WAYNE JOUBERT

Scientific Computing Group, National Center for Computational Sciences, Oak Ridge National Laboratory

PROFESSIONAL EDUCATION

Ph.D., Mathematics, University of Texas, May 1990.
Bachelor of Science, Mathematics, University of Louisiana, May 1981.

RESEARCH AND PROFESSIONAL EXPERIENCE

6/08 – present: Computational Scientist, National Center for Computational Sciences, Oak Ridge National Laboratory
5/07 – 5/08: Computational Scientist, U. S. Army Engineer Research and Development Center, Vicksburg, MS.
11/01 – 4/07: Computer Scientist, Xiylon Software Inc., Gable, SC.
1/00 – 10/01: Computer Scientist, Research Group, LizardTech Inc., Seattle, WA.
8/95 – 1/00: Technical Staff Member, Scientific Computing Group, Los Alamos National Laboratory.
9/92 – 8/95: Postdoctoral Fellow, Computer Research and Applications Group, Los Alamos National Laboratory.
1/90 – 8/92: Postdoctoral Fellow, Texas Institute for Computational Mechanics, Austin, TX.

AWARDS AND HONORS

Gordon Bell Awardee, CoMet application, 2018
ORNL Awards Night, Research Accomplishment and Director's Award, CoMet Exascale Accomplishment, 2018
ORNL Significant Event Award, Summit Acquisition, 2015
CUG Best Paper Award, 2015
Gordon Bell Finalist, uDeviceX project, 2015
ORNL Awards Night, Research Accomplishment, Westinghouse AP1000 Simulation, 2014
ORNL Significant Event Award, Titan Application Readiness, 2013
ORNL CCSD Distinguished Employee Award, May 2012
ORNL Significant Event Award, Jaguar Acceptance, 2009
Who's Who in America, 2008, 2018
Computer World Smithsonian Award, Falcon Project, 1998
R&D 100 Award, Falcon Project, 1997.
Mathematics collaborations: Erdos number 2 (Erdos > Faber > Joubert), 1996
LANL IPO Excellence in Industrial Partnerships Award, Falcon Project, 1996

PUBLICATIONS

Lixiang Luo et al., "Pre-exascale accelerated application development: the ORNL Summit experience," *IBM J. Res & Devel.*, submitted.

D. E. Womble, M. Shankar, W. Joubert, J. T. Johnston, J. C. Wells, J. A. Nichols , "Early Experiences on Summit: Data Analytics and AI Applications," *IBM J. Res & Devel.*, submitted.

Deborah Weighill, David Macaya-Sanz, Stephen Paul DiFazio, Wayne Joubert, Manesh Shah, Jeremy Schmutz, Avinash Sreedasyam, Gerald Tuskan, Daniel Jacobson, "Wavelet-based Genomic Signal Processing for Centromere Identification and Hypothesis Generation," *Frontiers in Genetics*, section *Bioinformatics and Computational Biology,* accepted.

Veronica G. Vergara Larrea, Wayne Joubert, Michael J. Brim, Reuben D. Budiardja, Don Maxwell, Matt Ezell, Christopher Zimmer, Swen Boehm, Wael Elwasif, Sarp Oral, Daniel Pelfrey, Oscar Hernandez, Dustin Leverman, Jesse Hanley, Mark Berrill, Arnold Tharrington, "Scaling the Summit: Deploying the World's Fastest Supercomputer," IWOPH19 Proceedings.

Veronica G. Vergara Larrea, Reuben Budiardja, Rahulkumar Gayatri, Christopher Daley, Oscar Hernandez, Wayne Joubert, "Porting mini-applications to OpenACC and OpenMP on heterogeneous systems," *Cray User Group CUG19 Proceedings*, Best Paper First Runner Up.

Wenlu Zhang, Wayne Joubert, Peng Wang, Matthew Niemerg, Bei Wang, William Tang, Sam Taimourzadeh, Lei Shi, Jian Bao, Zhihong Lin, "Heterogeneous Programming and Optimization of Gyrokinetic Toroidal Code Using Directives," Fifth Workshop on Accelerator Programming Using Directives WACCPD 2018 Workshop, LNCS 11381, Springer, 2019.

Verónica G. Vergara Larrea, Michael J. Brim, Wayne Joubert, Swen Boehm, Matthew Baker, Oscar Hernandez, Sarp Oral, James Simmons, Don Maxwell, "Are we witnessing the spectre of an HPC meltdown?", CUG18, C*oncurrency and Computation: Practice and Experience* 31 (2018).

Robert Searles, Sunita Chandrasekaran, Wayne Joubert, Oscar Hernandez, "MPI + OpenACC: Accelerating Radiation Transport Mini-Application, Minisweep, on Heterogeneous Systems," *Computer Physics Communications* 236 (2019), 176-187.

Wayne Joubert, Deborah Weighill, David Kainer,Sharlee Climer, Amy Justice, Kjiersten Fagnan, Daniel Jacobson, "Attacking the Opioid Epidemic: Determining the Epistatic and Pleiotropic Genetic Architectures for Chronic Pain and Opioid Addiction." *Supercomputing SC18*, Gordon Bell Award.

W. Joubert, J. Nance, D. Weighill, D. Jacobson, "Parallel Accelerated Vector Similarity Calculations for Genomics Applications," *Parallel Computing* 75 (2018), 130-145.

W. Joubert, J. Nance, S. Climer, D. Weighill, D. Jacobson, "Parallel Accelerated Custom Correlation Coefficient Calculations for Genomics Applications," *Parallel Computing* 84 (2019), 15-23.

Robert Searles, Sunita Chandrasekaran, Oscar Hernandez, Wayne Joubert, "Abstractions and Directives for Adapting Wavefront Algorithms to Future Architectures," *Proceedings of Platform for Advanced Scientific Computing Conference (PASC18)*, 2018.

Sudharshan S. Vazhkudai, et al., "The Design, Deployment, and Evaluation of the CORAL Pre-Exascale Systems," *Supercomputing SC18*.

D. I. Lyakh and W. Joubert, "Exascale Challenges in Numerical Linear and Multilinear algebras," in *Exascale Scientific Applications*, CRC Press, 2017.

Lopez, Matthew Graham, Joubert, Wayne, Vergara Larrea, Veronica G., Hernandez, Oscar R., Haidar, Azzam, Tomov, Stanimire, Dongarra, Jack J, "Evaluation of Directive-based Performance Portable Programming Models," *International Journal of High Performance Computing and Networking*, 2017.

Vergara Larrea, Veronica G., Joubert, Wayne, Berrill, Mark A., Boehm, Swen, Tharrington, Arnold N., Elwasif, Wael R., Maxwell, Don E., "Experiences evaluating functionality and performance of IBM Power8+ systems," *High Performance Computing*, Springer, 2017, pp 254-274.

Vergara Larrea, Veronica G., Joubert, Wayne, Lopez, Matthew Graham, Hernandez, Oscar R., "Early Experiences Writing Performance Portable OpenMP 4 Codes," *CUG 2016*.

Juckeland, Guido et al., "From Describing to Prescribing Parallelism: Translating the SPEC ACCEL OpenACC Suite to OpenMP Target Directives," *High Performance Computing*, Springer, 2016, pp. 470-488.

Lopez, Matthew Graham, Vergara Larrea, Veronica G., Joubert, Wayne, Hernandez, Oscar R., Haidar, Azzam, Tomov, Stanimire, Dongarra, Jack J., "Towards Achieving Performance Portability Using Directives for Accelerators," *2016 Third Workshop on Accelerator Programming Using Directives (WACCPD)*, Salt Lake City, UT, 2016, pp. 13-24.

O. E. B. Messer, E. D'Azevedo, J. Hill, W. Joubert, M. Berrill, C. Zimmer, "MiniApps Derived from Production HPC Applications Using Multiple Programming Models," *The International Journal of High Performance Computing Applications*, 2016.

W. Joubert et al., "Accelerated Application Development: The ORNL Titan Experience," *Computers and Electrical Engineering*, special issue on Optimization of Parallel Scientific Applications with Accelerated HPC, August 2015.

Veronica G. Vergara Larrea, Wayne Joubert, Chris Fuson, "Use of Continuous Integration Tools for Application Performance Monitoring," Cray User Group 2015 Proceedings, April 2015.

Thomas Evans, Wayne Joubert, Steven Hamilton, "Three-dimensional discrete ordinates reactor assembly calculations on GPUs," *Joint Intl. Conf. on Mathematics and Computation (M&C)* 2015.

C. Kartsaklis, W. Joubert, O. R. Hernandez, M. Eisenbach, W. R. Elwasif and D. E. Bernholdt, "CUDA Grid-Level Task Progression Algorithms," *2015 IEEE 17th International Conference on High Performance Computing and Communications, 2015 IEEE 7th International Symposium on Cyberspace Safety and Security, and 2015 IEEE 12th International Conference on Embedded Software and Systems*, New York, NY, 2015, pp. 1628-1632.

Messer, Bronson, D'Azevedo, Ed F., Hill, Judith C., Joubert, Wayne, Tharrington, Arnold N., "Developing MiniApps on Modern Platforms Using Using Multiple Programming Models," *IEEE Cluster Conference*, 2015, Chicago, IL, USA.

Diego Rossinelli et al., "The in-silico lab-on-a-chip: petascale and high-throughput simulations of microfluidics at cell resolution," In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC '15)*, Gordon Bell finalist, 2015.

Valentine Anatharaj, Fernanda Foertter, Wayne Joubert and Jack Wells, *Approaching Exascale: Application Requirements for OLCF Leadership Computing*, ORNL/TM-2013/186, July 2013.

Arthur Bland, Wayne Joubert, Don Maxwell, Norbert Podhorszki, Jim Rogers, Galen Shipman and Arnold Tharrington, "Titan: 20-Petaflop Cray XK-7 at Oak Ridge National Laboratory," in Jeff Vetter (ed.), *Contemporary High Performance Computing: From Petascale toward Exascale*, Chapman and Hall, 2013.

Christopher Baker, Gregory Davidson, Thomas Evans, Steven Hamilton, Joshua Jarrell and Wayne Joubert, "High Performance Radiation Transport Simulations: Preparing for TITAN," *Supercomputing SC12*, November 2012.

Wayne Joubert and Shiquan Su, "An Analysis of Computational Workloads for the ORNL Jaguar System," *International Conference on Supercomputing ICS12*, June 25-29, 2012, San Servolo Island, Venice, Italy.

Joubert, Wayne, Su, Shi-Quan, "Application Workloads on the Jaguar Cray XT5 System," *CUG2012*.

C. Kartsaklis, O. Hernandez, C. H. Hsu, T. Ilsche, W. Joubert and R. L. Graham, "HERCULES: A Pattern Driven Code Transformation System," *2012 IEEE 26th International Parallel and Distributed Processing Symposium Workshops & PhD Forum*, Shanghai, 2012, pp. 574-583.

Graham, Richard L., Messer, Bronson, Hernandez, Oscar R., Kartsaklis, Christos, Ilsche, Thomas, Mintz, Tiffany M., Joubert, Wayne, Whitten, Robert M., Kendall, Ricky A., "A Programming Environment for Heterogeneous Multi-Core Computer Systems," *CUG 2011*.

B. Vacaliuc et al., "Python for Development of OpenMP and CUDA Kernels for Multidimensional Data," *2011 Symposium on Application Accelerators in High-Performance Computing*, Knoxville, TN, 2011, pp. 159-167.

Arthur S. Bland, Wayne Joubert, Ricky A. Kendall, Douglas B. Kothe, James h. Rogers and Galen Shipman, "Jaguar: The World's Most Powerful Computer System -- An Update," *2010 Cray Users Group Conference*, Edinburgh, Scotland, May 24-27, 2010.

Joubert, Wayne, Kothe, Douglas B., Nam, Hai Ah, "Preparing for Exascale: ORNL Leadership Computing Application Requirements and Strategy," ORNL report ORNL/TM-2009/308 , December 2009.

Wayne Joubert, "Performance of Variant Memory Configurations for Cray XT Systems," Proceedings of the Cray Users Group (CUG), 2009.

Bobby Philip, Michael Pernice, Wayne Joubert and Bryan Lally, "A Comparison of Multilevel Preconditioners for Solving Multimaterial Equilibrium Radiation Diffusion Problems on Locally Refined Grids", *Nuclear Weapons Highlights, ADTSC*, 2007.

Wayne Joubert and Jane Cullum, "Scalable Algebraic Multigrid on 3500 Processors," *Electronic Transactions in Numerical Analysis*., vol. 23, 2006, pp. 105-128.

Michjael DeLong et al., "Petroleum Reservoir Management," in *Industrial Strength Parallel Computing*, Alice E. Koniges ed., Morgan Kaufmann, 2000.

A. Gajraj, W. Joubert and J. Jones, "A Parallel Implementation of Kriging with a Trend," *In situ* vol. 22, no. 2, 1998, pp. 239-261.

Gautam S. Shiralkar, R. E. Stephenson, Wayne Joubert, Olaf Lubeck and Bart van Bloemen Waanders, "Falcon: A Production Quality Distributed Memory Reservoir Simulator," SPE Paper 37975, presented at the *1997 SPE Reservoir Simulation Symposium*, Dallas, TX, 8-11 June, 1997.

A. A. Lorber, G. F. Carey and W. D. Joubert, "ODE Recursions and Iterative Solvers for Linear Equations," *SIAM Journal on Scientific Computing*, vol. 17, no. 1, January 1996.

Vance Faber, Wayne Joubert, Emanuel Knill and Thomas Manteuffel, "Minimal Residual Method is Stronger than Polynomial Preconditioning," *SIAM Journal on Matrix Analysis and Applications*, vol. 17, no. 4, October 1996.

Wayne Joubert, "A Robust GMRES-based Adaptive Polynomial Preconditioning Algorithm for Nonsymmetric Linear Systems," *SIAM Journal on Scientific and Statistical Computing*, vol. 17, no. 1, Jan. 1996.

Wayne Joubert, "On the Convergence Behavior of the Restarted GMRES Algorithm for Solving Nonsymmetric Linear System," *Numerical Linear Algebra with Applications*, vol. 1, no. 5, Sept-Oct 1994, pp 427-448.

Wayne Joubert and Graham F. Carey, "PCG: A Software Package for the Iterative Solution of Linear Systems on Scalar, Vector and Parallel Computers," in *Proceedings of the Scalable High Performance Computing Conference*, Knoxville, TN, May 22-25, 1994.

Wayne Joubert and Thomas Oppe, "Improved SSOR and Incomplete Cholesky Solution of Linear Equations on Shared Memory and Distributed Memory Parallel Computers," *Numerical Linear Algebra with Applications*, vol. 1, no. 3, May-June 1994, pp. 287-312.

Wayne Joubert and Graham F. Carey, "PCG: A Software Package for the Iterative Solution of Linear Systems on Scalar, Vector and Parallel Computers," in *Proceedings of the IMACS World Congress*, Atlanta, GA, 1994.

W. D. Joubert and G. F. Carey, "Embedded Gradient Iterative Solution of a Class of Nonlinear PDE's on the Connection Machine," *International Journal of High Speed Computing*, vol. 6, no. 2, 1994, pp. 277-286.

Wayne Joubert and Graham F. Carey, "PCG: A Software Package for the Iterative Solution of Linear Systems on Scalar, Vector and Parallel Computers," in *Proceedings of the Scalable High Performance Computing Conference*, Knoxville, TN, 1994.

Wayne D. Joubert and Graham F. Carey, "Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems. Part I: Theory," *International Journal of Computer Mathematics*, vol. 44, pp. 243-267, 1992.

Wayne D. Joubert and Graham F. Carey, "Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems. Part 2: Parallel Implementation," *International Journal of Computer Mathematics*, vol. 44, pp. 269-290, 1992.

Wayne Joubert and Graham Carey, "Parallelizable Restarted Iterative Methods for Nonsymmetric Linear Systems," in *Proceedings of the Fifth SIAM Conference on Parallel Processing for Scientific Computing*, Jack Dongarra, Ken Kennedy, Paul Messina, Danny C. Sorensen and Robert Voight, eds. Philadelphia: SIAM, 1992, pp. 138-143.

Joubert, Wayne and Highnam, Peter and Carey, Graham F. "PCG/CM: A Package for the Iterative Solution of Large Sparse Linear Systems Ond the Connection Machine," in *Proceedings of the Fifth SIAM Conference on Parallel Processing for Scientific Computing*, Jack Dongarra, Ken Kennedy, Paul Messina, Danny C. Sorensen and Robert Voight, eds. Philadelphia: SIAM, 1992.

G. F. Carey, E. Barragy, D. D. Cline,. W. Joubert, A. Lorber and A. K. Stagg, "Vector-Parallel Supercomputing Algorithms and Applications," in *Proceedings of the 1991 International Conference on Computational Techniques and Applications (CTAC 91)*, 1992.

Wayne D. Joubert, Thomas A. Manteuffel, Seymour V. Parter and Sze-Ping Wong, "Preconditioning Second-Order Elliptic Operators, Experiment and Theory," *SIAM J. Sci. and Stat. Comp.*, vol. 13, no. 1, Jan. 1992.

Wayne Joubert, "Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations," *SIAM Journal on Matrix Analysis and Applications*, vol. 13, no. 3, July 1992, pp. 926-943.

Wayne D. Joubert and Thomas A. Manteuffel, "Iterative Methods for Nonsymmetric Linear Systems," in *Iterative Methods for Large Linear Systems*, David R. Kincaid and Linda J. Hayes eds., Boston: Academic Press, 1990, pp. 149-171.

D. R. Kincaid, T. C. Oppe, and W. D. Joubert, "An Introduction to the NSPCG Software Package," International Journal for Numerical Methods in Engineering, vol. 27, no. 3, Dec. 1989, pp. 589-608.

D. R. Kincaid, T. C. Oppe, and W. D. Joubert, "An Overview of NSPCG: A Nonsymmetric Preconditioned Conjugate Gradient Package," *Computer Physics Communications*, vol. 53, 1989, pp. 283-294.

G. F. Carey, K. C. Wang and W. D. Joubert, "Performance of Iterative Methods for Generalized Newtonian Flows," *International Journal for Numerical Methods in Fluids*, vol. 9, 1989, pp. 127-150.

Wayne D. Joubert and David M. Young, "Necessary and Sufficient Conditions for the Simplification of Generalized Conjugate Gradient Algorithms," *Linear Algebra and its Applications*, vol. 88/89, 1987, pp. 449-485.

DISSERTATION

Title: Generalized Conjugate Gradient and Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations

Abstract: The solution of the linear system Au=b by iterative methods when A is nonsymmetric is known to be considerably more difficult than the case when A is symmetric. Some experimental studies have indicated that the Lanczos or biconjugate gradient method is an effective and economical technique for solving this problem. However, the Lanczos method may break down during the iteration process, and the iterates generated by the method may become arbitrarily large before convergence. In this thesis we present theoretical results on the phenomenon of breakdown of the Lanczos method. Results are given on the likelihood of breakdown as well as the causes and possible remedies of the problem of breakdown. Several new algorithms are defined which attempt to deal with the breakdown problem. The results of numerical experiments with these algorithms are presented.

Supervising Professor: David M. Young

SYNERGISTIC ACTIVITIES

Joubert specializes in the development of mathematical methods, algorithms and software to help researchers solve science problems more quickly and effectively on advanced computer systems. As member of the Center for Accelerated Application Readiness he developed the GPU-enabled S_n sweep code for the Denovo radiation transport application and was also part of the Summit application readiness team for the GTC fusion code. He is the principal author of the CoMet comparative genomics code which scales to ExaOp performance on Summit and was awarded a Gordon Bell Prize in 2018. His activities include mathematical algorithm development, mapping of algorithms to advanced computing hardware, application performance modeling and prediction, application readiness for future leadership systems, application requirements gathering, procurement support and acceptance testing of leadership-class systems. Previously he was developer of the LAMG algebraic multigrid solver code used by the LANL ASC program, developed linear solver algorithms and software for the R&D 100 Award-winning Falcon reservoir simulation code, and developed innovative Krylov solver methods and preconditioners for parallel computing systems.