

Erik Deumens

Professional Preparation

University of Antwerp	Physics	M. S., 1976
University of Brussels	Theoretical Nuclear Physics	Ph. D., 1982
University of Brussels	Computational Chemical Physics	D. Sc., 1984
University of Florida	Quantum Chemistry	1985-1988

Appointments

- Dec 2005: Director, High Performance Computing Center, University of Florida
- July 2000 - present: Scientist in the Departments of Chemistry and Physics, University of Florida.
- Jul. 1994 - Jun 2000: Associate Scientist in the Department of Chemistry and adjunct faculty in the Department of Physics, University of Florida.
- Jul. 1990 - Jun. 1994: Assistant Scientist in the Department of Chemistry and adjunct faculty in the Department of Physics, University of Florida.
- Sep. 1988 - Jun. 1990: Visiting Assistant Research Scientist with the Quantum Theory Project.
- Oct. 1984 - Nov. 1984: Researcher of the "Interuniversitair Instituut voor Kernwetenschappen" (a section of the Belgian National Science Foundation), University of Limburg, Belgium.
- Oct. 1977 - Sep. 1984: Teaching and research assistant to Prof. Dr. P. Van Leuven at the Theoretical Physics section of the University of Antwerpen (Rijksuniversitair Centrum Antwerpen), Belgium.
- Sep. 1982 - Mar. 1983: Fulbright Research Scholar, University of Florida.

Publications related to the project

- The super instruction processor parallel design pattern for data and floating point intensive algorithms, V. Lotrich, M. Ponton, L. Wang, A. Yau, N. Flocke, A. Perera, E. Deumens, R. J. Bartlett, Workshop on Patterns in HPC, University of Illinois at Urbana-Champaign, May 4-6, 2005, <http://charm.cs.uiuc.edu/patHPC/program.html>.
- Software integration in multi-scale simulations: the PUPIL system, J. Torras, E. Deumens, S.B. Trickey, in "Perspectives on simulations of Chemo-mechanical Phenomena", J. of Computer Aided Materials Design, 13, 201-212 (2006)
- Water molecule fragmentation induced by charge exchange in slow collisions with He⁺ and He²⁺ ions, R Cabrero-Trujillo, E. Deumens, Y. O'hrn, O. Quinet, J. R. Sabin, N. Stolterfoht, Phys. Rev. A75 052702 (13 pages) (2007) This article has been selected for the June 2007 issue of Virtual Journal of Ultrafast Science <http://www.vjulfrafast.org>

- PUPIL: A Systematic Approach to Software Integration in Multi-scale Simulations, J. Torras, Y. He, C. Cao, K. Muralidharan, E. Deumens, H.-P. Cheng, S. B. Trickey, Computer Physics Communications, 177265-279(2007)
- Parallel Implementation of Electronic Structure Energy, Gradient and Hessian Calculations, V. Lotrich, N. Flocke, M. Ponton, A. Yau, A. Perera, E. Deumens, R. J. Bartlett, J. Chem. Phys., 128, 194104 (15 pages) (2008).

Other significant Publications

- Dynamics of an atomic electron and its electromagnetic field in a cavity, D. Masiello, E. Deumens, and Y. Öhrn, Phys. Rev. A 71 032108(12 pages) (2005)
- Time-dependent theoretical treatments of the dynamics of electrons and nuclei in molecular systems, E. Deumens, A. Diz, R. Longo and Y. Öhrn, *Rev. of Mod. Phys.* 66 917-983 (1994).
- Teaching Quantum Mechanics, Erik Deumens, Adv. in Quant. Chem. 35 1999, 21-32.
- Charge transfer in low-energy collisions of He^{2+} with atomic hydrogen, deuterium and tritium, N. Stolterfoht, R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, R. Hoekstra, J. R. Sabin, Phys. Rev. Lett. submitted (2007)
- Fracture, water dissociation, and proton conduction in SiO₂ nano-chains, Chao Cao, Yao He, Juan Torras, Erik Deumens, S.B. Trickey, Hai-Ping Cheng, J. Chem. Phys. 126211101 (3 pages) (2007). This article has been selected for the June 15, 2007 issue of Virtual Journal of Biological Physics Research <http://www.vjbio.org>

Synergistic activities From 1998 until 2004, Erik Deumens acted as a consultant working with IBM on the installation, configuration and system administrator training of numerous high performance computing systems, IBM RS/6000 SP and eCluster 1600 systems, to many universities and research labs.

User training was also provided in the form of a 5 day course on parallel programming. This course was taught at Louisiana State University, University of Alaska Fairbanks

Development of the course Topics in High Performance Computing.

<http://www.qtp.ufl.edu/deumens/hpc-topics.html>

Collaborators and Other Affiliations Collaborators: R. Cabrera-Trujillo (U. Autonoma Mexica, Cuernavaca), Y. Öhrn (U. Florida), J. Sabin (U. Florida) N. Stolterfoht (Max Planck Inst. Berlin)

Graduate advisor: P. Van Leuven (retired)

Postdoctoral Sponsors: M. Bouten (retired) Y. Öhrn (U. Florida) J. Serneels (U. Limburg, Belgium)

Thesis Advisor: A. Diz (1992) R. Longo (1992) B. Mogensen (1997) J. Morales (1997, Texas Tech U.) J. Oreiro (1997) A. Blass (2001) D. Masiello (2004, Northwestern U.) B. Killian (2005, U. Maryland)

Postgraduate-Scholar Sponsor: D. Jacquemin (U. Namur, Belgium) O. Quinet (U. Florida)