MOLECULAR SIMULATIONS

1.1. Identification

University:	Alma Mater Studiorum – Università di Bologna																	
School:	School of Engineering																	
Course:	Molecular simulations																	
ECTS:	6																	
Semester:	*Winter*						X	*Summer*										
Category	*Fundamental course*							*Specialisation course*										X
Module	*MFI*		*MFII*		*MFIII*			*MSI*		*MSII*		*MSIII*	X					
Teachers:	Massimo Rudan																	
Language:	*English*	X	*Italian*	X	*Swedish*		*Spanish*											

1.2. Learning-outcomes

- knowledge of basic aspects of numerical modelling
- implementation of numerical routines to simulate physical problems
- development of a critical viewpoint on results of numerical simulations and

1.3. Competencies

- **General**
  - To have critical understanding of technical and scientific tools.
  - To be able to choose and apply numerical tools like Molecular Dynamics packages and Monte Carlo codes.
  - Communication skills.
  - To be able to work in an international context

- **Specific**
  - To understand the techniques used in numerical simulations of chemical or physical-related problems.
  - To identify the appropriate interactions existing among the components of a system under investigation.
  - To perform numerical analyses of systems ranging from isolated molecules to supramolecular complexes.
  - To develop analysis tools.

1.4. Contents

5. Introductory part to present numerical modelling techniques.
6. Monte Carlo simulations.
7. Molecular Dynamics simulations: an introductory overview.
8. Enhancing Molecular Dynamics codes: accelerating rare events.
9. Case studies

1.5. Teaching Methodology

- Lecture sessions.
- Laboratory sessions using freely-available Moleculard Dynamics software and self-implemented tools.

1.6. Evaluation

- Oral exams, including discussion of the laboratory work.

1.7. Bibliography

D. Frenkel and B. Smit, *Understanding Molecular Simulation – From Algorithms to Applications*, Academic Press, 2002.
A. R. Leach, *Molecular Modelling: Principles and Applications*, Prentice Hall, 2001.
M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids*, Oxford Science Publications, 1987.
A. Papoulis and S.U. Pillai, Probability, Random Variables and Stochastic Processes, McGraw Hill, 2002.