

# High Performance Computing

## Descriptive details concerning the subject

*Name of the subject:* High Performance Computing

*Code:* HPC

*Type of subject:* Optional

*ECTS:* 5

*Total hours:* 125 of which 30 hours will correspond to classroom attendance.

*Lecturing period:* January-March

*Building:* Mar

*Schedule:* The course comprises 9 weeks, with classes in the second semester (T2).

*Coordination:* Gianni De Fabritiis

*Department:* Ciències Experimentals i de la Salut, UPF

## Teaching details

*Language:* English

*Lecturers:* Ganni De Fabritiis

## **Synopsis**

The focus of this course is to provide the tools, knowledge and practice to perform biochemical experiments on proteins and other molecules (drugs) in-silico using molecular dynamics simulations on a high performance computing infrastructure.

- **Competences to be attained in the subject**
  - Practical knowledge on performing molecular dynamics simulations
  - Practical knowledge on analysing molecular dynamics simulations
  - Capacity to design and prepare a molecular simulation experiment
- **Target students**
  - Students with an interest in computing and simulation, structural biology, computational biophysics and biochemistry.
- **Requirements**
  - Courses: Attendance to the course MSI is recommended for this course.
  - Programming: Use of medium to high level scripting is used in order to perform analysis on large simulation data sets.
  - Knowledge: Interdisciplinary. Pharmaceutics, biochemistry, chemistry and biology will be an advantage to understand the molecular systems, computer science, physics and mathematics for the understanding of the fundamentals of the methodology.
- **Length**
  - Course length is 30 hours of classes (corresponding to 100 hours of

personal work including classes) of which 4 hours are for the final project revision and defense.

- **Evaluation**
  - 50% of final evaluation is based on exercises during the course
  - 50% of final evaluation is based on research projects carried out by groups and defended publicly.
- **Resources**
  - Hardware: Access to a GPU equipped machine and ACEMD will be given during the course
  - VMD user guide  
<http://www.ks.uiuc.edu/Research/vmd/current/ug.pdf>
  - ACEMD user guide <http://multiscalelab.org/acemd/manual>, ACEMD protocols <http://multiscalelab.org/acemd/protocols>
  - Octave: <http://www.gnu.org/software/octave/>
  - Nice books: Computer Simulation of Liquids, Allen and Tildesley. Understanding Molecular Simulation, Second Edition: From Algorithms to Applications, Frenkel and Smit.
- **Picture and video gallery**
  - You Tube channel: <http://www.youtube.com/user/ps3grid>
  - Flickr channel:  
<http://www.flickr.com/photos/multiscalelab/with/3542248429/>

**Course main page:** <http://multiscalelab.org/master/HPC>

### Course plan

- Class 1: Molecular dynamics hands-on
  - Concept of classical dynamics
  - The water molecule
  - Amber and Charmm forcefields (bond, angle, dihedral, improper, Lennard-Jones, Coulomb)
  - Charmm topology files [top\\_all27\\_prot\\_lipid.top](#)
  - Charmm parameter files [par\\_all27\\_prot\\_lipid.prm](#)
  - Molecular dynamics codes
- Class 2: Introduction to VMD
  - <http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/>  
(tutorial files <http://www.ks.uiuc.edu/Training/Tutorials/vmd/>)
  - Use of the user guide  
<http://www.ks.uiuc.edu/Research/vmd/current/ug.pdf>
  - Topics: Load molecule and navigate it, representations, selections (rename, name, type, resid), within of, same residue as, loading trajectories, keys (r,t,s,1,2)
  - Tcl scripting (tcl, mol, atomselect, measure)
  - Practice: [VMD\\_exercise.txt](#), [1NEY.pdb](#), TRJ:  
<http://www.gpugrid.net/download/trj.dcd>, PDB:

[http://www.gpugrid.net/download/TIM\\_sub\\_cry.pdb](http://www.gpugrid.net/download/TIM_sub_cry.pdb)

- Class 3: Preparing a molecular structure for MD simulations
  - Built from PDB in the Charmm format  
<http://www.multiscalelab.org/acemd/protocols/ACETK.BLDCHARMM>
  - Relaxation and production run  
<http://www.multiscalelab.org/acemd/protocols/ACETK.EQ>
  - Practice
- Class 4: Biased free energy calculations: Metadynamics
  - Theory behind metadynamics
  - Practice
- Class 5: Problem solving using metadynamics
  - Advanced practice, a problem is proposed and solved using this technique
- Class 6: Biased free energy calculations: Umbrella sampling
  - Theory behind umbrella sampling
  - Practice
- Class 7: Protein-ligand binding affinity calculations by umbrella sampling
  - Seminar
  - Practice
- Class 8: Markov state models
  - Theory behind Markov state models analysis
  - Practice using simple Brownian dynamics
- Class 9: Reconstructing the binding process by Markov state models
  - Seminar
  - Practice
- Class 10: Membrane and membrane proteins
  - Built a membrane using charmm-gui.org
  - Embed a protein into a lipid bilayer
  - Practice
- Class 11: Molecule parameterization
  - Molecule parametrization using the Amber force field  
<http://www.multiscalelab.org/acemd/protocols/ACETK.PRMMAMBER>
  - Molecule parametrization using the Charmm force field  
<http://www.multiscalelab.org/acemd/protocols/ACETK.PRMMAMBER>
  - Practice
- Class 12: Project review
- Class 13: Project review
- Class 14: Project defense
- Class 15: Project defense