

PhD Position: Quantum dynamics simulation algorithms for magnetic systems

Supervisor: Dr Ilya Kuprov

This project will use one of the biggest supercomputers in the UK to perform large-scale simulations of quantum system dynamics. Such simulations are essential in magnetic resonance research, materials engineering, nanotechnology, quantum systems engineering and computational drug screening because they allow the design work to be moved from physical reality into a virtual world inside a supercomputer that is set to evolve, just as the real world does, under the Schrödinger equation.

The primary difficulty with such simulations used to be their exponential scaling with the system size. Exponential scaling means that quantum systems with more than about 15 spins are overwhelming even the largest supercomputers – a major limitation, particularly in biomolecular NMR, ESR and DNP spectroscopy.

We have recently found a class of polynomially scaling algorithms that allow accurate simulations to be performed for large numbers of particles, and this project will be taking advantage of those algorithms. The results will provide basic theoretical and software infrastructure for large-scale quantum dynamics simulations and quantum control optimization of NMR and ESR pulse sequences, with applications to biomolecular NMR spectroscopy, magnetic resonance imaging, materials research and quantum device engineering.

This project is a part of the iMR CDT Doctoral Training Programme that provides high-level training courses, industry internship opportunities, conference and collaboration travel funds, high performance workstations as well as research networking opportunities within the six participating UK universities.

Further information on this project is available at <http://spindynamics.org>

For further information about applying contact Ilya Kuprov (i.kuprov@soton.ac.uk) or iMR.CDT@warwick.ac.uk.

The Centre for Doctoral Training in Integrated Magnetic Resonance is a collaboration between researchers at the Universities of Warwick, St Andrews, Dundee, Southampton, Aberdeen and Nottingham.