Juan C. Meza

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EDUCATION

Ph.D., M.A., Computational and Applied Mathematics, Rice University, 1986
M.S., Electrical Engineering, Rice University, 1979
B.S., Electrical Engineering (cum laude), Rice University, 1978

PROFESSIONAL EXPERIENCE

Department Head and Senior Scientist, High Performance Computing Research,
Lawrence Berkeley National Laboratory, Berkeley, CA, 2002 - Present

RESEARCH

- Lead PI for joint BES/ASCR project developing scalable methods for studying the electronic excitation and optical responses of nanostructures. In the first two years, this multi-institution project has produced over 55 publications and developed several new algorithms for studying nanostructures. Our research has resulted in new optimization techniques for electronic structure calculations, physics-based preconditioners for accelerating convergence of self-consistent calculations, and development of a new linear scaling 3D fragment electronic structure calculation that scales up to 2000 processors. This code was awarded a DOE INCITE award in 2007 for 1.5 Million hours on the Cray XT3 at ORNL.
- Research in parallel methods for simulation-based optimization problems, including a parallel optimization method for the determination of parameters used in fitting supernova spectral data, a surrogate optimization method used for structure determination problems for nanostructures, and a derivative-free method used for protein folding problems.
- Developed a new mixed integer nonlinear optimization method for detecting vulnerabilities in the electric power grid that is several orders of magnitude faster than previous methods.

ADMINISTRATIVE

- Provide leadership for department of 110 employees and a budget of $19M in computational science, mathematical modeling, algorithmic design, software implementation, computer system architectures and future technologies, scientific data management, and visualization.
- Point of Contact for DOE/ASCR Scientific Discovery through Advanced Computing (SciDAC) and Base Math and Computer Science Research programs.
- Oversaw the submission of the Computational Research Division's 50+ SciDAC-2 proposals in 2006, which resulted in a 15% increase of funding over previous levels.
- Established new collaborations with Environmental Energy Technologies Division, Earth Sciences Division, and Joint Genome Institute.

Distinguished Member Technical Staff, Sandia National Laboratories, Livermore, CA, 1987-2002

RESEARCH
- Principal investigator for MICS Large Scale Scientific and Engineering Design Optimization project resulting in the open-source object-oriented nonlinear optimization software OPT++.
- Research in parallel methods for simulation-based optimization problems for wide-ranging applications including thermal problems in chemical vapor deposition furnaces, molecular conformation problems, and 3D inverse geophysical problems.
- Developed semiconductor device simulation code for modeling of single-event upset phenomenon.

ADMINISTRATIVE
- Served one-year assignment as a Senior Technical Advisor to the DOE NNSA providing technical expertise to assist the Accelerated Strategic Computing Initiative (ASCI) program concerning high performance computing and applications related services. Assisted in the planning and coordinating of the ASCI Applications Program, a $250M program focused on the development of engineering codes by Sandia National Laboratories and performance and safety codes by the Los Alamos National Laboratory and Lawrence Livermore National Laboratory. Provided guidance to the Office of Advanced Simulation and Computing in the development of improved numerical algorithms for incorporation in engineering, performance and safety codes.
- Managed the Computational Sciences and Mathematics Research department from 1998-2000, and the Distributed Computing department from 1997-1998.
- Served as Program Manager for numerous technical programs including: Research Foundation/Network Research, Technology Transfer Initiative on 3D Geophysical Inverse Modeling, ASCI Advanced Simulation Development Environment Problem Solving Environment / Application Development Support, and the DOE 2000 Advanced Computational Toolkit.

Lecturer and Research Associate, Rice University, 1987

- Research on methods for large-scale linear systems and their applications to geophysical problems
- Taught 1 semester course on Numerical Methods for upper level undergraduates and graduate students

PROFESSIONAL MEMBERSHIPS

American Association for the Advancement of Science
Association for Computing Machinery
Mathematical Programming Society
Society for Industrial and Applied Mathematics
Society for Advancement of Chicanos and Native Americans in Science

AWARDS, SPECIAL RECOGNITIONS

Appointed to SIAM Committee on Science Policy, 2007
Appointed as a Visiting Lecturer by the Society for Industrial and Applied Mathematics, 2006
ACM Service Award for Conference Co-Chair of Richard Tapia Celebration of Diversity in Computing Conference, 2003
Appointed by the Secretary of DOE to the Advanced Scientific Computing Advisory Committee, 2000-2003
Award for Excellence for "significant achievement in the advancement of distributed computing capabilities to solve complex scientific and engineering problems", Sandia National Laboratories, 2002
Sandia National Laboratories Hispanic Leadership Committee Award, May 23, 2002
Sandia National Laboratories Royalty Award, 1996, 1997, 1998
Sandia Employee Recognition Award, 1995, 1993
Sandia Award for Excellence, 1993
Tau Beta Pi Engineering Honor Society

PUBLICATIONS

OPT++: An Object-Oriented Toolkit for Nonlinear Optimization, J. Meza, R. Oliva, P. Hough, P. Williams, ACM Trans. on Math. Software, Vol. 33, No. 2 (2007).

A Constrained Optimization Algorithm for Total Energy Minimization in Electronic Structure Calculation, C. Yang, J. Meza, L.-W. Wang, Journal of Computational Physics, 217, pp 709-721 (2006).

Motif-based Hessian Matrix for Aab Initio Geometry Optimization of Nanostructures, Z. Zhao, L.-W. Wang, J. Meza, Physical Review B, 73, 193309 (2006).

Using Pattern Search Methods for Surface Structure Determination of Nanostructures, Z. Zhao, J. Meza, M. van Hove, J. Phys. Condensed Matter, 18, pp 8693-8706 (2006).

Linear Scaling 3D Fragment Method for Large-scale Electronic Structure Calculations, L.-W. Wang, Z. Zhao, J. Meza, Technical Report LBNL-61691 (2006).

Identification of Severe Multiple Contingencies in Electric Power Systems, V. Donde, V. Lopez, B. Lesieutre, A. Pinar, C. Yang, J. Meza, Technical Report LBNL-60511, submitted to IEEE Transactions on Power Systems, (2006).

Identification of Severe Multiple Contingencies in Electric Power Networks, V. Donde, V. Lopez, B. Lesieutre, A. Pinar, C. Yang, J. Meza, Technical Report LBNL-57994, Proceedings 37th North American Power Symposium (2005).

Science-Driven Computing: NERSC's Plan for 2006-2010, Horst D. Simon, William T. C. Kramer, David H. Bailey, Michael J. Banda, E. Wes Bethel, Jonathon T. Carter, James M. Craw, William J. Fortney, John A. Hules, Nancy L. Meyer, Juan C. Meza, Esmond G. Ng, Lynn E. Rippe, William C. Saphir, Francesca Verdier, Howard A. Walter, Katherine A. Yelick, Technical Report LBNL-57582 (2005).

NERSC "Visualization Greenbook" Future Visualization Needs of the DOE Computational Science Community Hosted at NERSC, B. Hamann, E. Wes Bethel, Horst Simon, Juan Meza, Technical Report LBNL-51699 (2002)

Creating Science-Driven Computer Architecture: A New Path to Scientific Leadership, C. William McCurdy, Rick Stevens, Horst Simon, William Kramer, David Bailey, William Johnston, Charlie Catlett, Rusty Lusk, Thomas Morgan, Juan Meza, Michael Banda, James Leighton, and John Hules, Technical Report LBNL/PUB-5483 (2002).

A Class of Trust Region Methods for Parallel Optimization, P.D. Hough, J. C. Meza, SIAM Journal of Optimization, Vol. 13, No. 1, pp 264-282, 2002.

Can Data Recognize Its Parent Distribution? A.W. Marshall, J. Meza, I. Olkin, Journal of Computational and Graphical Statistics, Vol. 10, No. 3 (2001).

Simulation of Equipment Design Optimization in Microelectronics Manufacturing, J.C. Meza, C.H. Tong, C.D. Moen, Proceedings of the 30th Annual Simulation Symposium, Atlanta, Georgia, April 7-9, 1997.

Novel Applications of Optimization to Molecule Design, T.D. Plantenga, R.S. Judson, J.C. Meza, IMA Series "Large Scale Optimization with Applications, Part III", Ed. L. Biegler, T. Coleman, A. Conn, and F. Santosa, Vol. 94, 1997, Springer.

Parallel Optimization Methods for Agile Manufacturing. J.C. Meza, C.D. Moen, T.D. Plantenga, P.A. Spence, C.H. Tong, B.A. Hendrickson, R.W. Leland, G.M. Reese, Technical Report SAND97-8275, Sandia National Laboratories (1997).

Automatic Differentiation for Gradient-Based Optimization of Radiatively Heated Microelectronics Manufacturing Equipment. J.C. Meza, C.D. Moen, P.A. Spence, T.D. Plantenga, Proceedings of 6th AIAA/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Sept. 4-6, (1996), Bellevue, WA.

A Multigrid Preconditioner for the Semiconductor Equations. J.C. Meza and R.S. Tuminaro, SIAM J. Sci. Comput., Vol. 17, No.1, 118-132 (1996).

Asynchronous Global Optimization Techniques for Medium and Large Inversion Problems. V. Pereyra, M. Koshy and J.C. Meza, Technical Report SAND95-8591, Sandia National Laboratories (1995).

A Comparison of a Direct Search Method and a Genetic Algorithm for Conformational Searching. J.C. Meza, R.S. Judson, T.R. Faulkner and A.M. Treasurywala, J. Comp. Chem., Vol. 17, No. 9, 1142-1151, (1996)

Optimal Control of a CVD Reactor for Prescribed Temperature Behavior. J.C. Meza and T.D. Plantenga, Technical Report SAND95-8224, Sandia National Laboratories (1995).

Optimal Heat Transfer Design of Chemical Vapor Deposition Reactors. C.D. Moen, P.A. Spence and J.C. Meza, Technical Report SAND95-8223, Sandia National Laboratories (1995).

A Modification to the GMRES Method for Ill-Conditioned Linear Systems. Technical Report SAND95-8220, Sandia National Laboratories (1995).

Direct Search Methods for the Molecular Conformation Problem. M.L. Martinez and J.C. Meza, J.Comp. Chem., Vol. 15, 627-632 (1994).

OPT++: An Object-Oriented Class Library for Nonlinear Optimization. J.C. Meza, Technical Report SAND94-8225, Sandia National Laboratories (1994).

Numerical Procedures for Estimating the Parameters in a Multivariate Homogeneous Correlation Model with Unequal Variances. J.C. Meza and I. Olkin, Vol. 55, Part 3, 506-515 (1993).

A Parallel Network Computer Approach for 3D Geophysical Modeling. J.C. Meza, M. Koshy, and V. Pereyra, Technical Report SAND92-8467, Sandia National Laboratories (1992).

Conjugate Residual Methods for Almost Symmetric Linear Systems. J.C. Meza and W.W. Symes, Journal of Optimization Theory and its Applications, Vol. 72, No. 3, pp. 415-440, (1992).

Deflated Krylov Subspace Methods for Nearly Singular Linear Systems. J.C. Meza and W.W. Symes, Journal of Optimization Theory and its Applications, Vol. 72, No. 3, pp. 441-457 (1992).

Do Intelligent Configuration Search Techniques Outperform Random Search for Large Molecules? R.S. Judson, M.E. Colvin, J.C. Meza, A. Huffer, and D. Gutierrez, International Journal of Quantum Chemistry Vol. 44, 277-290 (1992).

Distributed Computing Applications in Forward and Inverse Geophysical Modeling. V. Pereyra, M. Koshy, J.C. Meza, Proceedings of the Society of Exploration Geophysicists' 1991 Annual Meeting, November 10-14, Houston, Texas.

DANCIR: A Three-Dimensional Steady-State Semiconductor Device Simulator. J.C. Meza and J.F. Grcar, Technical Report SAND89-8266, Sandia National Laboratories, (1990).

Towards the Development of Engineering Production Codes for the Connection Machine. R.E. Cline Jr., J.C. Meza, B.M. Boghosian, and B. Walker, Proceedings of the Fourth Conference on Hypercubes, Concurrent Computers and Applications, March 6-8 Monterey, California (1989).

Domain Decomposition Algorithms for Linear Hyperbolic Equations. J.C. Meza and W.W. Symes, Technical Report 87-20, Rice University (1987).

An Effective Methodology for PDE Software Development. L.K. Chen, T.K. Eccles, J.C. Meza, G.O. Morrell, A.H. Sherman, W.J. Silliman, In PDE Software: Modules, Interface and Systems, edited by B. Engquist and T. Smedsaas, Elsevier Science Publishing, New York (1984).

PRESENTATIONS

Surface Structure Determination Using Simplified Physics Surrogates, Second International Workshop on Surrogate Modeling and Space Mapping for Engineering Optimization, November 9-11, 2006. Copenhagen, Denmark.

An Introduction to Parallel Optimization Methods, SIAM Parallel Processing Conference, February 22-24, 2006. San Francisco, CA.

Generalized Pattern Search Methods for a Structure Determination Problem, SIAM Optimization Conference, May 15-19, 2005. Stockholm, Sweden.

LBNL, NERSC and ESnet Update, SOS9 Workshop, March 21-23, 2005, Davos, Switzerland

Optimization Methods for Simulation-Based Problems in Nanoscience, SIAM Computational Science and Engineering Conference, February 12-15, 2005, Orlando, FL

The Role of Mathematics in Amplifying Science Research, MSRI Workshop on Modern Mathematics, September 18, 2004, San Francisco, CA

Amplifying Science Research Through Computational Science, AGEP Seminar, Rice University, July 16, 2004, Houston, TX

The Art of Giving Talks: Some Thoughts, Advice, and Lessons Learned the Hard Way, Lawrence Berkeley National Laboratory, CS Summer Student Seminar, June 28, 2004, Berkeley, CA

Optimization Methods in Science and Engineering, SACNAS National Conference, October 2-5, 2003, Albuquerque, NM

OPT++: An Object-Oriented Toolkit for Nonlinear Optimization, Fourth Workshop on the DOE Advanced Computational Software Collection, August 24-27, 2003, Berkeley, CA

OPT++: A Toolkit for Nonlinear Optimization, 5th Annual International Conference on Industrial and Applied Mathematics Conference, July 7-11, 2003, Sydney Australia

Science Drivers for Networking: End-to-End Performance, DOE Science Networking: A Roadmap to 2008 Workshop, June 3-5, 2003, Reston Virginia

Giving a Good Talk Isn't as Hard as it Looks, Lawrence Berkeley National Laboratory Summer Student Seminar Series, July 22, 2002, Berkeley, CA

Challenges and Approaches for Simulation-Based Optimization Problems, SIAM Conference on Optimization, May 20-22, 2002, Toronto, Canada

Some New Approaches for Solving Simulation-Based Optimization Problems, San Diego State University, December 14, 2001

Parallel Optimization Methods for Simulation-Based Optimization, Richard Tapia Celebration of Diversity in Computing Symposium, October 19, 2001, Houston TX

Using Design of Computer Experiments to Quantify Uncertainty in Simulations, Sensitivity Analysis Workshop, August 17, 2001, Livermore, CA

The Role of Computational Mathematics in Industrial Problems, IMA Career Workshop in Computational Science and Engineering, May 4-6, 2001, Minneapolis, MN

Optimization Challenges and Opportunities in the ASCI Program, Workshop on PDE-constrained Optimization, April 4-6, 2001, Santa Fe, NM

Optimization Methods for Simulation-Based Problems, George Mason University, November 17, 2000, Washington DC

A Class of Trust-Region Methods for Simulation-Based Optimization, Old Dominion University, October 20, 2000, Norfolk, VA. I gave a very similar talk at Cornell University on March 31, 2000.

I want to be a Computational Mathematician, Second Minorities and Applied Mathematicians Conference-Connections to Industry and Laboratories, September 17-19, 1998, Berkeley, CA

Optimal Design and Control of Chemical Vapor Deposition Reactors. IMA Workshop, "Minorities and Applied Mathematics: Connections to Industry", October 4-6, 1996

In Search of Optimal Designs, University of California, Davis, Minority Undergraduate Research and Participation in the Physical and Mathematical Sciences, Davis, California, March 15, 1995

The Role of Mathematics in Computational Science and Engineering, University of California, Irvine, CAMP Seminar Series, Irvine, California, March 8, 1993

Massively Parallel Methods for Nonlinear Equations and Optimization, DOE/Office of Scientific Computing Workshop, Albuquerque, New Mexico, February 2-5, 1993

Massively Parallel Scientific Computation, Society for the Advancement of Chicanos and Native Americans in the Sciences, San Antonio, Texas, January 2-6, 1992

Three Dimensional Semiconductor Device Modeling, Conference on Numerical Optimization Methods In Differential Equations and Control, Raleigh, North Carolina, July 15-17, 1991

Semiconductor Device Modeling, Miniconference on Newton-Like Methods for Large-Scale Nonlinear Systems, Logan, Utah, August 27-29, 1989

Three-Dimensional Time-Dependent Semiconductor Device Modeling, Proceedings of the Fifth International Workshop on Physics of Semiconductor Devices, New Delhi, India, December 11-15, 1989

COMMITTEES

Member SIAM Science Policy Committee, 2007–2010
Member AAAS Electorate Nominating Committee Mathematics Section, 2007–2010
Member, SIAM Board of Trustees, SIAM, 2006–Present
Member, Committee on Opportunities in Science, AAAS, 2006–Present
Member, Center for Pure and Applied Mathematics, UC Berkeley, 2003-2007
Member, Department of Energy Advanced Scientific Computing Advisory Committee, 2000–2003. Also served as the chair of the ASCAC Subcommittee on Biotechnology.
Member, MSRI Human Resources Advisory Committee, 2001–2005
Member, SIAM Committee on Annual Meeting, 2001–2003
Member, SIAM Master Program Committee, 2001–2003
Co-Chair, SIAM Graduate Student Focus on Diversity Day Workshop, 2001, 2002
Co-Chair, SIAM 10th Conference on Parallel Processing for Scientific Computing, 2001
Member, Organizing Committee for SIAM Annual Meeting 2000
Member, Board of Governors, Institute for Mathematics and its Applications, 1999–2001
Member, National Partnership for Advanced Computational Infrastructure External Visiting Committee, 1999–2002
Member, External Advisory Committee for the Center for Research on Parallel Computation, 1996–1998

Editor, Society for Industrial and Applied Mathematics Special Interest Group in Optimization Views and News Newsletter, 1996–2001

Member, Parallel Tools Consortium Steering Committee, 1995–1997

Member, Advisory Board Science in California Communities Informal Science Education, 1995–1997

Editor, Society for Industrial and Applied Mathematics Special Interest Group in Linear Algebra Electronic Newsletter, 1995–1997

Member, AMS-SIAM Committee on Applied Mathematics, American Mathematical Society and Society for Industrial and Applied Mathematics 1994–1995

Member, Board of Trustees, Institute for Mathematical Sciences Education

Member, California Coalition for Mathematics Committee, 1991–1992

Member, Committee on Advising, Mathematical Association of America

Member, Committee on Materials on Careers, Mathematical Association of America