

## **Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina**

7 Aprile 2010, ore 15.30, Aula E. Majorana, Dip.to di Fisica,  
Ctr. Papardo Sperone, 31, S. Agata, Messina

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Conferenze organizzate con il supporto e il patrocinio culturale della  
**ACCADEMIA PELORITANA DEI PERICOLANTI**

### **ALGORITHMS FOR NON-HAMILTONIAN DYNAMICS**

In many instances, statistical averages in a variety of many-body problems can be efficiently calculated through deterministic dynamics. When thermodynamical constraints (such as constant-temperature and/or constant-pressure) must be enforced, energy-conserving non-Hamiltonian dynamics becomes the method of choice. The resulting associated equations of motion requires advanced algorithms to be integrated. It will be shown in a number of cases how to derive in detail both time-reversible algorithms and the very recent time-reversible measure-preserving integration method developed by Ezra [J. Chem. Phys. 125 034104 (2006)].