ACADEMIC PORTFOLIO: Pär Håkansson

Full name:	(Nils) Pär Håkansson
ResearchID:	A-6601-2011
Date of birth:	17 November 1971
Nationality	Swedish
Languages:	Swedish (mother tongue) English (fluent)

Current position

Marie Curie Individual Fellow: Mar 2016: University of Oulu (Finland), NMR Research unit.

Degrees

- **Ph.D in Physical Chemistry Jun 1999-May 2004**: University of Umeå (Sweden), Biophysical Chemistry. *Simulation of Relaxation Processes in Fluorescence, EPR and NMR Spectroscopy*
- **MSc in Computational/Theoretical Physics**: 1994-1999 University of Umeå (Sweden), department of Physics

ACADEMIC BACKGROUND

- **Research Fellow May 2011–31 Dec 2015**: University of Southampton (UK), Chemistry, Magnetic resonance section.
- **Research Fellow Apr 2008–Apr 2011**: Southampton University (UK), Engineering sciences, Computational Engineering and Design group.
- **Research Fellow Oct 2005–March 2008**: Cardiff University (UK), Chemistry, Theoretical and Computational chemistry.
- **Research Fellow Aug 2004–Aug 2005**: Umeå University (Sweden), Biophysical chemistry.
- **Ph.D position Jun 1999– Jun 2004**: Umeå University (Sweden), Biophysical Chemistry

QUALIFICATIONS

- Research funding: EU project 703446-QUNS: Marie Curie Individual Fellowship (2016-2018); Part of COST Action CA15209 European Network on NMR Relaxometry (2016-2020); Lennanders research fellowship (6-months 2005).
- Co-supervision of students in various topics: Quantum Monte Carlo (1 PhD, 1 Master); Brownian Dynamics modelling (2 PhD, 1 summer project); NMR relaxation experiments (1 Master).
- International activities: Group leader Theory and modelling (WG4) COST European Network on NMR Relaxometry.
- International activities: Organized and co-supervised COST short term scientific mission (one week April 2017)
- Journal Referee tasks (1-2 per year): Refereed papers on stochastic processes, quantum Monte Carlo, fluorescence energy transfer.

Software Development

- DEVIL/SATAN: My contribution has been optimization and "single walker implementation" and new subroutines [12]. In collaboration with Prof. Massimo Mella.
- MONSTER: Stochastic Liouville equation solver in C-code and MPI-format, to compute EPR/NMR or FRET observables with a wide range of Brownian Dynamics models. I am the only developer [14, 16].
- PCSOLVERS: parallel software library for construction of Weiner polynomial chaos expansions and its properties and iterative solution of random algebraic equations. Fortran (F90) and Matlab. My contribution are development of algorithms and numerical code, [23, c].

- TLLS: Library of Octave/Matlab functions to compute NMR relaxation rates from Quantum chemistry and molecular dynamics simulations, developed by me.

Teaching Activities & Curriculum Development

- **SESM6022**, **Uncertainty Quantification and Robust Design**, Year 4 Undergraduate and Postgraduate Students in Aerospace, Mechanical and Ship Science Engineering (2008 – 2011), University of Southampton, UK. Course module developed in collaboration with Dr Prasanth Nair for Year 4 MEng and postgraduate students. This is a topic that is not traditionally covered in Engineering degree programs. The objective behind developing this new module was to make our students more aware of the limitations of computational models and the need to rationally take uncertainty into account when designing engineering systems. My contributions are Monte Carlo simulation and Surrogate modelling (Polynomial Chaos) chapters aiming at graduate-level textbook. Development of Matlab exercises. *I held lectures on Polynomial Chaos 2009.*
- Brownian Dynamics for Biology students, developed a set of simulation exercises in Matlab (Umeå University).
- First-year chemistry teaching (problem solving/laboratory exercises) Umeå and Southampton Universities (Sweden and UK respectively).

Bibliometrics

Web of Science: citations 315, h-index: 11 (Aggregate citation metrics, June-2017)

Conference Oral presentations (updated June-2017)

(presenting author)

1. "Conjugate gradient methods for parameterized linear random algebraic equations", P. Håkansson and P. B. Nair, *23th Biennial Conference on Numerical Analysis, Strathclyde, Scotland, 2009*
2. "Conjugate gradient methods for parameterized linear random algebraic equations", P. Håkansson and P. B. Nair, *Workshop on Stochastic Partial Differential Equations: Modelling, Analysis, and Approximation (SPDE09), TU Darmstadt Germany, 2009*
3. "Prospects for overcoming the curse of dimensionality in polynomial chaos based stochastic projection schemes", P. B. Nair and P. Håkansson, *Proceedings of the 4th European Conference on Computational Mechanics (ECCSM IV), Paris , 2010*
4. "Reduced-order modelling of randomly parametrized PDEs", C. Audouze, P. Håkansson and P. B. Nair, *Proceedings of the 4th European Conference on Computational Mechanics, Paris, 2010*
5. "The Interplay of MD and QM calculations to elucidate singlet state relaxation" P. Håkansson, G. Pileio and Malcolm H Levitt, *8th Conference on FastFieldCycling Relaxometry, Turin, Italy, 2013*
6. "Recent progress in singlet state relaxation calculations merging MD and QM " P. Håkansson, G. Pileio and Malcolm H Levitt, *COST Meeting on Relaxation and Hyperpolarisation Theory, 2014*
7. "Merging MD and QM calculations to quantify singlet state relaxation" P. Håkansson, G. Pileio and Malcolm H Levitt, *XXXVI Finnish NMR symposium 2014, Oulu, Finland*
8. "Towards applications of long-lived nuclear spin-states guided by cost-efficient computational tools" P. Håkansson, J. Vaara, *XXXVI Finnish NMR symposium 2016, Jyväskylä, Finland*

9. "Correlated Brownian interface and translational dynamics simulation for nuclear spin relaxation in fluid membrane phases" P. Håkansson, T. Boirin,J. Vaara, *1st workshop COST European network of relaxometry, 2017, Olsztyn, Poland*
10. "Correlated Brownian interface and translational dynamics simulation for nuclear spin relaxation in fluid membrane phases" P. Håkansson, T. Boirin,J. Vaara, *Physics Days 2017, Aalto University, Helsinki, Finland*
11. "Brownian translational dynamics on flexible surface for nuclear spin relaxation study of fluid membrane phases" P. Håkansson, T. Boirin,J. Vaara, *10th Conference on Fast Field Cycling Relaxometry, Mikołajki, Poland, 2017*

Conference poster presentations

(presenting author)

1. "A direct simulation of EPR slow-motion spectra of spin labelled phospholipids in liquid crystalline bilayers based on a molecular dynamics simulation of the lipid dynamics" P. Håkansson, P.-O. Westlund *9th Chianti Workshop on Magnetic Resonance, Tirrenia, Italy, 2001*
2. "Itô diffusions on hypersurfaces with applications to the Schwarz-P surface and nuclear magnetic resonance theory" P. Håkansson, L. Persson, P.-O. Westlund *CCP5 LIQUIDS AND LIQUID INTERFACES , WARWICK, UK, 2001*
3. "Nuclear Magnetic Relaxation Study of the Microstructure of a Bicontinuous Cubic Phase" P. Håkansson, P.-O. Westlund *10th Chianti Workshop on Magnetic Resonance, San Miniato, Italy, 2003*
4. "Improved Diffusion Monte Carlo propagators for bosonic systems using Itô calculus" P. Håkansson and M. Mella, *13th International Symposium on Small Particles and Inorganic Clusters, Gothenburg, Sweden, 2006*
5. "Robust new solver for Stochastic Liouville equation in Langevin form: Scalability and application to transition metal EPR lineshape", P. Håkansson, T. N. Nguyen. P.B. Nair, R. Edge and E. Stulz, *World Wide Magnetic Resonance 2010, Florence, Italy*
6. "Dynamic nuclear polarization and NMR spectroscopy of solid $^{15}N_2O$ quantified with analytical line shape and Bayesian study", P. Håkansson, N. N. Kuzma, R. K. Ghosh, M. Pourfathi, H. Kara, S. J. Kadlecek, G. Pileio, M. H. Levitt and R. R. Rizi *The Third International Workshop on Metabolic Imaging, Philadelphia , 2012*
7. "The Interplay of MD and QM calculations to elucidate singlet state relaxation" P. Håkansson, G. Pileio and Malcolm H Levitt, *EUROMAR, Crete, 2013*