The Singapore Bioimaging Consortium (SBIC)
presents a seminar

on

"SpinDynamica : A Mathematica Environment for Spin Dynamical Calculations"

Speaker: **Professor Malcolm Levitt**
School of Chemistry
Southampton University
UK
Date : **Wednesday, 28 November 2012**
Time : **10.00am – 11.00am**
Venue : **SBIC Seminar Room**
11 Biopolis Way
Level 2, Helios Building
Singapore 138667
(Please use Level 1 entrance)

Abstract

SpinDynamica is a system for performing analytical and numerical spin dynamical simulations by computer. A set of open-source Mathematica routines are provided which include the following functionality:

- kets and bras for arbitrary spin systems
- matrix representations of spin operators in arbitrary bases
- matrix representations of spin superoperators in arbitrary operator bases
- angular momentum, rotation, projection and shift operators
- commutation, double commutation, coherence order filtration, rotation, projection superoperators
- high-level routines for numerical simulation of spectra, numerical simulation of operator trajectories, including arbitrary ensemble averages, arbitrary sequences of events, handling of continuous analytical functions
- arbitrary time-dependent Hamiltonians
- arbitrary time-dependent relaxation superoperators
- thermalization of superoperators
- Euler angle transformations, tensor transformations, Wigner matrices.
- Construction of axis systems and Euler angle determination

These routines allow the simulation of a wide variety of magnetic resonance experiments, including solution NMR, solid-state NMR, EPR, MRI, etc., all with the same platform, and embedded in the powerful Mathematica programming and graphical environment. An overview of SpinDynamica and its functionality will be presented. Some its drawbacks will also be highlighted.

About the Speaker

Dr Malcolm Levitt was born 1957 in Hull, England. He underwent undergraduate education (Chemistry) at Oxford University, received his BA in 1978), DPhil (1981) on Nuclear Magnetic Resonance with Ray Freeman. He worked as a postdoctoral research at the Weizmann Institute, Israel (with Shimon Vega) and ETH-Zürich (with Richard Ernst). Dr Levitt was a research staff member of the Francis Bitter Magnet Lab, MIT (1985-1990). He was research fellow in superconductivity research in Cambridge, UK, 1991. Lecturer and became professor at Stockholm University, Sweden (1991-2001). Dr Levitt is a Professor in Physical Chemistry at the University of Southampton since 2001. Honours include the LATSIS prize of the ETH-Zürich (1985), the Göran Gustafsson prize in Chemistry (1996), Fellowship of the Royal Society (2007), and the Laukien prize in Magnetic Resonance (2008).

--- Admission is free and all are welcome ---