Applied Mathematics

McGill Applied Mathematics Seminar
Joint with the Center for Physics of Materials

Sept. 11, 2006, 2:35 pm Monday
At McGill, Burnside Hall 1205

" Toward Quantitative Analysis and Simulation of Nanoelectronics"

Hong Guo
Center for the Physics of Materials and Dept. of Physics
McGill

Coffee and refreshments will be served after the seminar

Abstract: Nanoelectronic devices operate by the principle of quantum mechanics, their properties are also closely related to their atomic structure. It has been a theoretical challenge to calculate device characteristics including relevant microscopic details, especially when one wishes to predict these characteristics without using any phenomenological parameter.

I will speak about the present status of nanoelectronic device theory and numerical modeling, the existing numerical difficulties and some relevant problems. I will report some useful progress we have achieved toward quantitative predictions of non-equilibrium and non-linear charge/spin quantum transport in nanoelectronic devices from atomic point of view. This theoretical formalism is based on carrying out real space density functional theory (DFT) analysis within the Keldysh nonequilibrium Green's function (NEGF) framework. Several examples of calculating spin polarized quantum transport in magnetic nanostructures will be presented.