1-4, 1992.
- University of Delaware, Department of Computer Science, November, 1992.
- Pittsburgh Supercomputing Center, November, 1992.
- Carleton University (Ottawa, Canada), School of Computer Science, November, 1991.
- State University of New York at Geneseo, Department of Computer Science, April, 1991.
- University of Washington, Department of Computer Science, November, 1990.
- Carleton University (Ottawa, Canada), School of Computer Science, October, 1990.
- Kent State University, Department of Mathematical Sciences, April, 1990.
- State University of New York at Binghamton, Department of Mathematical Sciences, April, 1990.
- State University of New York at Buffalo, Department of Biophysics, September, 1989.
- State University of New York at Geneseo, Department of Computer Science, November, 1989.
- State University of New York at Buffalo, Graduate Group in Advanced Scientific Computing, 1988 (2), 1989 (2).
- Supercomputing Research Center, Lanham, Maryland, May, 1988.
- Niagara Frontier Chapter of the Association for Computing Machinery (NFC/ACM), March, 1988.
- Supercomputing Research Center, Lanham, Maryland, 1986.
- Ohio State University, Department of Computer Science, 1985.
- Purdue University, Department of Electrical Engineering, 1985.
- Rensselaer Polytechnic Institute, Department of Computer Science, 1985.

- Sperry, Reston, Virginia, 1985.
- State University of New York at Albany, Department of Computer Science, 1985.
- University of Kentucky, Department of Computer Science, 1985.
- University of Minnesota, Department of Computer Science, 1985.
- University of North Carolina at Chapel Hill, Department of Computer Science, 1985.

Departmental Committees (SUNY-Buffalo):

1. Grievance Committee (2010-2012 (Chair))
2. Brochure Committee (2009-2010)
3. Student Awards Committee (2007)
4. Alumni Speakers Selection Committee (2006)
5. Development and Outreach for CSE Retreat (2005)
6. Development Committee (1998-1999)
7. Distinguished Speaker Committee (2003-2004 (Chair), 2008-2009 (Chair))
8. Alumni Relations Committee (1998-1999 (Chair))
9. Teaching Quality Committee (1997-1998, 1998-1999)
10. Faculty Search Committee (1985-1986 (Chair), 1991-1992, 1996-1997 (Chair), 1998)
11. Graduate Affairs Committee (1985-1989, 1993-1995)
12. Facilities Committee (1986-1992, 1993-1994, 1996-1997, 1998-1999, 2000-2009)
13. Publications Committee (2004-2005)
14. Graduate Admissions Committee (1987-1988)
15. Undergraduate Affairs Committee (1989-1992)
16. RDF Expenditures Committee (1988-1989, 1989-1992 (Chair))
17. Computing Assessment Study Committee (1989-1990)
18. CISE Infrastructure Committee (1990-1992)
19. Library Committee (1991-1992 (Chair))
20. Colloquium Committee (1994-1996 (Chair))
21. Strategic Recruiting Committee (1999, Chair)

University Committees/Activities (SUNY-Buffalo):

1. Member, Furnas Scholar Athlete Award Committee (2003-2011)
2. Member, Information and Computing Technology Committee, UB 2020 (2005-2006)
3. Member, Internal Advisory Board, NIH National Program of Excellence in Biomedical Computing, pre-Center (2003-2004)
4. Member, Intercollegiate Athletic Board (2003-2006)
5. Participant, Faculty Development Program (1985)
6. FNSM (Faculty of Natural Sciences and Mathematics) Computing Committee (1987-1991)
7. FNSM Early Graduate Admissions Committee (1987-1989)

8. Co-founder: Interdisciplinary Graduate Group in Advanced Scientific Computing (1988)
9. Associate Director, Graduate Group in Advanced Scientific Computing (1988-1991)
10. Charter member, Graduate Group in Crystallography (1990-1991)
11. FNSM Search Committee for Chair of the Department of Computer Science (1989-1990)
12. Undergraduate Grievance Pool (1991-1992)
13. Graduate Grievance Pool (1991-1992 (Alternate))
14. Advocate in Tenure Case (1992-93)
15. Elected Personnel Committee (1995-1997, 1998-1999 (alternate))
16. Ad-Hoc Task Force on High-Performance Research Computing (1997-1998 (Chair))
17. UB/IBM Planning Session, Participant, 1999.
18. Faculty Research Advisory Council, Member, 1999-2000.
19. Bioinformatics Search Committee, 2001.
20. Buffalo Niagara Center of Bioinformatics Teams, "Industrial Partners, Informatics" (2001, co-chair)
21. Mentor, Honor's Program, 2001-2003.
22. Member, Search Committee, Electrical Engineer, Facilities Programming and Design, 2003.

Professional Service

Editorial Responsibilities

- Member of the IEEE CS Fellows Evaluation Committee, 2012.
- Associate Editor, *International Journal of Teaching and Case Studies*, 2007 - present.
- Member of the editorial board of *Parallel Processing Letters*, 1991 - present.
- Co-editor, with A. Schuster, Technion, Israel, for a special issue of *Parallel Processing Letters* on Dynamically Reconfigurable Architectures, vol. 5, no. 1, March, 1995.

Technical Committees

- Member of the *Advisory Committee* for the *IEEE Technical Committee on Parallel Processing*, 1997 - present.
- Member of the *Executive Committee* for the *IEEE Technical Committee on Parallel Processing*, 1992 - 1999. Co-ordinator for parallel processing education. Member of nomination committee.

Funding Panels:

- Panel Member, Department of Energy, Scientific Discovery through Advanced Computing (SciDAC), 2011.
- Panel Member, Cyber-Enabled Discovery and Innovation, National Science Foundation, 2009.
- Panel Member, Science Foundation Ireland, 2008.
- Panel Member, CLuE Bio Panel, National Science Foundation, 2008.
- Panel Member, Cyber-Enabled Discovery and Innovation, National Science Foundation, 2008.
- Chair of Programme Assessment Panel for Science Foundation Ireland (SFI), Irish National Centre for High Performance Computing (ICHEC), 2005.
- Reviewer for Science Foundation Ireland, National Centre for High Performance Computing, 2004.
- Chair of National Science Foundation committee for TeraGrid (ETF/Core) Panel Review, 2004.
- Reviewer for Science Foundation Ireland, Research Professors, 2003.
- Chair of the National Science Foundation review committee for *Partnerships for Advanced Computational Infrastructure (PACI)*, 2003.
- Chair of the National Science Foundation review committee for *Partnerships for Advanced Computational Infrastructure (PACI)*, 2002.
- Chair of the *Extensible Terascale Facility (ETF)* for the Partnerships for Advanced Computational Infrastructure (PACI) program, 2002.
- Chair of the *Committee of Visitors (COV)* for the Partnerships for Advanced Computational Infrastructure (PACI) program, 2002.
- Chair of the National Science Foundation review committee for *Partnerships for Advanced Computational Infrastructure (PACI)*, 2001.

- Member of National Science Foundation panel for the *Distributed Terascale Facility*, 2001.
- Member of the National Science Foundation review committee for *Partnerships for Advanced Computational Infrastructure (PACI)*, 2000.
- Chair of the National Science Foundation panel and member/chair of the site visit team for the *Terascale Computing System*, 2000.
- Member of the National Science Foundation review committee for *Partnerships for Advanced Computational Infrastructure (PACI)*, 1999.
- Member of the National Science Foundation panel on *Experimental Software Systems*, 1998.
- Member of the National Science Foundation review committee and site visit team for *Partnerships for Advanced Computational Infrastructure (PACI)*, 1996.
- Member of the National Science Foundation CISE Instrumentation Panel, 1988.

Advisory Councils:

- Member, Advisory Council for the Computational Center for Nanotechnology Innovations, Rensselaer Polytechnic Institute, 2006.
- Teragrid “Red Team” Review, September, 2004.
- Advisory Council to the Center for Integrated Biological, Chemical, and Technical Sciences, Niagara University, member, 2004-present.
- Shared Hierarchical Academic Research Computing Network (SHARCNET) High Performance Computing Strategic Council, 2003-present.
- Member of the SGI Innovator Program, charter member with 5 others from around the U.S., 2003.
- Member of the Dell HPCC Advisory Council, 2003.
- Member of the AAAS “National Workshop on Developing Guidance for NSF Advanced Networking Infrastructure Support,” 1999.

Evaluations:

- Department of Computer Science graduate program, Kent State University, 2004.
- AAAS Research Competitiveness Proposals for University Initiatives, 2004.

Conference Participation:

Program Committee

- Member of the program committee for *BioGrid’08*, a workshop of the 2008 HealthGrid Conference, Chicago, June, 2008.
- Member of the program committee for *BioGrid’07*, a workshop at *CCGrid07, Seventh IEEE International Symposium on Cluster Computing and the Grid - CCGrid 2007*, Rio de Janeiro, Brazil, May, 2007.
- Member of the program committee for the 19th *ISCA International Conference on Parallel and Distributed Computing Systems (PDCS 2006)*, 2006.

- Member of the program committee for *International Workshop on Scientific Instruments and Sensors on the Grid*, in conjunction with *eScience 2005, 1st IEEE International Conference on e-Science and Grid Computing*, Melbourne, Australia, December 5, 2005.
- Member of the steering committee for *BioGrid'06*, a workshop at *CCGrid2006, 6th IEEE/ACM International Symposium on Cluster Computing and the Grid*, Singapore, Japan, May, 2006.
- Member of the program committee for IPDPS'2006, the *International Parallel and Distributed Processing Symposium*, Rhodes, Greece, April, 2006.
- Member of the program committee for the 18th *ISCA International Conference on Parallel and Distributed Computing Systems* (PDCS 2005), 2005.
- Member of the program committee for *BioGrid'05*, a workshop at *CCGrid2005, 5th IEEE/ACM International Symposium on Cluster Computing and the Grid*, Cardiff, UK, May 9-12, 2005
- Member of the program committee for *BioGrid'04*, a workshop at *CCGrid2004, 4th IEEE/ACM International Symposium on Cluster Computing and the Grid*, Chicago, Illinois, April 19-22, 2004.
- Member of the program committee for *BioGrid'03*, a workshop at *CCGrid2003, 3rd IEEE/ACM International Symposium on Cluster Computing and the Grid*, Tokyo, Japan, May 12-15, 2003.
- Member of the program committee for the ICPP Workshop on High Performance Scientific and Engineering Computing with Applications, Toronto, Canada, 2000.
- Member of the program committee for *SUPER*CAN HPSC '96*, the 10th annual Conference on High Performance Computers, Ottawa, Canada, 1996.
- Member of the program committee for the *3rd Workshop on Reconfigurable Architectures*, as part of the *IEEE Tenth International Parallel Processing Symposium*, Hawaii, 1996.
- Member of the program committee for the *Seventh International Conference on Parallel and Distributed Computing and Systems*, Washington, D.C., 1995.
- Member of the program committee for the *2nd Workshop on Reconfigurable Architectures*, as part of the *IEEE Ninth International Parallel Processing Symposium*, Santa Barbara, California, 1995.
- Member of the program committee for the *12th International Conferences on Pattern Recognition*, Jerusalem, Israel, October, 1994.
- Member of the program committee for the *IEEE Eighth International Parallel Processing Symposium*, Cancun, Mexico, April, 1994.
- Member of the program committee for *Frontiers '92: The Fourth Symposium on Frontiers of Massively Parallel Computation*, Tyson's Corner, Virginia, October, 1992.
- Member of the program committee for the *International Conference on Computing and Information*, Ottawa, Canada, May, 1991.

Session Chair

- Session chair, *Second International Workshop on Semantic and Grid Computing (SGC07)*, The Fifth International Symposium on Parallel and Distributed Processing and Applications (ISPA-2007), Niagara Falls, ON, August, 2007.
- *New Trends in High Performance Computing*, Stony Brook, NY, August, 1999.
- *Fourth IEEE Symposium on Parallel and Distributed Processing*, Arlington, Texas, December, 1992.
- *1991 International Conference on Parallel Processing*, St. Charles, Ill.
- *The Fifth Distributed Memory Computing Conference*, Charleston, South Carolina, April, 1990.
- *1988 International Conference on Parallel Processing*, St. Charles, Ill.

- 1987 *International Conference on Parallel Processing*, St. Charles, Ill.

Panel Discussion

- Invited Panelist, *National Science Foundation Symposium: "Cyber-Enabled Discovery and Innovation"*, Albany, New York, Sept 5-6, 2007. Topic: "Education Issues of CDI." (The panel moderator is Lenore M. Mullin, National Science Foundation. The other panelists are Steven Gordon, Ohio Supercomputer Center, Prabhat Hajela, Rensselaer Polytechnic Institute, and John Sasso, New York State Office of Technology.)
- Invited Panelist, *GT'04 The Premier Enterprise Grid Computing Conference*, Philadelphia, Pennsylvania, May, 2004. Topic: "Storage Considerations for Grid Computing Environments." (The panel moderator is William Hurley, Senior Analyst, Enterprise Strategy Group. The other panelists are Kevin Deierling, Vice President, Product Marketing, Mellanox Technologies and Bruce Moxon, Chief Solutions Architect, Panasas.)
- Invited Panelist, *SC2003*, Phoenix, Arizona, November, 2003. Topic: "The Simplification of Supercomputing: Clustering, Appliances and Grid Computing"; Talk: "The WNY Bioinformatics Grid" (The other panelists were Marshall Peterson, CTO of the J. Craig Venter Science Foundation, Steve Oberlin, Founder and CEO of Unlimited Scale, Dr. Andrew Grimshaw, Founder and CTO of Avaki, and Mark Seager, Assistant Department Head for Terascale Systems, Lawrence Livermore National Laboratory. The chair was Bill Blake, SVP of Product Development, Netezza Corp.)
- Moderator, *The 9th International Parallel Processing Symposium*, Santa Barbara, California, April, 1995. Topic: "Different Approaches to Parallel Computing Education" (The panelists were Daniel C. Hyde, Bucknell University, David Kotz, Dartmouth College, Gordon Makinson, University of Kent, P. Takis Metaxas, Wellesley College, and Nan C. Schaller, Rochester Institute of Technology.)
- Moderator, *The 8th International Parallel Processing Symposium*, Cancun, Mexico, April, 1994. Topic: "The Right Stuff? Teaching Parallel Computing" (The panelists were Janet Hartman, Illinois State University, Elizabeth R. Jessup, University of Colorado at Boulder, Trevor Mudge, University of Michigan, John R. Nickolls, MasPar Computer Corporation, Ralph Roskies, Pittsburgh Supercomputing Center, and Nan C. Schaller, Rochester Institute of Technology.)
- Panelist, *The 8th International Parallel Processing Symposium*, Workshop on Reconfigurable Architectures, Cancun, Mexico, April, 1994. Topic: "The Future of Reconfigurable Architectures" (The panel chair was Hussein Alnuweiri, University of British Columbia, Canada, and the other panelist was Hossam ElGindy, University of Newcastle, Australia.)
- Invited panelist, *The 4th Symposium on the Frontiers of Massively Parallel Computation*, McLean, Virginia, October, 1992. Topic: "Issues on the Algorithm-Software Continuum" (The other panelists were Mike Atallah, Purdue University, Jan Cuny, University of Massachusetts, Amherst, Dennis Gannon, Indiana University, Joseph Ja'Ja', University of Maryland, and Virginia Lo, University of Oregon. The panel chair was Leah Jamieson, Purdue University.)
- Panelist, *From Pixels to Features II: Parallelism in Image Processing*, ESPRIT BRA 3035 Workshop, Bonas, France, August, 1990. Topic: "Parallel Architectures: A Moving Target" (The other panelists were Robert Hummel, New York University, Hans Burkhardt, Technische Universität Hamburg-Harburg, and Wolfgang K. Giloi, GMD-TUP FIRST, Berlin. The moderator was Lewis W. Tucker, Thinking Machines Corporation.)
- Invited panelist, 1986 *University of Rochester Computer Science Conference*, Topic: "General Purpose Parallel Computing" (The other panelists were Azriel Rosenfeld, University of Maryland, and R.C. Holt, University of Toronto. The moderator was Jerome Feldman, University of Rochester.)

Workshop/School Participation:

- Instructor, International School of Crystallography, *25th Course: Direct Methods of Solving Macromolecular Crystal Structures*, “Parallel Computing and Crystallography,” “*Shake-and-Bake: Applications and Advances*,” and “Tutorial: *Shake-and-Bake* using *SnB*,” Erice, Sicily, 1997.
- Instructor, *Computational X-Ray Crystallography Workshop*, Pittsburgh Supercomputing Center, July 24-27, 1994. The focus of the workshop was on *SnB* and X-PLOR. The other instructors were Herbert A. Hauptman, Medical Foundation of Buffalo, and Axel Brünger, Yale University.
- *Summer Workshop for Supercomputing* (1986), Supercomputing Research Center, Washington, D.C.

Reviewing:

- Reviewer for the following journals:
 - *IEEE Transactions on Computers (IEEE-TC)*
 - *IEEE Transactions on Pattern Analysis and Machine Intelligence (IEEE-PAMI)*
 - *IEEE Transactions on Software Engineering (IEEE-TSE)*
 - *IEEE Transactions on Parallel and Distributed Systems (IEEE-TPDS)*
 - *Journal of the Association of Computing Machinery (JACM)*
 - *Computer Vision, Graphics, and Image Processing (CVGIP)*
 - *Parallel Processing Letters (PPL)*
 - *Information Processing Letters (IPL)*
 - *Algorithmica*
 - *Journal of Parallel and Distributed Computing (JPDC)*
 - *Journal of Supercomputing*
 - *Machine Vision and Applications*
 - *SIAM Journal on Computing (SIAMJC)*
 - *Journal of Algorithms*
 - *Journal of Pattern Recognition and Artificial Intelligence*
 - *The Computer Journal*
 - *Acta Crystallographica*
- Reviewer for the following conferences:
 - *Distributed Memory Computing Conference (DMCC)*
 - *(IEEE) International Conference on Parallel Processing (ICPP)*
 - *IEEE International Symposium on Computer Architecture (ISCA)*
 - *International Parallel Processing Symposium (IPPS)*
 - *International Conference on Supercomputing (ICS)*
 - *IEEE Symposium on Parallel and Distributed Processing*
 - *Frontiers of Massively Parallel Computation (Frontiers)*
 - *International Conferences on Pattern Recognition*
 - *International Conference on Computing and Information (ICCI)*
- Reviewer of books for the following publishers:
 - McGraw-Hill
 - Academic Press
 - PWS-Kent
 - The MIT Press
- Reviewer of proposals for the following agencies:
 - National Science Foundation (NSF)
 - Air Force Office of Scientific Research (AFOSR)
 - Natural Sciences and Engineering Research Council of Canada (NSERC)

Teaching:

State University of New York at Binghamton

- *Undergraduate Courses Taught:*
 - Computer Programming I
 - Computer Programming II
 - Data Structures
 - Independent Study: Microcomputers
- *Graduate Courses Taught:*
 - Independent Study: Software Engineering
 - Independent Study: Data Structures

State University of New York at Buffalo

- *Undergraduate Courses Taught:*
 - Introduction to Scientific Computing (1995, with Eberlein and Pitman)
 - Analysis of Algorithms (1986, 1987, 1988 (2 sections), 1996, 1997, 2010, 2011, 2012)
 - Advanced Data Structures (1989, 1990, 1991 (2 sections))
 - Data Structures (2009)
 - Independent Studies, including Cluster Computing (1999, 2000), High-Performance Computing (2000), Registering and Downloading on the World Wide Web (1996), Monitoring a Distributed System (1991), X-Ray Crystallography on Parallel Machines (1989, 1990), Intermediate-Level Image Processing on Distributed-Memory Machines (1989, 1990), and The Intel iPSC/2 Operating System (1988).
- *Graduate Courses Taught:*
 - Theory of Computation (1985)
 - Analysis of Algorithms (1986, 1987, 1988, 1994, 1996, 1997, 2010, 2011, 2012)
 - Introduction to Parallel Algorithms (1986, 1987, 1988, 1989, 1990, 1992, 1995, 2007, 2008, 2009, 2010)
 - Special Topics: Cyberinfrastructure (2007)
- *Seminars Directed:*
 - High-End Computing (2012)
 - Cyberinfrastructure (2006, 2007, 2008, 2011)
 - Grid Computing (2003, 2004, 2005)
 - Cluster Computing (2000)
 - Introduction to the World Wide Web (1997)
 - Optimization Algorithms (1994, with Eberlein)
 - Parallel Computing (1989, 1994 (with Eberlein))
 - Parallel Algorithms and Architectures for Image Analysis (1992)
 - Minimization Techniques and Parallel Computing (1991)

- Computational Geometry (1990)
- Advanced Scientific Computing (1988, with Eberlein, Furlani, Kazarinoff, King, McIver, Zubrow)
- Hypercube Multiprocessors (1987-1988, with Eberlein)
- Hypercubes (1986-1987, with Eberlein)
- Parallel Algorithms (1986)

Other Teaching Activities:

- Designed and Introduced CSE514: Cyberinfrastructure, 2007.
- Designed, Introduced, and Refined, CSE712: Grid Computing, 1998-pres.
- Introduced experimental cluster computing into CSE633: Parallel Algorithms, 2006.
- Designed and Introduced CS633: Parallel Algorithms, 1985-1986.
- Co-Designed and Introduced CS350: Advanced Data Structures, 1985-1989.
- Co-Designed CS515: Introduction to Parallel Computing, 1991-1992.
- Co-Designed and Introduced CS237: Introduction to Scientific Computing, 1993-1994.
- Co-Initiated Advanced Certificate in Computational Science.
- Co-Initiated COR 501: Introduction to High-Performance Computing I.
- Co-Initiated COR 502: Introduction to High-Performance Computing II.

Student Supervision:⁴

Post-Doctoral Students:

- Hongliang (Jimmy) Xu, Direct Methods Crystallography, 1997-1999.
- Mark L. Green, Grid Computing, 2002-2004.
- Henrique Bucher, Grid Computing & Traffic Simulation, 2004-2005.

Major Professor for Ph.D. Students:

- C.-S. Chang, "Structure Determination Algorithms in Computational X-Ray Crystallography," 1994.
- Yanina Vekhter, "Application of the Two-Channel Maximum Entropy Method for the Reconstruction of Electron Density, The Phase Extension Procedures Coupled to the Isomorphous Replacement Method," 2000.
- Ioana Sirbu, "A Perturbation Approach to the Electron Correlation Cusp," 2002.

Committee Member for Ph.D. Students:

1. Cesar Bandera, "Computer Vision Using Fovial Space-Variant Sampling," Electrical and Computer Engineering, 1990.
2. Anil Shende, "Digital Analog Simulation of Uniform Motion in Representations of Physical n -Space by Lattice-Work MIMD Computer Architectures," 1991.
3. S. Sunder, "Parallel Algorithms for Scheduling Problems," 1994.
4. C.-H. (Vincent) Huang, "Communication-Efficient Bulk Synchronous Parallel Algorithms," 2001.

M.S. Students with Thesis:

1. Laurence Boxer, "Parallel Algorithms for Dynamic Computational Geometry," 1987.
2. Pam Thuman, "Solutions to the Phase Problem of X-Ray Crystallography on a Variety of Parallel Machines," 1992.
3. Catherine L. Ruby, "Three Data Grid Initiatives for the Advanced Computational Data Center," 2006.

M.S. Students with Projects:

1. Susan E. Miller, "Hypercube Algorithms for Determining Geometric Properties of Digitized Pictures," 1987.
2. Norm Wahl, "Component Labeling on the Intel Hypercube," 1987.
3. Mark Gunning, "The All-Nearest Neighbor Problem on an Intel iPSC/1 Hypercube," 1987.
4. Elias Sarraf, "Convexity Algorithms for Planar Point Data on the Intel iPSC," 1988.
5. Diane Wise, "Computing the Voronoi Diagram on a Shared-Memory Machine," 1988.
6. Rick Fenrich, "NP-Hard Packing Problems on the Intel iPSC/2 Hypercube," 1989.

⁴Unless otherwise indicated, degrees were awarded from the Department of Computer Science (and Engineering).

7. Steve Gallo, "*SnB*: Portability and User Interface," 1996.
8. Martins Innus, "Scientific Visualization," 2001.

Undergraduate Research Students Supervised:

John Delgado (1988), Jeff Horvath (1989), Pam Thuman (1990), Noushin Bashir (1990), Todd Sabin (1990), Babak Falsafi (1990), Marc Poulin (1992), Steve Gallo (1993), Thomas Tang (1997), Adam Fass (1998), David Walia (2003-2004), Mark Cianchetti (2003-2004), Catherine Ruby (2003-2004), Noah Milman (2006-2007), Matt Lehner (2005-2007)

Major Community Service (Non-Professional)

1. Co-Chair, Fox Valley Club Handicap Committee, 2011.
2. Member, Fox Valley Club Grounds Committee, 2011.
3. Manager, Lou Gehrig Little League, 1993-1999.
4. Manager, Mathewson-McCarthy Little League, 2000-2003.
5. Head Coach, Amherst Youth Basketball, 1997-2004.
6. Board of Directors, Amherst Youth Basketball, 1998-present.
7. President, Amherst Youth Basketball, 1999-2005.
8. Head Coach, WNY Warriors AAU Travel Basketball, 2002-2004.
9. President, WNY Warriors AAU Basketball Organization, 2002-2004.

Commercial Software Packages:

- 1980: A surveying package was developed for Benro Survey Ltd., Huntington, New York. This package allowed surveying firms to produce more efficient and more accurate bids that met New York State specifications.
- 1981: A cargo and driver protection package was developed for Elk Routemaster, Inc., Farmingdale, New York. This software package, coupled with the Routemaster hardware, disables a vehicle that deviates from its predetermined route. Further, the cargo doors of a vehicle equipped with the Routemaster system cannot be opened unless the vehicle is at a predetermined destination. This package has been used on shipments by trucking companies transporting tobacco and by the United States Postal Service.
- 1982: A package combining inventory control, automated mailings, and customer selection was developed for the Sound Approach, Inc., an audio store in Commack, New York.
- 1994: *SnB* is a molecular structure determination package developed jointly with members of the Hauptman-Woodward Medical Research Institute (HWI). This package, which is based on our *Shake-and-Bake* method of structure determination, has proven to be quite effective in solving molecular structures containing up to 2500 non-hydrogen atoms in the asymmetric unit cell, given atomic resolution data, and up to 200 Se atoms used to solve 600 kDa structures given Se-Met data. *SnB* has been distributed to more than 500 laboratories worldwide. For more details, please see <http://www.hwi.buffalo.edu/SnB/>.
- 2002: *BnP* is The Buffalo 'n Pittsburgh Interface for complete protein phasing. It combines the *SnB* structure determination package with the Bill Furey's PHASES suite of routines. *BnP* provides a seamless interface between *SnB* and other crystallographic software. This interface provides a coordinated control of several steps in the protein structure determination pathway, and it facilitates a high degree of automation. The package has been made available for single processor, multiprocessor, cluster, and grid computing environments. It runs under the SGI, Linux, and Mac OS X platforms.

Center for Computational Research (CCR)

In the 21st century, leading academic institutions will embrace the digital data-driven society that we live in and empower their students to compete in our knowledge-based economy. In order to support research, scholarship, education, and community outreach, institutions must be prepared to deliver high-end cyberinfrastructure that will enable the efficient collection, management, organization, analysis, and visualization of data.

Through Dr. Miller's vision and foresight, and with support of strong University leadership, the Center for Computational Research was established in 1998. Dr. Miller served as (founding) Director from 1998–2006. CCR providing a competitive advantage for the faculty, students, and staff at the University, as well as the WNY community. One only needs to look at funding, recruiting, government relations, and community outreach to see the enormously positive impact that CCR had on the University and the Western New York region.

The mission of CCR was to 1) enable Research and Scholarship, 2) provide Education, Outreach, and Training, and 3) effect Technology Transfer to local industry in areas that require high-end computing, storage, networking, and visualization.

- **Founding Director.** The Director was responsible for oversight, planning, and budgetary decisions of the Center. The mission of CCR was to enable world-class computationally-intensive research (*i.e.*, research that requires high-performance computing and high-end visualization) at the University, thereby improving the reputation of UB in WNY/NYS, the national stature of the University, and the rankings of programs in computationally-intensive areas. This was accomplished by
 - providing state-of-the-art resources and support to high-technology computationally-intensive research projects,
 - providing opportunities for industrial partnerships that include access to center resources, including CPU cycles, high-end visualization hardware and software, application software, and technical consulting, and
 - serving as a focal point for technology transfer within the UB/WNY community by offering seminars, workshops, and courses on high-performance computing, computer modeling and simulation.

While the initial mission of CCR was to provide high-performance computing to UB faculty with computationally-intensive research programs, the Director worked with the UB administration and CCR staff to greatly enhance the mission of CCR to include economic development in WNY, education and outreach, increased funding, and national visibility for UB.

- **Research and Scholarship Supported.** CCR annually supported on the order of 140 research groups spanning approximately 40 departments at UB, as well as 20 external groups. This extensive coverage included traditional computational science and engineering disciplines, nontraditional disciplines (classics, art, media study, and so on), local institutions (RPCI, HWI, Children's Hospital, Buffalo General Hospital, Niagara College, Brockport, Columbia, U. Rochester, Geneseo, RIT, U. Toronto), and local and national industry (MTV, Q-Chem, Bergmann, Parsons, Praxair, TVGA, NYSTA, IBC Digital, eMedia, First Interstate Data, Veridian, Tops Markets, etc.).
- **CCR-Based Funding:** In excess of \$300M of external funds were brought into the University, and \$400M into the Western New York region, for which either CCR staff had a lead scientific role, projects relied on CCR resources, vendors provided in-kind donations to CCR, or CCR staff played a major role in the acquisition of funds. Funding agencies included NSF, NIH, NIMA, EPA, and NASA, to name a few. Vendor contributions came from Dell, SGI, IBM, Sun Microsystems, Alias|Wavefront, Myricom, Nortel, Platform Computing, Q-Chem, and Performance Technologies. Foundation support was provided by Oishei, Keck, and Wendt. NYS support, led by Governor Pataki and Assembly Speaker Sheldon Silver, was provided for a number of CCR-centric activities, including the Center

of Excellence in Bioinformatics and High-End Visualization. Federal support, led by Congressman Thomas M. Reynolds, Senator Hillary Rodham Clinton, and Senator Charles E. Schumer, was also provided for CCR-centric activities.

- **Major Infrastructure.** During Miller's tenure as Director, CCR maintained 25TF of computing, 300TB of storage, and a variety of high-end visualization systems. This included the following.
 - A 2100 processor Dell Linux cluster of Myrinet-connected Irwindale processors, with a peak performance of over 13TF.
 - A 600 processor Dell Linux cluster of Myrinet-connected Pentium4 processors, which was listed in the November, 2002 top500 list as the 22nd fastest supercomputer in the world.
 - A 2000 processor Dell Linux cluster of PIII and P4 nodes connected with Ethernet.
 - A 532 processor IBM BladeCenter cluster of Intel Xeon processors.
 - A 150 processor SGI PentiumIII cluster of Myrinet connected 1 GHz chips.
 - A 64 processor SGI Altix3700 supercomputer.
 - A 78 processor IBM RS/6000 SP.
 - An 80 processor Linux/Solaris SUN Microsystems cluster.
 - An HP storage area network (SAN) with 75TB (raw) of disk and 250TB of tape.
 - A 35TB (raw) EMC Storage System.
 - A heterogeneous bioinformatics system.
 - High-end SGI Onyx2 and Onyx300 3D visual supercomputers attached to display environments including a Fakespace Immersadesk and an SGI 3300W.
 - A 20-projector tiled display wall.
 - A visDuo passive stereo display system.
 - Two access grid nodes.
- **Western New York Community Projects.** CCR provided an immersive 3D visualization of the proposed Peace Bridge and Plaza options to the public in CCR and offered videos and stills of the simulations via the CCR Web site. CCR has also worked on high-profile projects involving moving the Williamsville Toll Plaza, Accident Reconstruction, Traffic Flow and Simulation, Medical Visualization, and Scientific Simulation and Visualization. CCR worked with various government agencies to provide models and simulations of numerous projects in the Western New York Region, including TVGA, Bergmann Associates, 3DScape, the New York State Thruway Authority, Children's Hospital, The Medical Corridor, various Departments of Transportation, the Photonics Institute, Parsons, Niagara College, eMedia, and IBC Digital.
- **Education and Outreach.** Efforts in this area have been substantial.
 - CCR developed and deployed a year-long High School course in bioinformatics. This project involves Mt. St. Mary's Academy, City Honors, and Orchard Park High School.
 - CCR operated a highly successful annual summer workshop for High-School students. During 1999 & 2000, the workshop focused on Computational Chemistry, while in 2001 & 2002, the focus was on high-end visualization, and in 2003 & 2004, the focus was on bioinformatics.
 - CCR hosted students and faculty from SUNY-Brockport and SUNY-Geneseo during the Winter 1999-2000 intersession, providing an intensive workshop on high-performance computing.
 - CCR regularly provided workshops and seminars on aspects of high-performance computing of interest to our current and potential users.

- CCR hosted workshops on Bioinformatics software, computational chemistry software, and banking software.
 - CCR hosted a session of SGI's Linux University and a session of IBM's IBM SP supercomputing workshop.
 - CCR provided tours to approximately 2500 people per year. People passing through CCR include elected officials, scout troupes, elementary, middle, and high-school classes, local industry, and a wide range of interested citizens.
- **National Presence.** CCR staff were invited to give presentations at numerous national meetings, vendor-based events, high-schools, community organizations, and so forth.
 - **Publicity.** The Director interfaced with various public relations organizations on campus and faculty/industry utilizing CCR resources. On the order of 1500 news articles appeared during this period, including print and electronic media both locally and nationally. The Director represented CCR and UB on television on a wide variety of occasions.

Russ Miller: Future of Computing

In the 21st century, leading academic institutions will embrace our digital data-driven society and empower students to compete in this knowledge-based economy. In order to support research, scholarship, education, and community outreach, Miller's Cyberinfrastructure Laboratory (CI Lab) is dedicated to the integration of research in disciplinary domains, including science, engineering, economics, health care, transportation, multimedia, and national security, with research in enabling technologies and interfaces. The goal of the CI Lab is to allow end-users to transparently collect, manage, organize, analyze, and visualize data without having to worry about details such as where the data is stored, where the data is processed, or where the data is rendered. This ease of use and high availability of data and information processing tools will allow for revolutionary advances in science, engineering, and beyond.

Cyberinfrastructure sits at the core of modern simulation and modeling, enabling entirely new methods of investigation that allow scholars to address previously unsolvable problems. Specifically, the development of necessary software, algorithms, portals, and interfaces that will enable research and scholarship by freeing end-users from dealing with the complexity of various computing environments is critical to extending the reach of high-end computing, storage, networking, and visualization to the general user community.

Computational environments must be driven by disciplinary research and scholarship. In order to produce effective systems, such an approach requires 1) teams of users focused on disciplinary research and scholarship who will partner with 2) teams of computationally-focused enabling scientists and engineers, both of whom will work with 3) a team of personnel who can implement critical technical tasks. The resulting systems must be robust (hardware and software) and include easy-to-use tools for producing efficient as well as effective applications. These systems should be comfortably extended to new and non-standard user communities in an effective fashion. While there is a need to continue to focus on high-performance computing (single systems and collections of multiple heterogeneous systems), significant advances need to be made in areas that include data, visualization, interfaces, virtual organizations, education, and outreach. For example, extremely efficient and generally-applicable high-performance computing-based algorithms need to be developed that serve as building blocks to a wide variety of efficient applications by crossing disciplinary boundaries. Further, applications need to be developed using tools that will allow for ease of portability.

The Grid currently serves as critical infrastructure for most activities in cyberinfrastructure. The Grid is a rapidly emerging and expanding technology that allows geographically-distributed and independently-operated resources to be linked together in a transparent fashion. These resources include CPU cycles, data storage systems, sensors, visualization devices, and a wide variety of Internet-ready instruments.

The New York State Grid (NYS Grid) was designed and deployed under Miller's direction, following extensive efforts in developing a Buffalo-based grid (ACDC-Grid) and a Western New York Grid (WNY Grid). NYS Grid includes a heterogeneous collection of resources from institutions throughout New York State and is available in a simple and seamless fashion to users worldwide. Major features of NYS Grid include that following: it integrates a computational grid with a data grid in a simple and transparent fashion; it incorporates a Web Portal for ease-of-use; it includes a user-friendly grid monitor; and it includes a grid-enabling application template in order to expedite the porting of applications to the grid.

As we move forward, computing will serve as a magnet that is used to foster and transform transdisciplinary research to generate new knowledge from large and growing data sets, will be used to derive fundamental insights on multi-component systems, and will enhance discovery by continuing to create significant virtual organizations that cross boundaries of all varieties.

An academic institution can contribute to the ubiquitous future that computing will play in our daily lives by creating computing-centric infrastructures that are dedicated to the advancement of research, scholarship, education, and outreach in areas that can take advantage of compute, networking, visualization, storage, sensors, and a wide-variety of integrated instrumentation resources.

Under Miller's leadership while (Founding) Director of the Center for Computational Research, SUNY-Buffalo made significant advances with respect to many of these initiatives. Further, Miller provided a number of proposals to enhance cyber-enabled discovery to the SUNY-Buffalo administration. These proposals were viewed by a faculty review panel as being of top priority.

Russ Miller: Brief Biography

Dr. Miller maintains appointments as Distinguished Professor of Computer Science and Engineering at SUNY-Buffalo and senior scientist at the Hauptman-Woodward Medical Research Institute (HWI).

Dr. Miller is world-renowned for his seminal work in areas of parallel algorithms for the mesh, pyramid, hypercube, and reconfigurable architectures covering domains that include computational geometry, image analysis, and fundamental data movement operations. Miller's current focus is on cyberinfrastructure, grid computing, and molecular structure determination.

Prof. Miller's publications number approximately 200, including peer-reviewed papers, chapters, and abstracts of presentations at national or international conferences. He has also published 2 textbooks covering parallel and sequential algorithms.

Miller's work in parallel algorithms led to a collaboration with world-class scientists at the HWI working on solutions to problems in molecular structure determination. This revolutionary work produced algorithms and community codes that have been used to solve molecular structures several orders of magnitude larger than had previously been possible, as well as solving numerous structures with a wide variety of properties that were previously thought to be unsolvable. This work was recognized by the IEEE with its inclusion in the IEEE poster "Top 10 Algorithms of the 20th Century."

Dr. Miller founded the Center for Computational Research (CCR) at SUNY-Buffalo, where he served as Director from 1998-2006. During his tenure, CCR was continuously ranked as one of the leading supercomputing centers worldwide and served as a model for universities providing key infrastructure to enable 21st century discovery. On an annual basis, CCR supported nearly 140 projects covering approximately 40 academic departments, as well as projects from a variety of local and national colleges, universities, non-profit organizations, government agencies, and private sector companies.

Dr. Miller played a significant role in bringing approximately \$0.5 billion dollars to Western New York in the form of peer-reviewed funding, appropriations, and contracts. In fact, he was instrumental in the establishment of the \$290M New York State Center of Excellence in Bioinformatics. Note that in establishing the Center of Excellence in January of 2001, New York State Gov. George E. Pataki stated that "This Center [of Excellence in Bioinformatics] will, through the University of Buffalo's Center for Computational Research, create academic and industrial partnerships..."

Dr. Miller was listed on HPC Wire's 2003 *Top People and Organizations to Watch*. The computational crystallographic algorithm *Shake-and-Bake*, which is co-authored by Prof. Miller, was listed on the IEEE poster "Top 10 Algorithms of the 20th Century." Miller was elected to the European Academy of Sciences (Computer Science) in 2002 with the citation "for an outstanding and lasting contribution to parallel algorithms and computer science education" and was presented with International Scientist of the Year, Cambridge, England, in 2003.

Russ Miller: Education and Outreach

Dr. Miller has been teaching courses to graduate and undergraduate students since 1981. He has taught courses in areas that include data structures, algorithms, computational science, cyberinfrastructure, and high-performance computing. He has served on departmental teaching evaluation committees and been awarded the Best Presentation Award for a talk he gave at the 1987 International Conference on Parallel Processing. Prof. Miller has given many hundreds of presentations to professional as well as non-technical audiences, including invited talks at international conferences and workshops, as well as presentations to elected officials, cub scout troops, defense contractors, high-school AP classes, prospective students and student/athletes, citizens interested in urban planning, and so forth.

Prof. Miller has been involved in education and outreach for over 20 years. He produced a report on parallel processing education, a summary of which appears in [28], and organized a panel discussion at the 1994 *International Parallel Processing Symposium* [85]. He is currently a member of the editorial board of the *International Journal of Teaching and Case Studies*, was coordinator for parallel processing education from 1992-1999 for the *IEEE Technical Committee on Parallel Processing*, has introduced approximately 10 courses involving cyberinfrastructure, high-performance computing, and computational science, has published a number of articles on parallel processing education, has given invited talks on parallel computing education, and has organized workshops at international conferences on parallel processing education. Under Miller's leadership as Director of the Center for Computational Research, CCR offered summer workshops for high-school students, summer workshops for high-school teachers, developed a year-long High-School course in bioinformatics for a number of schools including some involving underrepresented students, has offered training sessions for faculty, students, and staff from area colleges and institutions, and organized regular workshops targeting interests of the local community, to name a few,

Dr. Miller was instrumental in the establishment and advancement of the EOT-PACI program, which focused on education, outreach, and training, predominantly in the area of computational science, high-performance computing, and high-end visualization. Miller set up similar programs through the Center for Computational Research in the Western New York area, reaching out to an all-girls school, an inner city school, a private inner city school, and a suburban school. In addition, when CCR was established, the first program that CCR hosted was a high-school workshop. This series of workshops ran for 6 consecutive years on topics that include computational chemistry, bioinformatics, and visualization.

Dr. Miller has published two textbooks in the area of parallel and sequential algorithms and has contributed a number of chapters to various collections.

Russ Miller: Research Program (1985-2007)

My research program is concerned with *i*) developing efficient parallel algorithms to solve fundamental problems on a variety of feasible parallel models of computation, *ii*) developing efficient solutions to computationally intensive problems, and *iii*) cyberinfrastructure, including the development, analysis, and deployment of critical middleware, as well as the development and deployment of a series of grids in Buffalo, Western New York, and throughout New York State.

The focus of the parallel algorithms research is on developing solution strategies and fundamental operations that can be applied to a variety of problems. Using this approach, efficient solutions to problems in image analysis, graph theory, and computational geometry have been obtained.

The focus of the research in computational science has been on optimization problems. The highlight of this effort has been the development of a solution strategy to a difficult minimization problem that provides a powerful means to determining molecular structures, which is an important ingredient in the cure and prevention of disease via rational drug design. Note that our *Shake-and-Bake* algorithm was recently listed on the IEEE poster *Top Algorithms of the 20th century*.

The focus of my Cyberinfrastructure Laboratory is on providing the infrastructure necessary to perform high-end simulation and modeling, including the development of algorithms, portals, interfaces, and middleware. In addition, my Cyberinfrastructure Laboratory has led in the development of several grids, including an experimental Buffalo-based grid, a Western New York Grid, and most recently, a heterogeneous and persistent New York State Grid, upon which a grass-roots New York State Cyberinfrastructure Initiative has been established. In terms of middleware, the focus has been on the design, analysis, and implementation of efficient grid monitoring and scheduling tools, as well as on the dynamic integration of resources in order to create a coherent grid that is transparent to the users.

A brief overview of this work is presented below. [The citations in brackets refer to the enumerated papers listed earlier in the CV.]

Cyberinfrastructure and Grid Computing

Cyberinfrastructure provides for the transparent and ubiquitous application of technologies central to contemporary science and engineering, including high-end computing, networking, and visualization, as well as data warehouses, science gateways, and virtual organizations, to name a few. The focus of my Cyberinfrastructure Laboratory is on providing the infrastructure necessary to perform high-end simulation and modeling, including the development of algorithms, portals, interfaces, and middleware. In addition, we have led in the development of several grids, including an experimental Buffalo-based grid, a Western New York Grid, and most recently, the New York State Grid, upon which a grass-roots New York State Cyberinfrastructure Initiative has been established.

Cyberinfrastructure sits at the core of modern simulation and modelling, providing entirely new methods of investigation that allow scholars to address previously unsolvable problems. Specifically, the development of necessary software, algorithms, portals, and interfaces that will enable research and scholarship by freeing end-users from dealing with the complexity of various computing environments is critical to extending the reach of high-end computing, storage, networking, and visualization to the general user community.

The Grid currently serves as critical infrastructure for most activities in cyberinfrastructure. The Grid is a rapidly emerging and expanding technology that allows geographically distributed and independently operated resources (CPU cycles, data storage, sensors, visualization devices, and a wide variety of Internet-ready instruments) to be linked together in a transparent fashion. The power of the Grid lies not only in the aggregate computing power, data storage, and network bandwidth that can readily be brought to bear on a particular problem, but on its ease of use.

The *Advanced Computational Data Center Grid (ACDC-Grid)* [52,53,54,55,18,115,116], which spans organizations throughout Western New York, is a heterogeneous grid initially designed to support *SnB*. ACDC-Grid was part of Grid3+, Open Science Grid (OSG), the IBM NE BioGrid, and serves as the cornerstone of the Western New York Grid (WNY-Grid) and the emerging New York State Grid (NYS Grid). ACDC-Grid

incorporates an integrated computational and data grid, lightweight job monitoring, predictive scheduling, and opportunities for improved Grid utilization through an elegant backfill facility.

The ACDC-Grid was developed with critical grid components that allow for the deployment of a general-purpose regional enterprise grid residing over generally available IP networks. An effective and efficient grid monitoring system was developed during the early stages of the prototype ACDC-Grid. This monitoring system was critical to the grid development group and proved useful to early application adopters. The ACDC-Grid monitoring system exploits the development of robust database servers. The monitoring system utilizes a MySQL database server, which can maintain millions of records and hundreds of simultaneous connections in a fast and stable manner.

The ACDC-Grid predictive scheduler uses a database of historical jobs to profile the usage of a given resource on a user, group, or account basis. Determining accurate quality of service estimates for grid-enabled applications can be defined in terms of a combination of historical and runtime user parameters in addition to specific resource information. Such a methodology is incorporated into the ACDC-Grid Portal, which continually refines the predictive scheduler parameters based, in part, on the data stored by the monitoring system.

The ACDC-Grid enables the transparent migration of data between various storage element resources while preserving uniform access for the user, where basic file management functions are provided via a platform-independent Web interface.

The ACDC-Grid introduced the concept of dynamic resource allocation during the GRID3 intensive application period during Supercomputing 2003 and Supercomputing 2004. The amount of computational resources provided to the GRID3 user base was dynamically rolled into and out of production on a daily basis.

The ACDC-Grid exploits a grid-enabling template framework that includes a dynamically created HTML grid console for the detailed monitoring of computational grid jobs. Results from previous studies have been used in the design of the Globus-based ACDC-Grid that serves researchers at the Center for Computational Research and the Hauptman-Woodward Medical Research Institute, located in Buffalo, NY. The Grid-enabling Application Templates (GATs) used for porting scientific and engineering applications to the ACDC-Grid use abstraction as the process of combining multiple smaller operations into a single unit that can be referred to by a stage. Each stage is named and may contain a template for imposing fine-grained application input file generation, automated parallelization, intermediate result file monitoring, exception handling, and overall application performance metrics. Using the ACDC-Grid GAT abstraction allows programmers to solve problems at a high level, while deferring non-critical details.

To date, a variety of applications have been incorporated into the ACDC-Grid. These applications come from domains that include structural biology, earthquake engineering, groundwater modeling, and computational chemistry, to name a few.

The ACDC-Grid membership in the international Virtual Data Grid Laboratory (iVDGL) provides access to international heterogeneous computing and storage resources for the purpose of experimentation in grid-enabled data-intensive scientific computing. The ACDC-Grid team participates in the (i) iVDGL iGOC, which is used as the central coordination point for grid technical problem resolution, (ii) grid monitoring technical working group, and (iii) grid troubleshooting working group.

The ACDC-Grid is a founding participant of the Open Science Grid (OSG), a cooperative venture that brings together laboratory and university facilities, grid technology providers, and the application communities, for the purpose of engineering and building a common Grid infrastructure that will ensure the necessary robust, persistent, computational, and data services needed by laboratories, experiments, and application managers.

The New York State Grid (NYS Grid) was designed and deployed by my Cyberinfrastructure Laboratory, in collaboration with the Center for Computational Research while I was director of CCR. NYS Grid was an expansion of our Western New York Grid, a heterogeneous grid that included SUNY-Buffalo (Dell Cluster), the Hauptman-Woodward Medical Research Institute (Apple Cluster), Niagara University (Dell Cluster), and SUNY-Geneseo (Sun Cluster). NYS Grid includes resources from a dozen institutions throughout New York State and is available in a simple and seamless fashion to users worldwide. NYS Grid contains a

heterogeneous set of resources and utilizes general-purpose IP networks.

A major feature of NYS Grid is that it integrates a computational grid (compute clusters that have the ability to cooperate in serving the user) with a data grid (storage devices that are similarly available to the user) so that the user may deploy computationally-intensive applications that read or write large data files in a very simple fashion. In particular, NYS Grid was designed so that the user does not need to know where data files are physically stored or where the application is physically deployed, while providing the user with easy access to their files in terms of uploading, downloading, editing, viewing, and so on.

The core infrastructure for NYS Grid includes the installation of standard grid middleware, the use of an active Web portal for deploying applications, dynamic resource allocation so that clusters and networks of workstations can be scheduled to provide resources on demand, a scalable and dynamic scheduling system, and a dynamic firewall, to name a few.

NYS Grid currently supports a variety of applications and users from NYS Grid institutions as well as from users sponsored through Open Science Grid.

Computational Crystallography

Direct Methods are commonly used by crystallographers to determine relatively small crystal structures. However, traditional approaches do not appear to be extensible to larger structures. The combination of a new formulation of the phase problem of x-ray crystallography based on Hauptman's *minimal principle* [25, 84], and advances in massively parallel computing [20, 83, 102, 105, 106], have led to the development of the *Shake-and-Bake* [26, 84] solution strategy. This approach to crystal structure determination consists of a cyclical process which alternates phase refinement in reciprocal space with the imposition of phase constraints through an atomic interpretation of the electron density in real space in an effort to determine the set of phases that minimize the minimal function.

Our computer program *SnB* [27], which is based on our *Shake-and-Bake* method of molecular structure determination, has been used successfully to solve more than three dozen structures over a variety of space groups. Highlights of *SnB* include *i*) solving two previously complex and important unknown 100-atom structures (Ternatin_E and Ternatin_D) [19, 22], which had escaped solution for over a decade, in about an hour, *ii*) solving numerous other previously unknown structures [32, 33, 38, 44], including SeMet structures, some of which could not be solved by traditional direct methods, *iii*) solving vancomycin [36], the antibiotic of last resort, *iv*) solving a variety of difficult and large small molecules [35, 36, 37], *v*) dramatically improving the success rates over traditional direct methods, and *vi*) re-solving Crambin, a 400-atom structure, in a matter of several hours [31]. The original solution to Crambin relied on special properties of the Crambin molecule and the measurement of additional x-ray data. Further, previous attempts to solve this structure by direct methods in other laboratories had failed. These attempts were significant in that more than 500,000 ambiguities were considered without success, while we obtained a success rate of approximately 4%.

A number of phase refinement techniques have been considered within the *Shake-and-Bake* framework, including the tangent formula, where the minimal function is used only as a passive figure-of-merit. Experimentation has shown that the tangent formula can be a cost-effective alternative to traditional phase refinement approaches. For this reason, the tangent formula has been incorporated as an optional phase refinement technique into *SnB* [12].

Recently, traditional optimization strategies have been successfully revisited, including genetic algorithms [107] and simulated annealing [108], for exploiting the minimal function to solve the phase problem within the framework of *Shake-and-Bake*. Previous attempts at using traditional optimization strategies with the minimal function, but without the alternation between real and reciprocal space, had failed.

SnB has been shown to be more robust than traditional methods in terms of solving structures based on partial structure information [30]. In addition, *SnB* can be successfully applied to difficult electron diffraction data sets. Direct methods break down when the quality of the data is worse than about 1.3Å. The current focus of this research is on *i*) breaking the 1.3Å barrier, *ii*) coupling low-cost special purpose hardware with *SnB*, and *iii*) designing a cost-effective multiprocessor system that will be amenable to a significant set of problems in scientific computing, including the phase problem.

BnP is The Buffalo 'n Pittsburgh Interface for complete protein phasing. It combines the *SnB* structure determination package with the Bill Furey's (University of Pittsburgh) PHASES suite of routines. Specifically, *BnP* provides a seamless interface between *SnB* and other crystallographic software. This interface provides a coordinated control of several steps in the protein structure determination pathway, and it facilitates a high degree of automation. This package has been distributed world-wide and used to solve numerous SeMet structures.

Initially, experimentation that led to the development of the *Shake-and-Bake* method was performed on an Intel iPSC/2, Intel iPSC/860, Thinking Machines Corporation CM-2, and Thinking Machines Corporation CM05. The current version of *SnB* and *BnP* are available on a variety of workstations, networks of workstations, clusters, shared-memory machines, and grids.

Computational Geometry

Given planar input (i.e., nonimage input) representing points, sets of points, circles, convex figures, hyperplanes, simple polygons, orthogonal polygons, or iso-oriented rectangles, optimal mesh algorithms have been developed [4, 6, 63, 69, 73] to solve problems involving convexity, smallest enclosing figures, linear separability, proximity, area, and intersection. These algorithms involved developing new mesh paradigms that have additional applications, as well as giving mesh implementations for several existing paradigms. A powerful *grouping technique* was developed to solve many of the area and intersection problems. This is a general technique that can be used in situations where multiple nondisjoint binary searches would naturally occur. It was also shown how to exploit the *slab* method for solving problems in computational geometry on the mesh, and how to avoid the natural explosion of data that is possible with recursion in order to exploit Bentley's versatile *multidimensional divide-and-conquer* technique.

The *multisearch problem* is defined as follows. Given a data structure D modeled as a graph with n constant-degree nodes, perform $O(n)$ searches on D . Let r be the length of the longest search path associated with a search process, and assume that the paths are determined "on-line." That is, the search paths may overlap arbitrarily. In [23, 80], it is shown that the multisearch problem for certain classes of graphs can be solved in $O(n^{1/2} + rn^{1/2}/\log n)$ time on a mesh of size n . For many data structures, the search path traversed when answering one search query has length $r = O(\log n)$. For these cases, our algorithm processes $O(n)$ such queries in asymptotically optimal $\Theta(n^{1/2})$ time. The classes of graphs amenable to this technique include many important data structures that arise in practice, ranging from simple trees to Kirkpatrick hierarchical search DAGs. Multisearch is a useful abstraction that can be used to implement parallel versions of standard sequential data structures on a mesh. For example, this technique can be used for parallel on-line tree traversals, as well as to provide hierarchical representations of polyhedra, which can be exploited to yield optimal algorithms for three-dimensional convex hull, lines-polyhedron intersection queries, multiple tangent plane determination, and convex polyhedra intersection.

Optimal algorithms to solve the planar point input convex hull problem have been developed for a variety of architectures [4, 73], including the EREW PRAM and a fixed interconnection machine. In addition, optimal mesh algorithms, and efficient PRAM algorithms, have been developed for solving problems involving equally-spaced collinear sets [18, 82].

The work in dynamic computational geometry [7, 10, 70, 75, 97] focuses on developing techniques for a variety of architectures to solve problems involving point objects that are moving along known trajectories. The problems involve properties such as collision, convexity, containment, and proximity, where the solution is a function over time. Some of the results and subalgorithms developed for problems in dynamic computational geometry were used to give efficient solutions to static problems, such as the circle-cover minimization problem [9] and problems involving intersections of polygons [11].

Efficient and often optimal scalable algorithms have been developed for Dehne's Coarse-Grained Multiprocessor (CGM). Solutions have been developed to solve problems in computational geometry and image processing [39, 42].

Finally, parallel algorithms to solve convexity and domination problems on fine-grained (theoretical) hypercubes and on a medium-grained Intel hypercube were studied [15, 96]. The medium-grained results

show that for such problems efficient solutions are constructed as a combination of communication patterns associated with the theoretical parallel algorithms, efficient serial data reduction techniques, and efficient parallel data reduction techniques. Through experimentation, the behavior of different algorithms with respect to the distribution of the input has been studied.

Image Analysis and Graph Theory

The initial concentration in this area was on developing efficient algorithms, as well as time and processor bounds, for the mesh and pyramid computers. New techniques and fundamental data movement operations were developed that formed the foundation of the algorithms [1, 2]. Optimal mesh algorithms were developed [1, 62] for intermediate-level image problems involving convexity, internal paths, proximity, diameter, and largest empty circle. Given a gray-scale image, two asymptotically optimal algorithms were developed for labeling the connected components [24, 81]. The first of these algorithms operates directly on the image using a traditional divide-and-conquer paradigm, while the second operates on a graph representation of the image, exploiting a variety of new graph algorithms that were developed, such as finding independent sets and coloring graphs.

Optical clustering is a technique based on the principal of optical resolution, and is of particular interest in picture analysis. Results in computational geometry and graph theory are exploited in [14] to derive an optimal mesh algorithm to determine the optical clusters with respect to a given separation parameter, and to determine the range of the separation parameter that will result from a desired range of optical clusters.

An interesting result in terms of scalable parallel algorithms was presented in [66], which shows that a mesh computer with a reduced diameter is an optimal interconnection scheme for solving problems in image analysis and graph theory. Current work on scalable algorithms focuses on a practical model of computation for which optimal scalable parallel algorithms have been developed for a variety of problems in image processing and computational geometry.

While the pyramid was initially proposed for performing low-level image processing, efficient algorithms [2, 61, 64, 65, 114] to solve problems in intermediate-level image processing and graph theory demonstrated that pyramids can be exploited for more than just low-level image processing. Problems in image processing involve connectivity, convexity, proximity, diameter, and smallest enclosing figures, while problems in graph theory include determining the bridge edges, articulations points, and cyclic index of a graph, as well as determining whether or not a graph is bipartite or biconnected.

Convexity properties of digitized pictures on a pyramid computer have also been studied for the purpose of showing that the pyramid is very sensitive to the rate at which data can be compressed [13]. For example, given an $n \times n$ image, algorithms have been developed that range from $\Theta(\log n)$ time to find the extreme points of a convex figure in a digitized picture, to $\Theta(n^{1/3})$ time to find the diameter of a labeled figure, to $\Theta(n)$ time to find, for every label, the extreme points of the processing elements with that label.

Researchers in image processing are often able to develop efficient single figure pyramid algorithms that are difficult to extend to the multiple figure per image case. This is due to the fact that severe bottlenecks are created at the apex of the pyramid if one tries to naively generalize a single figure algorithm to a multiple figure algorithm. However, it was shown [3, 72] that by systematically simulating the effect of having a separate “essential” pyramid over every object, optimal or nearly optimal image algorithms for pyramids, hypercubes, mesh-of-trees, meshes with buses, the reconfigurable mesh, and the PRAM can be obtained. This approach should greatly simplify algorithm development for image processing in that one can concentrate on *single* figure pyramid algorithms and use this simulation technique to extend the solution to *multiple* figure algorithms for a wide variety of architectures.

While the pyramid is an interesting architecture for implementing image algorithms, the hypercube has a number of well-known advantages over the pyramid. Hypercube (and mesh-of-trees) algorithms were developed [94] for problems involving images and graphs. The image problems involve convexity, proximity, separability, diameter, and smallest enclosing figures, while the graph problems involve bridge edges, articulations points, minimal spanning forests, biconnected components, the cyclic index, as well as determining properties of a graph such as whether or not it is bipartite. These algorithms rely on efficient data movement

operations and simulation techniques. Unfortunately, optimal hypercube algorithms are not yet known for problems such as sorting/routing data or labeling the figures of an image. However, given a labeled image, optimal hypercube algorithms have been developed [78] to determine the extreme points, area, perimeter, centroid, diameter, width, and smallest enclosing rectangle of every figure. These algorithms rely on new fundamental operations and implementations of interesting paradigms.

For many applications, it is desirable to have an interconnection scheme that may be reconfigured during an algorithm. A mesh with reconfigurable broadcast bus (i.e., a *reconfigurable mesh*) was proposed [71] as a model of computation that captures some of the salient features of the CAAPP, polymorphic-torus network, and CHiP project. Further, due to the reconfigurability of the bus, which is controlled locally within the processors, this model combines the advantages of the mesh, pyramid, mesh-of-trees, and mesh with multiple broadcast buses. Fundamental operations and algorithmic techniques for this model have been developed [74, 76]. Based on these operations and techniques, polylogarithmic time algorithms have been presented [21, 4, 5] to solve problems involving digitized pictures or graphs given as adjacency matrices. Recently, I have proposed a *systolic reconfigurable mesh*. This is a practical model that can be effectively realized as a co-processor coupled to a workstation, and for which optimal algorithms have been developed to solve fundamental problems involving images and graphs[86].

Finally, a variety of algorithms have been implemented on an Intel hypercube to evaluate solution strategies and data reduction techniques for solving convexity and labeling problems [8, 68, 95, 104]. The results show that for such problems, efficient solutions are constructed as a combination of theoretical parallel algorithms, efficient serial algorithms, efficient serial data reduction techniques, and efficient parallel data reduction techniques. Through experimentation, the performance of algorithms with respect to certain properties of the input image has been studied.

Languages

The interconnection scheme among processors (or between processors and memory) of a parallel computer significantly affects the running time of programs. Therefore, efficient parallel algorithms must take the interconnection scheme into account. This in turn entails tradeoffs between efficiency and portability among different architectures. Based on experience with parallel algorithms, a high-level data parallel programming language called Seymour was presented for use in designing, expressing, and implementing efficient portable parallel algorithms. The foundation of Seymour is based on the approach of designing parallel algorithms based on standardized global operations such as prefix, broadcast, sort, compression, and associative read. Seymour also incorporates fundamental paradigms, such as divide-and-conquer, reduce-and-create-cross-product, and reduce-and-compress, which are derived from theoretical parallel algorithms. The intent is to redirect the difficulties of portability and efficiency into similar difficulties for the global operations and paradigms since the cost of developing efficient implementations of standardized operations on the various target architectures can be amortized over numerous algorithms. [12, 67, 77, 93, 98, 101]

NP-Hard Approximation Algorithms

This research focuses on the design, analysis, and implementation of approximation solutions to NP-Hard problems on medium-grained machines. The problems studied include the multiprocessor scheduling problem [5] and the 2-dimensional (rectangle) packing problems [100, 103]. Interesting results have been obtained that consider not only the standard time and accuracy of solution tradeoff, but a third parameter, namely, the number of processors.

Parallel Computing at SUNY-Buffalo

During the Summer and Fall of 1986, I was engaged in discussions and negotiations with Intel Scientific Computing. The result of this effort was that Intel agreed to loan me a hypercube for research and educational purposes. This machine, a hybrid iPSC/1 hypercube, was the first general purpose parallel computer to be installed (during the Spring of 1987) at SUNY-Buffalo.

During the Summer and Fall of 1986, I was also intimately involved with a multidisciplinary and interinstitutional grant proposal involving Computer Science (Eberlein, Miller), Chemistry (George, King, McIver), and the Calspan Advanced Technology Center (Furlani, Lordi). The proposal was sent to the National Science Foundation in December, 1986, and the award was made effective September, 1987. With these funds, the following 3 hypercubes were obtained.

1. A 16-node iPSC/1 in which each 80286-based processor was configured with 4.5Mbytes of memory.
2. A 32-node iPSC/2 in which each 80386-based processor was configured with 4Mbytes of memory.
3. A 4-node iPSC/2 in which each 80386-based processor was configured with 4Mbytes of memory and coupled to a vector board.

During 1986, I served on a committee that was responsible for making recommendations to the Department of Computer Science for replacing some of its time-sharing Unix machines. After considering numerous alternatives, a few of the committee members, including myself, supported the acquisition of a shared-memory multiprocessor that could handle a heavy course load and support shared-memory multiprocessor research. While there was strong opposition to this approach within the committee, the Department supported our position and University funds were used to purchase an 8-processor shared-memory Encore Multimax for the Department. The machine has been used successfully since its installation in the Spring of 1987 for both courses and research.

In the Summer of 1987, an equipment proposal was submitted to the National Science Foundation by 3 members of Computer Science (Eberlein, Miller, Srihari) for the purchase of a departmental distributed-memory research machine. The award was made in the Spring of 1988, and a 16-node transputer machine from Topologix was purchased.

Work in parallel computing has been supported by the Graduate Group in Advanced Scientific Computing (later renamed the Graduate Group in High Performance Computing), which was officially recognized (and funded) by the University in the Fall of 1988. I was Associate Director of the Group during its first 3 years (1988-1991).

In the mid-1990s, due to the wide variety of software and hardware platforms available, the focus of my experimental parallel computing efforts have been on parallel machines that are available off-site. Due to my affiliation with Thinking Machines Corporation, a variety of CM-2, CM-200, and CM-5s have been available for use at Thinking Machines Corporation. In addition, based on a number of supercomputing grants that I have obtained, including a prestigious MetaCenter Allocations Grant for Grand Challenge Problems, students working under my direction have used a CM-5 at the Pittsburgh Supercomputing Center and at the National Center for Supercomputing Applications, as well as a Cray C90 and the new massively parallel Cray T3D at the Pittsburgh Supercomputing Center. Finally, a variety of distributed computing platforms have been exploited using RPC, Linda, and PVM.

Please refer to the section "Center for Computational Research," which appears earlier in this CV, for information pertaining to my involvement with high-end computing at SUNY-Buffalo during the period 1998-2006. In 2007, once the University makes the appropriate space available, my cyberinfrastructure laboratory has plans to purchase significant high-performance computing systems with NSF CRI and ITR funds.

Multidisciplinary Research at SUNY-Buffalo

SUNY-Buffalo embraces multidisciplinary and interinstitutional research efforts. I have been involved in such activities since the Summer of 1986, when regular meetings involving members of the Department of Computer Science, the Department of Chemistry, and the Calspan Advanced Technology Center focused on possibilities of using parallel machines to solve scientific problems. These meetings resulted in an NSF-funded proposal that supported the acquisition of 3 Intel hypercubes. As the meetings continued and the new machines arrived, I began to work closely with scientists in other departments at the University and at neighboring institutions.

These early discussions also led to the formation of the **Graduate Group in Advanced Scientific Computing**, a University-recognized multidisciplinary graduate group funded by the University and local corporate affiliates. I was one of the founding members of the group and was its Associate Director during its first three years (1988-1991). The members of the Graduate Group shared a common interest in large-scale scientific computing, with participants representing a wide variety of academic units including Computer Science, Chemistry, Mathematics, Physics, Engineering, Anthropology, Management, and Geography, as well as neighboring research institutions, including the Medical Foundation of Buffalo and the Calspan Advanced Technology Center. This group of mathematicians, computer scientists, crystallographers, theoretical chemists, and others have collaborated in the study of parallel algorithms and their application to problems in several different fields of science. This has led to the design, analysis, and implementation of parallel solutions to a number of problems. Relationships forged as a result of this Graduate Group have stimulated multidisciplinary and interinstitutional research in Western New York. In fact, as a result of the relationships formed by key members of the Graduate Group, I chaired an ad-hoc committee of faculty and staff who developed a report that led to the formation of the Center for Computational Research.

I am currently involved in a number of multidisciplinary projects, which have been described on the preceding pages. In addition, through the Center for Computational Research, I have played a role in supporting research and scholarship involving on the order of 140 research groups spanning approximately 40 different academic departments, 20 companies and institutions, and a variety of government agencies.