Jack C. Wells (wellsjc@ornl.gov)
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Education and Training

Oak Ridge National Laboratory (ORNL)	Wigner Fellowship	1997-1999
Harvard-Smithsonian Astrophysical Observatory	Postdoctoral Fellowship	1994-1997
Vanderbilt University	Theoretical Physics, Ph.D.	1994
Vanderbilt University	Theoretical Physics, M.S.	1989
Centre College	Physics, B.A., *Magna Cum Laude*	1985

Professional Experience

01.2020 –	Director, Strategic Planning and Performance Management, Office of the Laboratory Director, ORNL.
07.2011 – 12.2019	Director of Science, National Center for Computational Sciences (NCCS), Oak Ridge Leadership Computing Facility (OLCF), ORNL.
08.2009 – 10.2011	Director, Office of Strategic and Institutional Planning, ORNL.
08.2009 – 10.2011	Director, Advanced Research Projects Agency Programs, ORNL.
02.2009 – 09.2010	Director, Electrochemical Energy Storage Initiative, Laboratory Director's R&D (LDRD) Program, ORNL.
10.2008 – 08.2009	Director, Nanomaterials Theory Institute (NTI), Center for Nanophase Materials Sciences (CNMS), ORNL.
10.2008 – 08.2009	Group Leader, Computational Materials Sciences (CMS Group), Computer Science and Mathematics Division (CSMD), ORNL.
08.2006 – 08.2008	Legislative Fellow, Office of U.S. Senator Lamar Alexander (R-TN), U.S. Senate.
2005 – 2011	Senior Staff Scientist, NTI, CNMS & CMS Group, CSMD, ORNL.
2003 – 2006	Technical Assistant to the Associate Laboratory Director, Computing and Computational Science Directorate, ORNL.
2002 – 2005	Research Staff Scientist, CMS Group, CSMD, ORNL.
2000 – 2001	Group Leader, Computational Nanotechnology (CN), Center for Engineering Science Advanced Research (CESAR), CSMD, ORNL.
1999 – 2002	Research Staff Scientist, CN Group, CESAR, CSMD, ORNL.
09.1997 – 08.1999	Wigner Fellow, Center for Computational Sciences, ORNL.
08.1996 – 12.1996	Institute for Theoretical Physics (ITP), University of California at Santa Barbara: Program: New Ideas for Particle Accelerators.
09.1994 – 08.1997	Postdoctoral Fellow, Institute for Theoretical Atomic and Molecular Physics (ITAMP), Harvard-Smithsonian Astrophysical Observatory, Harvard University
09.1994 – 08.1997	Visiting Scientist, Theoretical Physics Group, Physics Division, ORNL.
10.1990 – 08.1994	Graduate Research Fellow, Theoretical Physics Group, Physics Division, ORNL.
01.1994– 05.1994	Assistant Professor, Pikeville College, Pikeville, Kentucky.
1991	Pre-doctoral Fellow, ITAMP, Harvard University.

08.1991 – 12.1991 Institute for Theoretical Physics (ITP), University of California at Santa Barbara: Program: Time Dependent Phenomena in Atomic, Molecular, and Optical Physics.

1989 – 1990 Research Assistant, Department of Physics, Vanderbilt University.

Professional, Society Leadership, & Service Activities

- Vice-Chair of Division of Computational Physics (DCOMP), Executive Committee, American Physical Society (APS), 2019. First year of four-year chair rotation for DCOMP Executive Committee. https://www.aps.org/units/dcomp/governance/officers/index.cfm
- Vice-President, OpenACC. OpenACC is a nonprofit organization founded to enable and educate researchers do more science and less programming by providing a high-level directives-based programming model for high performance computing. https://www.openacc.org/about
- Co-Organizer & Chair, APS Division of Computational Physics (DCOMP) Focus Session at APS March Meeting, (2019, 2020), "Building the Bridge to Exascale: Applications and Opportunities for Materials, Chemical, and Biophysical Sciences".
- Co-Organizer & Chair, APS Division of Plasma Physics (DPP) Mini-Conference at 2019 DPP Meeting (2019), "Building the Bridge to Exascale Computing: Applications and Opportunities for Plasma Science". https://www.aps.org/units/dpp/meetings/annual/mini.cfm
- Co-Organizer & Co-chair, International Workshop on OpenPOWER for HPC at ISC Conference (IWOPH'16, IWOPH'17, IWOPH'18, and IWOPH'19) https://indico-jsc.fz-juelich.de/event/87/.
- Steering Committee, Platform for Advanced Scientific Computing (PASC) Conference, 2018-2020. https://www.pasc-conference.org/about/steering-commitee/
- Co-Organizer, US-Japan Joint Institute for Fusion Theory Workshop on Exascale Computing, Nagoya (2015), Oak Ridge (2016), Tokyo (2017), Princeton (2018), Kobe (2019).
- Member, Data Working Group, Neutron Sciences Directorate, ORNL, 2019.
- Chair, Internal Review Committee on Data Lifecycle Management for Neutron Sciences Directorate, ORNL, 2018.
- Co-Organizer & Chair, APS Division of Computational Physics (DCOMP) Focus Session at APS March Meeting, (2014, 2015, 2016, 2017, 2018) "Petascale Science and Beyond: Applications and Opportunities for Materials, Chemical, and Biophysical Sciences".
- Co-Chair, Papers Program & Mini-symposium and Posters Program, Platform for Advanced Scientific Computing (PASC) Conference PASC-18, Basel, Switzerland, July 2018. https://pasc18.pasc-conference.org/ .
- Chair, Papers Program, Platform for Advanced Scientific Computing (PASC) Conference: PASC-17, Lugano, Switzerland, June 2017, and PASC18, Basel, Switzerland, July 2018.
- Chair, International Advisory Committee, BEAM-ME Project - Developing speed-up methods from Applied Mathematics and Computer Science for the optimization of energy systems models, German Federal Ministry for Economic Affairs and Energy (BMWi); Stuttgart (2016), Frankfurt (2017).
- Member, ORNL Research Conflict of Interest (RCOIAC) Advisory Committee, 2012 - present.
- Organizing Committee, DOE Exascale Requirements Review, 2015-2017, https://exascaleage.org/.
- Member, ORNL Information Technology Advisory Committee, 2012 - 2016.
- Member, Advisory Board, L&N STEM Academy, Knoxville, TN, 2011 –2013.
- Technical Program Committee, Applications Subcommittee, SC14 (The Supercomputing Conference).

- Program Committee, Smoky Mountain Computational Sciences and Engineering Conference (2011-2017), Gatlinburg, TN.
- Program Committee: Symposium on Energy Storage Beyond Lithium Ion (BLI) 2010 – 2014.
- General Chairman; Symposium on Energy Storage Beyond Lithium Ion, BLI-III: Materials Perspectives, October 7 – 8, 2010, Oak Ridge National Laboratory.
- Program Committee Chairman, Symposium on Energy Storage Beyond Lithium Ion, BLI-II: Computational Perspectives, May 3 – 4, 2010, Argonne National Laboratory.
- Program Chair, Accelerating Computational Sciences Symposium, March 29-30, 2012, Washington DC.
- Member, Advisory Board, NanoScience Center, University of South Carolina, 2009-2010.
- Editor and Working Group Member, SciDAC-2 Strategic Plan, DOE, Office of Advanced Scientific Computing Research, 2005.
- Program Committee, Fall Creek Falls Conference on Computational Science, 2004 – 2005.
- Review Panel for National Science Foundation (NSF), Information Technology Research (ITR), Revolutionary Computing (RC) Program, 2001; NSF/AMO Theory Program, 1998-2003: DOE, Nanoscale Science, Engineering, and Technology Research (NSET) Program, 2001; DOE, Small Business Innovation Research (SBIR) Program, 2001.
- Referee for: DOE SBIR, The Physical Review, Physical Review Letters, Chemical Physics Letters, and Computer Physics Communications.
- Member: APS, AAAS, ACM-SIGHPC.

Honors & Awards

- HPCWire 2019 "People to Watch," https://www.hpcwire.com/people-to-watch-2019/ .
- Wendell G. Holladay Award & Lecture, (Distinguished Alumnus Award) Vanderbilt University Department of Physics and Astronomy, 2009.
- Lockheed-Martin Development Accomplishment Award, ORNL, 1999.
- DOE Travel Award, 1998.
- Wigner Fellow, ORNL, 1997 – 1999.
- National Science Foundation Travel Award to attend NATO Advanced Study Institutes (1993, 1989).
- Dissertation Enhancement Award, Vanderbilt University, 1989.
- Sigma Pi Sigma, Vanderbilt University, 1988.
- Phi Beta Kappa, Centre College, 1985.
- Trustee Scholar, Centre College, 1982 – 1985.
- Harold P. Brown Engineering Fellowship, Washington University in St. Louis, 1984.

Teaching Experience

- "Introductory Quantum Mechanics," an undergraduate course offered through the Oak Ridge Science Semester, Great Lakes College Association, 2002.
- "Introductory Physics", an undergraduate course offered at Pikeville College, 1994.

Diversity, Equity, and Inclusion (DEI)

Demonstrates commitment to diversity, equity, and inclusion through actions.

- Professional mentorship and collaboration with colleagues from under-represented groups.
- Experienced in communicating values with leaders, collaborators, and partners internal and external to my organization.
- Participation in continuing DEI education, e.g., ORNL's Courageous Leaders' Summit, April 2019.
- Participation in community science and technology outreach and awareness activities.
- Lead community and educational tours of the Oak Ridge Leadership Computing Facility.

Research Support

Date	Agency/Project	Funding($)	Status
FY11 – FY20	DOE/ASCR, Oak Ridge Leadership Computing Facility	~100M/year	Ongoing
07/16 – 06/19	DOE/ASCR, Big PanDA Workflow Management (Co-PI)	1.4M/year	Complete
FY17 – FY18	LDRD, Understanding HPC Apps, (CAASCADE project) (PI)	573 total	Complete
FY16	PD, Exascale Computing Project (ECP) – App. Dev. (PI)	146K total	Complete
FY16	PD, Exascale Computing Project (ECP) – Codesign Centers (PI)	32K total	Complete
FY05 – FY09	DOE/BES, Center for Nanophase Materials Sciences (Co-PI)	19M/year	Complete
FY03 – FY06	DOE/BES, Design and Synthesis of Nanomaterials (Co-PI)	300K/year	Complete
FY03 – FY04	ORNL/Seed, Global Optimization for Remote Sensing (PI)	125K total	Complete
FY03 – FY04	ARDA/NSA, Oriented Polymer Nanostructures (Co-PI)	60K/year	Complete
FY00 – FY03	DOE/BES, Robotics and Intelligent Machines (Co-PI)	300K/year	Complete
FY02	ARDA/NSA, Molecular Single-Electron Latching Switches (PI)	50K total	Complete
FY03	Charge Transport in Conducting Polymer Nanostructures (co-PI)	80K total	Complete
FY02 – FY03	ORNL/LDRD, Growth of Carbon Nanotubes (Co-PI)	400K total	Complete
FY01 – FY03	DOE//BES, Nano-structural Photonics (PI)	120K total	Complete
FY00 – FY02	ORNL/LDRD, Computing with Arrays of Quantum Dots (Co-PI)	720K total	Complete
FY00 – FY01	ORNL/SEED, Correlated Structure in Quantum Dots (PI)	100K total	Complete

Supercomputing Resource Support

CY10 DOE INCITE Program, "Understanding the Ultimate Battery Chemistry: Rechargeable Li/Air" (PI)
- Jaguar, Cray XT (12,000,000 processor hours)
- Intrepid, IBM Blue Gene/P (12,000,000 processor hours)

CY11 DOE INCITE Program, "Understanding the Ultimate Battery Chemistry: Rechargeable Li/Air" (PI)
- Jaguar, Cray XT (10,000,000 processor hours)
- Intrepid, IBM Blue Gene/P (15,000,000 processor hours)

PUBLICATION LIST: Dr. Jack C. Wells

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ResearcherID: D-3675-2016

Edited Volumes

1. A. Korkin, P.S. Krstic, and J.C. Wells, *Nanotechnology for Electronics, Photonics, and Renewable Energy*, Editors, Springer (2011). (http://www.spinger.com/materials/nanotechnology/book/978-1-4419-7234-7). DOI 10.1007/978-1-4419-7454-9.
2. O. R Hernandez, M. G. Lopez, D. Pleiter, J.C. Wells, "International Workshop on OpenPOWER for HPC (IWOPH'16)," High Performance Computing: ISC High Performance 2016 International Workshops, Germany, June 23, 2016, Revised Selected Papers. Vol. 9945, Pages. 170. Springer. https://link.springer.com/content/pdf/10.1007%2F978-3-319-46079-6.pdf
3. O. R Hernandez, M. G. Lopez, D. Pleiter, J.C. Wells, "International Workshop on OpenPOWER for HPC (IWOPH'17)," High Performance Computing: ISC High Performance 2017 International Workshops, Germany, June 22, 2019, Revised Selected Papers. Springer. https://link.springer.com/content/pdf/10.1007%2F978-3-319-67630-2.pdf
4. O. R Hernandez, M. G. Lopez, D. Pleiter, J.C. Wells, "International Workshop on OpenPOWER for HPC (IWOPH'18)," High Performance Computing: ISC High Performance 2018 International Workshops, Germany, June 28, 2018, Revised Selected Papers. Springer. https://link.springer.com/content/pdf/bfm%3A978-3-030-02465-9%2F6%2F1.pdf

Journal Papers

1. J.C. Wells, V.E. Oberacker, A.S. Umar, C. Bottcher, M.R. Strayer, J.-S. Wu, and G. Plunien, "Nonperturbative Electromagnetic Lepton-Pair Production in Peripheral Relativistic Heavy-Ion Collisions." *Phys. Rev. A* **45**, 6296 (1992). DOI: 10.1103/physreva.45.6296
2. V.E. Oberacker, A.S. Umar, J.C. Wells, M.R. Strayer, and C. Bottcher, "Study of Nuclear Dissipation via Muon-induced Fission: a Relativistic Lattice Calculation," *Phys. Lett. B* **293**, 270 (1992). DOI: 10.1016/0370-2693(92)90882-5
3. J.C. Wells, A.S. Umar, V.E. Oberacker, C. Bottcher, M.R. Strayer, J.-S. Wu, J. Drake, and R. Flanery, "A Numerical Implementation of the Dirac Equation on a Hypercube Multicomputer," *Int . J Mod. Phys. C* **4**, 459 (1993). DOI: 10.1142/s0129183193000501
4. D.J. Dean, C. Bottcher, M.R. Strayer, and J.C. Wells, "Parallel Implementation of 3+1-Dimensional Relativistic Hydrodynamics." *Int. J. Mod Phys. C* **4**, 1023 (1993). DOI: 10.1142/s0129183193000793
5. V.E. Oberacker, A.S. Umar, J.C. Wells, C. Bottcher, M.R. Strayer, and J. Maruhn, "Muon-induced fission: a probe for nuclear dissipation and fission dynamics." *Phys. Rev. C* **48**, 1297 (1993). DOI: 10.1103/physrevc.48.1297
6. D.J. Dean, C. Bottcher, M.R. Strayer, J.C. Wells, A. von Keitz, Y. Pursun, D.-H. Rischke, and J.A. Maruhn, "Comparison of Flux-correcting and Spline Algorithms for Solving (3+1)-dimensional Relativistic Hydrodynamics," *Phys. Rev. E* **49,** 1726 (1994). DOI: 10.1103/physreve.49.1726
7. J.C. Wells, V.E. Oberacker, M.R. Strayer, and A.S. Umar, "Spectral Properties of Derivative Operators in the Basis-Spline Collocation Method," *Int. J. Mod. Phys. C* **6**, 143 (1995). DOI: 10.1142/s0129183195000125
8. M.C. Guclu, J.C. Wells, A.S. Umar, M.R. Strayer, and D.J. Ernst, "Impact-Parameter Dependence of Multiple Lepton-Pair Production from Electromagnetic Fields." *Phys. Rev. A* **51**, 1836 (1995). DOI: 10.1103/physreva.51.1836

9. P. Gavras, M.S. Pindzola, D.R. Schultz, and J.C. Wells, "Direct Solution of the Time-dependent Schroedinger Equation for Proton-Hydrogen Collisions in two-dimensional Cartesian Space," *Phys. Rev. A* **52,** 3868, (1995). DOI: 10.1103/physreva.52.3868

10. J.C. Wells, V.E. Oberacker, M.R. Strayer, and A.S. Umar, "Convergence of a lattice Calculation for Bound-free Muon-pair Production in Peripheral Relativistic Heavy-ion Collisions," *Phys. Rev. A* **53**, 1498 (1996). DOI: 10.1103/physreva.53.1498

11. D.R. Schultz, P.S. Krstic, C.O. Reinhold, and J.C. Wells, "Ionization of hydrogen and hydrogenic ions by antiprotons," *Phys. Rev. Lett.* **76**, 2882 (1996). DOI: 10.1103/physrevlett.76.2882

12. J.C. Wells, D. R. Schultz, P. Gavras, and M.S. Pindzola, "Numerical Solution of the Time-dependent Schrödinger Equation for Intermediate-Energy Collisions of Antiprotons with Hydrogen," *Phys. Rev. A* **54**, 593 (1996). DOI: 10.1103/physreva.54.593

13. D.R. Kegley, V.E. Oberacker, M.R. Strayer, A.S. Umar, and J.C. Wells, "Basis-Spline Collocation Method for Solving the Schrödinger Equation in Axially Symmetric Systems," *J. Comp. Phys.* **128**, 197 (1996). DOI: 10.1006/jcph.1996.0203

14. J.C. Wells, I. Simbotin, and M. Gavrila, "Multistate High-Frequency Floquet Theory," *Laser Phys.* **7**, 525 (1997).

15. J.C. Wells, I. Simbotin, and M. Gavrila, "High-frequency Floquet Theory Content of Wave-packet Dynamics," *Phys. Rev. A* **56**, 3961 (1997). DOI: 10.1103/physreva.56.3961

16. D.R. Schultz, J.C. Wells, P.S. Krstic, and C.O. Reinhold, "Lattice Schrödinger-equation approach to excitation and ionization in antiproton-He+ collisions," *Phys. Rev. A* **56**, 3710 (1997). DOI: 10.1103/physreva.56.3710

17. B. Segev and J.C. Wells, "Light-fronts approach to electron-positron pair production in ultra-relativistic heavy-ion collisions," *Phys. Rev. A* **57**, 1849 (1998). DOI: 10.1103/physreva.57.1849

18. J.C. Wells, I. Simbotin, and M. Gavrila, "Physical reality of light-induced atomic states," *Phys. Rev. Lett.* **80**, 3479 (1998). DOI: 10.1103/physrevlett.80.3479

19. A. Kolakowska, M.S. Pindzola, F. Robicheaux, D.R. Schultz, and J.C. Wells, "Excitation and charge transfer in proton-hydrogen collisions," *Phys. Rev. A* **58**, 2872 (1998). DOI: 10.1103/physreva.58.2872

20. J.C. Wells, B. Segev, and J. Eichler, "Asymptotic channels and gauge transformations of the time-dependent Dirac equation for extremely relativistic heavy-ion collisions," *Phys. Rev. A* **59**, 346 (1999). DOI: 10.1103/physreva.59.346

21. J.C. Wells, I. Simbotin, and M. Gavrila, "Comment on 'Light-induced atomic states' - Reply," *Phys. Rev. Lett.* **82**, 665 (1999). DOI: 10.1103/PhysRevLett.82.665

22. B. Segev and J.C. Wells, "Exact Z^2 scaling of pair production in the high-energy limit of heavy-ion collisions," *Phys. Rev. C* **59**, 2753 (1999). DOI: 10.1103/physrevc.59.2753

23. D.R. Schultz, M.R. Strayer, and J.C. Wells, "Lattice, time-dependent Schrödinger equation for ion-atom collisions," *Phys. Rev. Lett.* **82**, 3976 (1999). DOI: 10.1103/physrevlett.82.3976

24. D.J. Dean, M.R. Strayer, and J.C. Wells, "Quantum dots in magnetic fields: Thermal response of broker symmetry phases," *Phys. Rev. B* **64**, 125305 (2001). DOI: 10.1103/physrevb.64.125305

25. M.S. Hussein, M.P. Pato, J.C. Wells, "Causal classical theory of radiation damping," *Mod. Phys. Lett. A* **17**, 1635-1642 (2002). DOI: 10.1142/s021773230200806x

26. K. A. Stevenson, G. Muralidharan, L. Maya, J.C. Wells, J. Barhen, and T.G. Thundat, "Covalent Attachment of Gold Nanoparticles to DNA Templates," *J. Nanosci. Nanotech* **2**, 397-404 (2002). DOI: 10.1557/proc-635-c4.2

27. H.X. Zhong, J.C. Wells, and Y. Braiman, "Surface Diffusion and Size Evolution of Nanostructures in Laser-focused Atomic Deposition," *J. Vac. Sci. Technol. B* **20**, 2758-2762 (2002). DOI: 10.1116/1.1520558

28. H.X. Zhong, J.C. Wells, Q. Niu, and Z. Zhang, "Dependence of Surface Strain on Island Geometry in Embedded Quantum-Dot Systems," *Surf. Sci.* **539**. L525-L530 (2003). DOI: 10.1016/s0039-6028(03)00784-2

29. Q.-M. Zhang, J.C. Wells, X.-G. Gong, and Z. Zhang, "Adsorption of a Carbon Atom on the Ni_{38} Magic Cluster and Three Low-index Nickel Surfaces: a First-Principles, Comparative Study," *Phys. Rev. B* **69**, 205413 (2004). DOI: 10.1103/physrevb.69.205413

30. M.D. Barnes, P.S. Krstic, P. Kumar, A. Mehta, and J.C. Wells, "Far-field Modulation of Fluorescence Decay Rates in Pairs of Oriented Semiconducting Polymer Nanostructures," *Phys. Rev. B* **71**, 241303(R) (2005). DOI: 10.1103/physrevb.71.241303

31. Y.-S. Leng, P.S. Krstic, J.C. Wells, P.T. Cummings, and D.J. Dean, "Interaction between benzenedithiolate and gold: classical force field for chemical bonding," *J. Chem. Phys.* **122**, 244721 (2005). DOI: 10.1063/1.1942468

32. I.A. Merkulov, A.V. Meleshko, J.C. Wells, H. Cui, V.I. Merkulov, M.L. Simpson, and D.H. Lowndes, "Two Growth Models of Graphitic Carbon Nanofibers with Herring-bone Structure," *Phys. Rev. B* **72**, 045409 (2005). DOI: 10.1103/physrevb.72.045409

33. M. Fuentes-Cabrera, B.G. Sumpter, and J.C. Wells, "Size-Expanded DNA bases: An ab-initio study of their structural and electronic properties," *J. Phys. Chem. B* **109** (44) 21135-21139 (2005). DOI: 10.1021/jp055210ie

34. M. Fuentes-Cabrera, B.G. Sumpter, P. Lipkowski, and J.C. Wells, "Size-expanded yDNA bases: An Ab Initio Study," *J. Phys. Chem. B* **110**, 6379-6384 (2006). DOI: 10.1021/jp057356n

35. X.G. Zhang, P.S. Krstic, R. Ziki, J.C. Wells, and M. Fuentes-Cabrera, "First-principles transversal DNA conductance deconstructed," *Biophysical Journal* **91**, (1) L04-L06 (2006). DOI: 10.1529/biophysj.106.085548

36. X.G. Zhang, P.S. Krstic, R. Ziki, J.C. Wells, and M. Fuentes-Cabrera, "Comment on 'First-principles transversal DNA conductance deconstructed' - Reply," *Biophysical Journal* **91**, (2) p.777 (2006). DOI: 10.1103/PhysRevE.76.013902

37. R. Ziki, P.S. Krstic, X.G. Zhang, M. Fuentes-Cabrera, J.C. Wells, and X.C. Zhao, "Characterization of the tunneling conductance across DNA bases," *Phys. Rev. E* **74** (1), 011919 (2006). DOI: 10.1103/physreve.74.011919

38. R. Ziki, P.S. Krstic, X.G. Zhang, M. Fuentes-Cabrera, J.C. Wells, and X.C. Zhao, "Comment on 'Characterization of the tunneling conductance across DNA bases'- Reply," *Phys. Rev. E* **76** (1), 013902 (2007). DOI: 10.1103/physreve.76.013902

39. M. Fuentes-Cabrera, P. Lipkowski, O. Huertas, B.G. Sumpter, M. Orozco, F.J. Luque, J.C. Wells, and J. Leszczynski, "Aromaticity-induced changes in the electronic properties of size-expanded bases: The Case of xC," *Int. J. Quantum Chem.* **106**, (11), p.2339-2346 (2006). DOI: 10.1002/qua.20966

40. C. D'Helon, V. Protopopescu, J.C. Wells, and J. Barhen, "GMG – A guaranteed global optimization algorithm: Application to remote sensing," *Math. Comput. Modell*. **45**, (3-4), p.459-472 (2007). DOI: 10.1016/j.mcm.2006.06.005

41. M. Fuentes-Cabrera, B.G. Sumpter, J.E. Sponer, J. Sponer, L. Petit, and J. C. Wells, "Theoretical study on the structure, stability, and electronic properties of the guanine-Zn-Cytosine base pair in M-DNA," *J. Phys. Chem B* **111** (4), p.870-879 (2007). DOI: 10.1021/jp066465e

42. R.F. Wood, S. Pannala, J.C. Wells, A.A. Puretzky, and D.B. Geohegan, "Simple Model of the Interrelation Between Single- and Multi-Wall Carbon Nanotube Growth Rates for the CVD Process," *Phys. Rev. B* **75**, 235446 (2007). DOI: 10.1103/physrevb.75.235446

43. T. Hu, Q.M. Zhang, J.C. Wells, X.G. Gong, Z.Y. Zhang, "A Comparative First-principles study of the adsorption of a carbon atom on copper and nickel surfaces," *Phys. Lett. A* **374**, 4563-4567 (2010). DOI: 10.1016/j.physleta.2010.09.0

44. 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. & Dev. (submitted, February 2019).

45. E. A. Huerta, G. Allen, I. Andreoni, J. M. Antelis, E. Bachelet, G. B. Berriman, F. B. Bianco, R. Biswas, M. C. Kind, K. Chard, M. Cho, P. S. Cowperthwaite, Z. B. Etienne, M. Fishbach, F. Förster, D. George, T. Gibbs, M. Graham, W. Gropp, R. Gruendl, A. Gupta, R. Haas, S. Habib, E. Jennings, M. W. G. Johnson, E. Katsavounidis, D. S. Katz, A. Khan, V. Kindratenko, W. T. C. Kramer, X. Liu, A. Mahabal, Z. Marka, K. McHenry, J. M. Miller, C. Moreno, M. S. Neubauer, S. Oberlin, A. R. Olivas Jr., D. Petravick, A. Rebei, S. Rosofsky, M. Ruiz, A. Saxton, B. F. Schutz, A. Schwing, E. Seidel, S. L. Shapiro, H. Shen, Y. Shen, L. P. Singer, B. M. Sipöcz, L. Sun, J. Towns, A. Tsokaros, Wei Wei, J. C. Wells, T. J. Williams, J. Xiong, and Z. Zhao, "Enabling real-time multi-messenger astrophysics discoveries with deep learning," *Nat. Rev. Phys.* 1 (10), 600-608. DOI: 10.1038/s42254-019-0097-4

46. 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. & Dev. VOL. 63, No. 6, Paper 2, November/December 2019. DOI: 10.1147/JRD.2019.2944146

47. L. Luo, T.P. Straatsma, L. E. Aguilar Suarez, R. Broer, D. Bykov, E. F. D'azevedo, S. S. Faraji, K. C. Gottiparthi, C. de Graaf, A. Harris, R. W. A. Havenith, H. J. Aa. Jensen, W. Joubert, R. K. Kathir, J. Larkin, Y.-W. Li, D. I. Lyakh, O. E. B. Messer, M. R. Norman, J. C. Oefelein, R. Sankaran, A. F. Tillack, A. L. Barnes, L Visscher, J. C. Wells, M. Wibowo, "Pre-exascale accelerated application development: The ORNL Summit Experience," IBM J. Res. & Dev., (in preparation).

Peer-Reviewed Conference Papers

1. J.C. Wells, V.E. Oberacker, A.S. Umar, C. Bottcher, M.R. Strayer, and J.-S. Wu, "Nonperturbative Electromagnetic Muon-Pair Production with Capture in Relativistic Heavy-Ion Collisions," in Proceedings of Conference on Computational Quantum Physics, Vanderbilt University, Nashville, TN, May 22-25, 1991. AIP Conf. Proc. (USA), AIP Conference Proceedings, no. 260, p. 215-227 (1992). DOI: 10.1063/1.42600

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