TUCKER CARRINGTON, Queen's University
Using sparse grids to solve the vibrational Schroedinger equation

In principle, it is straightforward to compute the vibrational spectrum of a molecule without neglecting coupling and anharmonicity: one must calculate eigenvalues and eigenvectors of a matrix representing the Hamiltonian in an appropriate basis. In practice, this is difficult because the matrix is very large. To obviate the N^2 memory and N^3 CPU costs of standard diagonalisation methods, it is now common to use iterative algorithms (e.g. Lanczos, Davidson, Filter Diagonalisation) for computing eigenvalues and eigenvectors. It is easy to efficiently implement iterative algorithms when a direct product basis is used. However, for a molecule with more then four atoms, a direct product basis set is large and (although iterative algorithms eliminate the need to store the matrix) minimising the number of basis functions required to obtain converged eigenvalues would be advantageous. Can this be done without jeopardizing the efficiency of the matrix-vector products required by all iterative algorithms? One way to reduce the number of basis functions is to discard unimportant functions from a direct product basis. In this talk I shall present new basis-size reduction ideas of this type that are compatible with efficient matrix-vector products.

IAN CUNNINGHAM, Western University
Advances required to improve image quality in medical radiography – a statistical problem

Image quality in medical radiography is a statistical problem. Images are formed when x-ray quanta deposit energy into a detector that normally consists of a large two-dimensional array of small (100-um square) discrete detector elements. The physical processes of energy transfer are statistical in nature and can be represented as a complex cascaded of random point processes that describe photon scatter, conversion to secondary quanta, and liberation of charge pairs. Spatial correlations in image signals introduced by these processes are largely responsible for image quality. Detector performance and the ability to produce high-quality images for low x-ray exposures is described by the Fourier-based detective quantum efficiency (DQE) which is derived from statistical decision-making theory. This talk will summarize the link between detector design and image quality through the DQE and cascaded-systems analysis. The physical processes that currently limit image quality in modern systems will be identified with attention drawn to how these detectors must be redesigned for improved image quality and dose reduction.

JOHN FEDERICI, New Jersey Institute of Technology
Image and beam correction algorithms for THz computed Tomography Imaging

For the past decade, there has been a considerable improvement in Terahertz (THz) imaging. In particular, the technique of 3-D computed tomography has been adapted to the THz range. However, the finite refractive index of materials in the THz range can severally refract probing THz beams during the acquisition of tomography data. Due to Fresnel reflection power losses at the boundaries as well as steering of the THz beam through the sample, refractive effects lead to anomalously high local absorption coefficients near the material boundaries of a reconstructed THz tomography image. These boundary phenomena can dominate the reconstructed THz-CT images making it difficult to distinguish any hidden finer structural defect(s) inside the material. In order to eliminate boundary effects, an algorithm has been developed to remove the effects of refraction in THz-CT reconstructed images. The algorithm is successfully implemented on cylindrical shaped inhomogeneous objects.

FRANÇOIS FILLION-GOURDEAU, CRM
Recent advances in numerical solutions of the molecular relativistic time-dependent Dirac equation

Due to recent and prospected technological advances, it is now possible, to consider laser intensities of 10^{23} W/cm^2 and higher. In this new regime, relativistic and quantum electrodynamics effects start to be important, requiring a theoretical description in terms of the time-dependent Dirac equation. In this presentation, I will present recent advances on the numerical solution of this equation for 3-D axisymmetric geometries using cylindrical coordinates. The numerical method is based on a split-step scheme in coordinate space, which is free from the "fermion doubling" problem and which can be parallelized very efficiently. A new technique to circumvent the coordinate singularity at $r = 0$ using Kirchhoff's formula will also be described. The numerical method is then utilized to simulate the quantum relativistic dynamics of an electron bound in a diatomic molecule potential and interacting with an ultraintense counterpropagating laser field. These simulations may have applications in quantum imaging for ultraintense laser-matter interaction.

DANIEL LEVESQUE, University of Sherbrooke
Immersive Environment for Molecular Visualization

.

JEAN-MARC LINA, University of Montreal
Wavelet-based Localization of Oscillatory Brain Activities in Electro-Magnetic Imaging

.

EMMANUEL LORIN DE LA GRAND MAISON, Carleton University
Absorbing boundary conditions for quantum relativistic mechanics

In this work microlocal analysis is used to derive pseudodifferential transparent and absorbing boundary conditions for the 1-d and 2-d Klein-Gordon and Dirac equations modeling particles subject to classical electromagnetic fields.

ALFRED MAQUET, Université Pierre et Marie Curie, Paris, France
Status of the time variable in quantum mechanics and the new generation of experiments with attosecond pulses of radiation

Whether time is a parameter or an operator in Quantum Mechanics is a long-standing question since the foundation of the theory. In fact, it remains open to decide if time is a parameter (as in classical mechanics) or a measurable quantity associated to a hermitian operator expressed in terms of dynamical variables. For years, the question remained rather academic and it attracted mainly the specialists' attention.

Things have changed first in the 1980s, with the related concept of "Tunnelling Time", i.e. how to measure "the time it takes a particle to tunnel through a potential barrier"? It turns out that no consensus has been reached yet on how to define such tunnelling times. It is in the 2010s, with the advent of sources of coherent radiation delivering "attosecond" (1 as = 10-18 s) pulses, that one has investigated photoionization in the time domain. At a fundamental level, this has opened the possibility to "clock" the response of a quantum system to the annihilation (absorption) of one photon.

We shall address some issues raised by this new generation of measurements and we shall present a theoretical analysis of recent experiments. These have evidenced the existence of attosecond time delays between the emission times of electrons ejected from different sub-shells in atoms, upon the absorption of one photon [1], [2].

[1] M. Schultze et al. "Delay in Photoemission", Science 328 1658-1662 (2010).

[2] K. Klünder et al. "Probing Single-Photon Ionization on the Attosecond Time Scale", Phys. Rev. Lett. 106, 143002 (2011).

TUNG NGUYEN, Université Laval
Quantum dynamics of correlated electrons for time-resolved imaging of laser-driven molecules: Formal and computational challenge

The description of the time-resolved electron dynamics of a many-electron atom or molecule subjected to an intense ultrafast laser pulse requires solving the multi-dimensional, many-body Time-Dependent Schroedinger Equations. We show how the many concepts and tools of ab-initio stationary-state Quantum Chemistry, the object of which is to describe stationary molecular electronic structures, can be adapted to this time-dependent context. While that adaptation is straightforward in so far as the dynamics of bound electrons (described by L^2 wavefunctions) is concerned, using for example our non-variational Time-Dependent Multi-Configuration Self-Consistent Field (TDMCSCF) approach [Nguyen-Dang T.T et al, J. Chem. Phys. 127, 174107 (2007).], it presents severe computational problems when large amplitude electron motions, corresponding to ionizations and laser-induced re-scattering processes, are considered. To deal with this problem, a multi-level partition of the many-electron state space is introduced to allow for separate treatments, with separate accuracy criteria with regards to the electron correlation, of the bound and continuum components of the N electron wavefunction. We show how to solve the coupled integral equations resulting from this type of partitioning in such a manner that norm conservation is well enforced, and how concepts derived from the Graphical Unitary Group Approach (GUGA) can be used to organize the computational tasks. Illustrations of the methodology are given on the H_2 (2 electrons) and LiH (4 electrons) molecules.