McGill Computational Science and Engineering Seminar

Friday, October 22, 2004 at 10:45 a.m.
McConnell Engineering Bldg. Room 603

Macromolecules, Microparticles, and Flexible Approximation

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The talk consists of two main parts. The first one − intended to inspire new research in engineering, physics and computational methods − is an overview of interesting molecular-, nano- and microscale phenomena and related simulation challenges. The problems include electromagnetic interactions of charged and magnetized colloidal particles; electrostatics of protein molecules in solvents (explicit and implicit solvent models); electromagnetic waves in photonic crystals; electronic structure calculation.

In the second part of the talk, after a brief review of traditional approaches to solving some of the above problems, new "Flexible Local Approximation MEthods" (FLAME) are introduced. The guiding principle is as follows. Physical quantities frequently have salient features that are qualitatively known *a priori*: dominant dipole components near polarized or magnetized spherical particles; singularities at point sources, edge and corners; boundary layers; discontinuities at material interfaces; cusps of electronic wave functions at the nuclei; electrostatic double layers around colloidal particles, and much more. FLAME incorporates this *a priori* knowledge into numerical schemes through a judicious choice of basis functions. In many cases the solution accuracy is improved, both quantitatively and qualitatively. Moreover, simple regular grids often suffice because the solution is represented *algebraically*, by relevant approximating functions, rather than *geometrically*, on conforming meshes.

Various computational examples will be presented: charged and polarized particles in solvents (the Poisson-Boltzmann equation); super high-order schemes for the Schrödinger equation; high order "Mehrstellen"-Collatz schemes; electromagnetic wave propagation and scattering.

Coffee and snacks will be served at 10:30 a.m. in Room 603 before the seminar.