SECCIÓN DEPARTAMENTAL DE ASTRONOMIA Y GEODESIA

Ciclo de Seminarios

Andreas Pedersen

Reykjavik University, Iceland & UCM Abel Extraordinary Chair

"Atomistic dynamics using applied mathematics"

Abstract:

In a series of three lectures I will present how atomistic dynamics can be approached with mathematical modeling. In the first lecture (October 15th) I will give an introduction to the theory behind atomistic simulations. The introduction is based on statistical mechanics and we start from an ensemble average, which can be used to determine the thermodynamical value of a property of the system, temperature as an example. It is then assumed that the Ergodic Hypothesis holds. By doing so it is possible to determine the value of a thermodynamical property from a time average of a single system rather than as an ensemble average.

In the following two lectures I will present two classes of methods that are based on either Monte Carlo or Molecular Dynamics. Both methods are numerical schemes, because the dimensionality of the problem scales as 3N – where N is the number of particles and each is defined by x, y and z – it is not feasible to apply analytical methods. The second lecture (October 29th) will revolve around the adaptive kinetic Monte Carlo method where dynamics is obtained by locating low energy saddle points on the potential energy surface. A saddle point represents the barrier for the system to overcome in order to undergo a transition and it corresponds to the less probable configuration along this transition. For the method to be applicable the height of the energy barriers has to be several times larger than the thermal energy. I will explain the method in greater details and show you results obtained with this method. In the last lecture (November 5th) Molecular Dynamics will be in focus. This method is a more direct approach, where the equation of motion – set of differential equations – is evolved in discrete time steps using the Velocity Verlet algorithm as an example. This method is not limited by the restrictions mentioned above. However, the total time that can be simulated limits to a couple of nano-seconds since the discrete time step is limited to the femto-second scale due to lattice vibrations. I will show you some results already obtained and also explain what we expect to achieve in the near future.

Organizado por la sección departamental de Astronomía y Geodesía, y el IMI.

Fechas: 15 y 29 de octubre y 5 de noviembre de 2009, a las 13.00 horas

Sala de Grados (250 C)

Facultad de Ciencias Matemáticas, UCM.