Nicholas J. Wright

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Experience

San Diego Supercomputer Center, University California San Diego. *Aug 2006→*
Staff Scientist PMaC Group   *Prof Allan Snavely*
- Research into understanding and modeling performance of HPC codes.
- Co-principle investigator on $1.5M NSF grant "SDCI HPC Improvement: IPM- A Performance Monitoring Environment for Petascale High-Performance Computing Systems". Responsibilities included
    o Writing proposal, in collaboration with other PI's
    o Porting IPM to machines with the NSF computing portfolio
    o Using IPM to understand the performance differences these machines exhibit
    o Extending the capabilities of IPM to 10,000+ MPI tasks
- Member of Performance team for SDSC's proposal efforts for NSF Track 2 awards (2006 & 2007) and Track 1 award (2007).
- Senior Personnel on SDSC's 2008 winning track 2 proposal efforts. Responsibilities included
    o Liaising with vendors, both to choose a partner and to design a machine
    o Writing performance and science justification sections of proposal
- Member of WRF team that was a finalist for 2007 Gordon Bell Prize.
- Reviewer for NSF and HPCMO Challenge board.

San Diego Supercomputer Center, University California San Diego. *July 2005→Aug 2006.*
User Services Consultant.
- User Support, with special emphasis on performance analysis tools.

University of Illinois at Urbana-Champaign.   *Jan 2001→ Sept 2004.*
Postdoctoral Research Assistant.   *Professor Nancy Makri.*
- Research in semiclassical mechanics.

Hebrew University, Jerusalem, Israel & University of California, Irvine. *Jan 1999→Dec 2000.*
Postdoctoral Research Assistant.   *Professor R. Benny Gerber.*
- Research into using electronic structure methods to calculate anharmonic vibrational spectra.

Education

Ph.D. Chemistry   **University of Durham, England.** *Dec 1998*
Professor Jeremy M. Hutson   Thesis title: "Bound States of Van der Waals Trimers."
- Developed a method for calculating the spectroscopic properties of weakly-bound molecules to enable the determination of the intermolecular forces holding them together.

BSc Chemistry   **University of Durham, England**. *July 1995*
- Research project: "Non-Additive Intermolecular Forces in $Ar_2 HF$ and $Ar_2 HCl$".

Awards
- Postdoctoral research fellowship. Royal Society, UK.
- Graduate scholarship. University of Durham Chemistry Department.

Publications
1. *Characterizing Parallel Scaling of Scientific Applications using IPM.* N. J. Wright, W. Pfeiffer and A. Snavely. The 10th LCI International Conference on High-Performance Clustered Computing. Denver, March 10-12 2009.
2. W. Pfeiffer and N. J. Wright. *Modeling and Predicting Application Performance on Parallel Computers Using HPC Challenge Benchmarks.* 22nd IEEE International Parallel and Distributed Processing Symposium, Hyatt Regency Hotel, Miami, FL, April 14-18, 2008.
3. *WRF Nature Run* J. Michalakes, J. Hacker, R. Loft, M. O. McCracken, A. Snavely, N. J. Wright, T. Spelce, B. Gorda and R. Walkup.. Proceedings of the 2007 ACM/IEEE Conference on Supercomputing, (SC07), Reno, Nevada, November 10-13, 2007. pp. 32-41.
4. *The effects of orientational and energetic disorder on Forster energy migration along a one-dimensional lattice.* T-S Ahn, N. J. Wright and C. J. Bardeen. Chem. Phys. Lett. 446, 43-48 (2007)
5. *Phase space features and statistical aspects of forward-backward semiclassical dynamics.* N. J. Wright, and N. Makri. J. Phys. Chem. B. 2004, **108**, 6816-6825
6. *Forward-Backward Semiclassical Simulation of Dynamical Processes in Liquids.* N. Makri, A. Nakayama, and N. J. Wright. J. Theor. Comp. Chem. 2004, **3**, 391-417.
7. *Forward–backward semiclassical dynamics for condensed phase time correlation functions.* N. J. Wright, and N. Makri. J. Chem. Phys. 2003, **119,** 1634-1641
8. *An upper limit to the concentration of an SO_2 complex at the air–water interface at 298 K: infrared experiments and ab initio calculations.* H. Yang, N. J. Wright, A. M. Gagnon, R. B. Gerber and B. J. Finlayson-Pitts. Phys. Chem. Chem. Phys., 2002, **4,** 1832-1838
9. *Extending the vibrational self-consistent field method: using a partially separable wave function for calculating anharmonic vibrational states of polyatomic molecules.* N. J. Wright and R. B. Gerber. J. Chem. Phys., 2001, **114**, 8763-8768
10. *The potential energy surface and ro-vibrational states of He-CH$^+$.* M. Meuwly and N. J. Wright. J. Phys. Chem. A, 2000, **104**, 1271-1277
11. *Direct calculation of anharmonic vibrational states of polyatomic molecules using potential energy surfaces calculated from density functional theory* N. J. Wright and R. B. Gerber.. J. Chem. Phys, 2000, **112**, 2598-2604
12. *Regular and irregular vibrational states: Localized anharmonic modes and transition-state spectroscopy of Na_3* N. J. Wright and J. M. Hutson.. J. Chem. Phys, 2000, **112**, 3214-3219
13. *Regular and irregular vibrational states: Localized anharmonic modes in Ar_3* .N. J. Wright and J. M. Hutson. J. Chem. Phys, 1999, **110**, 902-911