

Curriculum Vitæ

Mark A. Novotny

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*Research
Interests:*

- Computational Science, Quantum Computing, Computational Materials, Nanoscale Materials, Algorithm Development, Statistical Mechanics, Metastability, Parallelization of Algorithms, Dynamics of Materials, Magnetic Materials, Electrochemistry, Small-world Nanomaterials, Network Theory, High Performance Computing, Non-equilibrium Statistical Mechanics, Transport through Materials, Engineering Applications of Nanomaterials, Nucleation and Growth, Discrete Event Simulations.

Education:

- Ph.D., Physics, Stanford University, 1978, advisor W. A. Little, Thesis title: *I. Matrix Products with Applications to Classical Statistical Mechanics; II. Reflectivity of One-Dimensional Solids.*
- B.S., Physics, North Dakota State University, 1973.

*Employment
History:*

- Professor and Head, Department of Physics and Astronomy, Mississippi State University, 2001–present.
- Director, HPC² Center for Computational Sciences, Mississippi State University, 2002–2005.
- Scholar/Scientist, Supercomputer Computations Research Institute (SCRI), Florida State University, 1991–2001.
- Associate Scholar/Scientist, SCRI, Florida State University, 1988–1991.
- Senior Scientist, IBM Bergen Scientific Centre, Bergen, Norway, 1986–1988.
- Assistant Professor, Northeastern University, 1981–1986.
- Visiting Assistant Professor, University of Georgia, 1979–1981.
- Lecturer/Postdoctoral Research Associate, University of Georgia, 1978–1979.
- Research Assistant, Stanford University, 1974–1978.

- Professional Societies:*
- **Fellow:** American Physical Society (units DCOMP, DCMP, SSE, FIAP, FED, GMAG); **Fellow:** AAAS.
- Current Funding:*
- US Air Force Research Laboratory, Award FA8750-18-0096, “QuAnCo Applied to Boltzmann Machines”, 2018-2019 (12 months), PI with co-PI Prof. Y. Koshka (MSU ECE), \$484,819.
- Select Previous Funding:*
- National Science Foundation, DMR-12062033, 2012-2016, “Computational Studies of Nonequilibrium Dynamics of Classical and Quantum Systems”, \$248,341.
 - Idaho Bailiff, Task E4, Boltzmann machines, \$600,000, May 2015-May 2016 (1 year), Pacific Northwest National Laboratory.
 - National Science Foundation, DMR-1339172, 2013-2014, co-PIs M. Jarrell (LSU and C. Roland (NCSU), “Young Investigator Support to Attend the XXV IUPAP Conference on Computational Physics”, \$18,200, funded four young US investigators to attend conference in Moscow, Russia.
 - Ultralife Corporation (CERDECC, US Army), 12/2009–12/2011, \$249,866, with co-PI Prof. David Wipf (MSU Chemistry), “Confirmation and Development of a Fast-Charging Method for Li-Ion Cells”.
 - National Science Foundation, 2005–2009, \$360,000, with co-PI Prof. P.A. Rikvold (FSU physics, MARTECH), “Computational Studies of Dynamical Phenomena in Nanoscale Ferromagnets”, funded by the DMR (Division of Materials Research).
 - National Science Foundation, 2004–2007, \$550,000, with co-PI Prof. G. Korniss (RPI physics), “ITR-(ASE+NHS)-(sim+dmc): Non-Equilibrium Surface Growth and the Scalability of Parallel Discrete Event Simulations for Large Asynchronous Systems”, funded by the DMR and ITR (Information Technology Research) for National Priorities.
 - ABSL, 2006–2007, \$209,990, “MSU Center for Advanced Portable Electric Power”, Task 2, Supercomputer Simulation and Modeling, co-PI, PI Mark White (MSU Chemical Engineering), funded by company ABSL (from U.S. Army).
 - U.S. Department of Energy, 2006–2007, \$100,113, Funded through MSU Southeastern Energy Center (SEC), “Renewable Hydrogen Production from Biorefinery Co-products and Effluents”, co-PI, PI Sandun Fernando (MSU Ag and Bio Engineering), Task 1.2.2, Development of Mathematical Models and Simulation of Nanodroplets.
 - National Science Foundation, 2001–2004, \$450,000, “ITR/AP(MPS) Non-Equilibrium Surface Growth and Scalability of Parallel Discrete Event Simulations”, with co-PI Prof. G. Korniss (RPI physics), funded by the DMR and ITR (Information Technology Research).
 - National Science Foundation, 2001–2004, \$330,000, with co-PI P.A. Rikvold (FSU physics, MARTECH, SCR1), “Computational Studies of

Dynamical Phenomena in Nanoscale Ferromagnets”, funded by the DMR.

- U.S. Department of Energy, 2000, Computational Materials Science Network (CMSN), \$19647, to fund 1/2 post-doc.
- National Science Foundation, 1998–2001, \$450,000, with co-PI Prof. P.A. Rikvold (FSU physics, MARTECH, SCRI), “Computational Studies of Dynamical Phenomena in Nanoscale Ferromagnets”, funded by the DMR and NCC (New Computational Challenges) within the KDI (Knowledge & Distributed Intelligence) initiative.
- National Science Foundation, 1995–1998, \$434,000, Computational Approaches to Real Materials, CARM95, with co-PI Prof. P.A. Rikvold “Computational Studies of Dynamical Phenomena in Nanoscale Ferromagnets”, funded by the DMR, ASC (Division of Advanced Scientific Computing), DMS (Division of Mathematical Sciences), and OMA (Office of Multidisciplinary Activities)
- National Science Foundation, 1999, \$12,000, with co-PIs B. Berg, H. Meirovitch, and P.A. Rikvold (FSU), “Monte Carlo and Structure Optimization Methods for Biology, Chemistry, and Physics”, to support workshop held at Florida State U, March, 1999.
- U.S. Department of Energy, 1994–1997, \$135,000, with J.R. Schrieffer and L. Gor’kov, “Theoretical Studies of Magnetic Systems”.

Publications:

Over 205 refereed publications:

- 10 in *Physical Review Letters*; 2 in *Europhysics Letters*; 1 in *Science*; 3 in *Physical Review A*; 33 in *Physical Review B*; 23 in *Physical Review E*, and 1 in *Physical Review Applied*.
- 40 invited publications.
- 1 US patent (issued in 2006, U.S. patent number #6,996,504); 2 provisional US patent applications (both in 2014).
- Many papers, reprints and preprints available online.

Mentorship:

- Undergraduate students mentored in research – 16
- Undergraduate student co-authors – 5
- High school students mentored – 5
- High school student co-authors – 4
- Graduate students mentored – 23
- Graduate student co-authors – 15
- Post-Doctorate associates mentored – 14
- Post-Doctorate associates as co-authors – 16

Presentations:

- All recent presentations: 6 in 2018, 5 in 2017, 7 in 2016, 5 in 2015, 2 in 2014, 7 in 2013, 2 in 2012, 9 in 2011, 5 in 2010, 6 in 2009, 3 in 2008, 5 in 2007, 13 in 2006, 9 in 2005, 7 in 2004, 7 in 2003, 5 in 2002, 12 in 2001, 11 in 2000, and 8 in 1999.
- Invited conference talks: 3 in 2018, 2 in 2017, 2 in 2016, 1 in 2015, 1 in 2014, 1 in 2012, 2 in 2011, 1 in 2010, 2 in 2009, 3 in 2008, 5 in 2007,

11 in 2006, 2 in 2005, 1 in 2004, 2 in 2003, 1 in 2002, 3 in 2001, 2 in 2000, and 3 in 1999.

Selected Invited Presentations:

- Qubits 2018, D-Wave Users Conference, *Classical and Noncommutative Boltzmann Machines: An Update from the Magnolia State*, Knoxville, TN, Sept. 2018.
- 42nd International Conference of Theoretical Physics: Correlation and Coherence at Different Scales, *How to Approach a Quantum Dragon*, Ustron, Poland, Sept., 2018.
- Canary Center at Stanford, *Quantum Computing: All Hype or Huge Advance?*, Stanford, CA, Jan. 2018.
- Qubits 2017, D-Wave Users Conference, *Cyber Security --- Just Do It*, National Harbor, MD, September 2017.
- Univerzita Karlova, Matematico-fyzikální fakulta, Strouhalovskou přednášku, (Strouhal Lecture, Charles University), *Adiabatic Quantum Computers in 2017: Huge Advance or All Hype?*, Prague, Czech Republic, March 1, 2017.
- Faculty of Mathematics and Physics, Charles University, *Quantum Dragons: Fictional? Factual? Physics? Phantasy?*, Prague, Czech Republic, October 13, 2016
- International Workshop on Quantum Annealing and its Applications in Science and Industry (QuASSI'16), *Explorations on Quantum Annealers: Past, Present, and Future*, Jülich, Germany, July 26-27, 2016.
- Looking Beyond CMOS Technology for Future HPC, *Adiabatic Quantum Computers: Testing and Selected Applications*, sponsored by Oak Ridge National Laboratory, Hanover, MD, April 5-6, 2016.
- International Conference on Computer Simulations in Physics and Beyond, *Spanning Trees, Continents, and the Quantum-Classical Divide on D-Wave 2 Machines*, Moscow, Russia, Sept. 6-9, 2015.
- 25th Annual Workshop on 'Recent Developments in Computer Simulation Studies in Condensed Matter Physics', *When Exabytes Are Not Enough: An Efficient Quantum Algorithm for Dynamics of a Spin System Coupled to Specific Spin Baths*, Athens, GA, February 20-24, 2012.
- Mardi Gras Conference on Computational Materials & Biosystems, *Surprises, Computational Methods, and Results for Metastable Phenomena and Homogeneous Nucleation and Growth*, Baton Rouge, LA, February 16-18, 2012.
- VI Brazilian Meeting on Simulational Physics, *Matrix and RG Methods for Calculating Quantum Transport*, Cuiabá, Brazil, Aug. 2-6, 2011.
- Telluride Summer School on 'Searching for Reaction Coordinates and Order Parameters', *Projective Dynamics for Long-Time Simulations*, Telluride, CO, June 21-25, 2010.
- Workshop on Computations in Nanotechnology, *Going through Rough Times: Parallel Discrete Event Simulations — a Physicist's Perspective*, Technion, Israel, April. 21-24, 2009.

- Workshop on Long-Time Simulations in Engineering and Physics, *Rejection-Free and Monte Carlo with Absorbing Markov Chain Methods for Long Time Simulations*, Tokyo, Japan, Feb. 2, 2009.
- Workshop on Novel Aspects of Phase Transitions with Long-range Interactions, *Can Pseudo-long-range Interactions make Small-world Nanomaterials Possible?*, Tokyo, Japan, Oct. 28-30, 2008.
- Workshop on Complexity in Materials Far from Equilibrium, *Far from Equilibrium Processes in Magnetic Nanomaterials and Thin Films*, Virginia Tech, Blacksburg, VA, May 13-16, 2008.
- Workshop ‘Practice and Theory of Stochastic Simulation’, *Advanced Algorithms for Dynamic Monte Carlo Simulations*, American Institute of Mathematics (AIM), Palo Alto, CA, Oct. 22-26, 2007.
- 3rd International Workshop on Simulation Physics 2006 Hangzhou, *Non-equilibrium Statistical Physics Applied to Parallel Computing*, Zhejiang University, Hangzhou, China, Nov. 16-18, 2006.
- International Workshop on Simulation Physics, *Dynamic Phase Transition: Simulations and Experiments in Magnetic Thin Films*, Shaanxi Normal University, Xi’an, China, Nov. 12, 2006.
- Workshop on Microfluidics and Kinetic Monte Carlo and SSA, *Projective Dynamics for Accelerated Dynamic Simulations*, Dept. of Mathematics, Princeton University, Princeton, NJ, Oct. 14-16, 2006.
- 232nd American Chemical Society National Meeting, *Projective Dynamics and Rejection-Free Methods for Accelerated Dynamic Monte Carlo Simulations*, San Francisco, CA, Sept. 10-14, 2006.
- Cyberinfrastructure in Materials Science Workshop, *Perfect Scalability: from Materials to Informatics and Back*, National Science Foundation (Division of Materials Research), Arlington, VA, Aug. 3-5, 2006.
- US-Japan bilateral Seminar on Simulations of Complex Behavior from Simple Models, *Complicated Behavior in Mixing Random Deposition with other Non-equilibrium Surface Growth Processes*, Kaanapali Beach, Maui, HI, July 17-20, 2006.
- IV Brazilian Meeting on Simulation Physics, *Finite-size Scaling of Ising Models Associated with Physical Small-World Nanomaterials*, Ouro Preto, Brazil, August 10–12, 2005.
- Workshop on Current Topics in Micromagnetics, Courant Institute of Mathematical Sciences, *Advanced Computational Methods for Finite-Temperature Magnetization Dynamics*, New York, NY, June 1–3, 2005.
- GDIN 2004 (Global Disaster Information Network), *Perfectly Scalable Discrete Event Simulations for ‘at the right time’ Information*, Washington, DC, March 25–29, 2004.
- NATO ARW on *Nanostructured Magnetic Materials and Their Applications*, Istanbul, Turkey, July 1–4, 2003.
- Symposium on Non-Equilibrium Statistical Mechanics in the New Millennium, Boston U., Boston, MA, March 2003.
- NATO ASI and Euroconference on *Computer Simulations of Surfaces and Interfaces*, Albena, Bulgaria, Sept. 10–20, 2002, two lectures.

- 46th Annual Conference on Magnetism and Magnetic Materials, Seattle, WA, Nov. 2001.
- Conference on Computational Physics (CCP), Aachen, Germany, Sept. 2001.
- Workshop on Micromagnetics, Math Department, Princeton University, NJ, June, 2001.
- American Chemical Society 220th national meeting, Washington D.C., August, 2000.
- Ising Centennial Seminar, Cologne, Germany, June 2000.
- International Materials Research Conference, Cancun, Mexico, August 1999.
- US-Japan bilateral seminar on ‘Understanding and Conquering Long Time Scales in Computer Simulations’, Maui, Hawaii, July 1999.
- International Conf. Computational Physics, Atlanta, GA, March 1999.

*Conferences
Co-Organized:*

- 9th Mississippi State - UAB Conference on Differential Equations and Computational Simulations, Local Committee Member, Starkville, MS, Oct. 4-6, 2012.
- “Monte Carlo and Structure Optimization Methods for Biology, Chemistry, and Physics”, March 28–30, 1999, Tallahassee, Florida. Partially funded by the NSF and SCRI. Workshop had 86 registered participants. Workshop financial support provided to 44 junior researchers (graduate students and post-docs) and 18 invited speakers.
- VECPAR 98, 3rd International Meeting on Vector and Parallel Processing, 1998, Porto, Portugal, member of Scientific Committee.
- STATPHYS 16, August 11–15, 1986; Boston, MA, member of local organizing committee.

Select Service:

- 2011-2013, International Advisory Board, XXV Conference on Computational Physics, Moscow, Russia, held August 20-24, 2013.
- 2011-2012 member of Program Committee for APS DCOMP.
- 2008, 2009, 2010, 2011: Panel reviewer at National Science Foundation on eXtreme Digital, tasks CMS/AUSS/TEOS, successor to Teragrid.
- 2009 Panel review at National Science Foundation on XD TeraGrid TAIS task.
- 2007-2011 Metropolis Prize Committee (graduate dissertations), DCOMP (Division of Computational Physics), American Physical Society (APS); Chair of committee in 2010.
- 2006 Chaired award committee for the SESAPS (Southeastern Section of the American Physical Society) Jesse W. Beams research award.
- 2006 member of steering committee for National Science Foundation Division of Materials Research on cyberscience and cyberinfrastructure.
- 2005 ran for Vice-Chair of the Division of Computational Physics (DCOMP) of the American Physical Society (APS).

- 2004, lead author on report entitled *Materials Research Cyberscience enabled by Cyberinfrastructure* for the Division of Materials Research of the National Science Foundation;
See: <http://www.nsf.gov/mps/dmr/csci.pdf>.
- 2002-2005 served as elected Member-at-Large of Division of Computational Physics (DCOMP) of the APS.
- 2001-2006 served at various times on different committees of the Division of Computational Physics (DCOMP) of the American Physical Society (APS): Nominating Committee (twice, once as chair), Metropolis Prize Committee, Rahman Prize Committee.
- 1999 served on NSF preproposal panel for KDI (Knowledge and Distributed Intelligence) initiative.
- 1999 chair of Nominating Committee for Division of Computational Physics of the APS.
- 1998 served on NSF proposal panel for KDI (Knowledge and Distributed Intelligence) initiative.
- 1998 vice-chair of Nominating Committee for Division of Computational Physics of the APS.

Personal Honors:

- 2016-2017, Fulbright Distinguished Chair award, spending 2016-2017 sabbatical year in the Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic
- 2013 designated William L. Giles Distinguished Professor, highest honorary distinction awarded to Mississippi State University faculty.
- 2013 Elected Fellow of AAAS, Physics Division
- 2012 ‘Dynasty Foundation Visiting Scientist’: one of 40 foreign physicists, mathematicians, and biologists awarded travel grant to spend a fortnight visiting and speaking at academic institutions in Russia.
- 2011 selected as ‘Outstanding Referee’ by the American Physical Society.
- 2006 Faculty Research Award, College of Arts & Sciences, MSU (one award given annually from the college).
- 2000 Elected Fellow of the American Physical Society (through DCOMP).
- 2000 listed in Marquis “Who’s Who in the World”.
- 1995 ‘Distinguished Foreign Researcher Study Grant’, Tokyo Metropolitan University, Japan.

Other Honors:

- Undergraduate co-author, Christina White, awarded a two year Goldwater Fellowship, 1999.
- Undergraduate co-author, Dean M. Townsley, whom I mentored in research for 3 years, 1998 NSF Graduate Fellowship.
- Co-supervised graduate student and co-author, H.L. Richards, 1995 Sigma Xi Fisher award for best FSU student research paper.

Select

Administration:

Department Head, Physics and Astronomy, MSU, 2001-present:

- Hired and retained quality faculty and staff; faculty include winners of both research and teaching awards at college, university, and regional levels. The quality and quantity of scholarship has grown over the years. MSU total student main-campus enrollment grew from 14,395 in Fall 2005 to 20,100 in Fall 2014. Encouraged interdisciplinary and multidisciplinary research, education, and grantsmanship where appropriate.
- Ph.D. program in Physics under the College of Arts & Sciences initiated, first admitted class in Fall 2014.
- Dramatically increased graduate student numbers. From 10 in Fall 2000 to 45 in Fall 2011. Graduate students won university-wide research awards. Increase number of permanent TA positions, 6.5 in 1999-2000 to 8.5 in 2011-2012. Increased substantially number of MS and PhD degrees awarded.
- Grantsmanship in the department increased in number of grants and average amount of grants. Through the Department in 2000 faculty had 3 external grants for \$264,397; in Spring 2012 all but one tenured/tenure-track faculty were supported by external funds with 2011 expenditures of \$1,329,257. In addition, in 2011 faculty utilized \$1,531,379 in external research dollars through MSU interdisciplinary and multidisciplinary centers and institutes (only counting dollars spent directly by departmental faculty and students, not including umbrella grants or infrastructure monies or monies spent by adjunct faculty). Note: *NSF Science and Engineering Indicators: 2010* lists MSU with \$211 million as 83rd in R&D expenditures by academic institutions. MSU has just been reclassified by the Carnegie Foundation as RU/VH: Research Universities (very high research activity), the highest classification of US Universities.
- Provided excellent instruction to all MSU students. Student teaching evaluations of faculty are excellent (average 4.2 out of 5.0 as Fall 2010 average), compared to 4.2 for Fall 2010 average for all MSU classes. This in spite of physics being a traditionally difficult class with high failure rates and guarding against grade inflation.
- Ensured quality education for department majors, with many being successful in top-ranked graduate schools.
- Encouraged undergraduate research.
- Encouraged technological enhancements, one example lead to MSU-wide eInstruction clickers.
- Endowed funds of Department currently 3.7 times the amount in 2000. Worked across departments and colleges with several donors.
- Fostered and maintained collegial and entrepreneurial atmosphere.
- Fostered and maintained commitment to excellence and integrity.
- Fostered and maintained welcoming environment for underrepresented and international students and faculty.
- Enhanced Department outreach. Annual physics competition for high school students. Funded summer workshops and classes for K-12

teachers. Demonstrations performed in middle and high school classes. Public viewing nights at Howell Observatory. Encouraged miscellaneous service: judging science fairs, serving as reviewers of proposals and articles, and *Physics of Football* on JumboTron during games. Service in aftermath of hurricanes Katrina and Rita, and other disasters.

- Longest serving Head in College of Arts & Sciences. Annual confidential evaluations of administrators consistently rank among the top MSU Department Heads.
- Served on various MSU committees, a few include committees for search for MSU President (twice), Faculty Research Advisory Committee (last 3 years), Chaired search for head of Department of Mathematics and Statistics (2006), elected to Academic Department Heads Executive Committee (2012).

Director, HPC² Center for Computational Sciences (CCS), MSU, 2002-2005:

- Founding Director of CCS, under the College of Arts & Sciences. Directed HPC² (High Performance Computing Collaboratory) in concert with Directors of other HPC² centers and institutes (which reported to College of Engineering, College of Agriculture, and Office of the Vice President for Research).
- HPC² is a follow-on to the MSU NSF-funded ERC, 1990-2001. After one year of inadequate leadership after the ERC graduation from NSF, HPC² was formed by engineers, scientists, and agricultural faculty interested in high performance computing. The HPC² has flourished since 2002, including faculty and students from across MSU.
- HPC² centers and institutes have annual external funding of about \$50 million.
- Currently a member of CCS, and make use of the HPC² machines: including a 34.4 TeraFLOP computer (3072 processor cores running at 2.8 GHz) installed May 2010 at a cost of about \$2 million. Currently HPC² is in the process of purchasing a new high performance computer.

Group Leader: IBM Bergen Scientific Centre, 1986-1988:

- Built computational physics group from zero to an active and productive group of six permanent scientists, plus many visitors. Excellent working relationships with research groups in academia and industry in Norway and other Nordic countries.