Laboratoire de Biochimie Théorique
Institut de **B**iologie **P**hysico-**C**himique
13, rue Pierre et Marie Curie
75005 PARIS

S E M I N A I R E

Vincenzo Barone
Scuola Normale Superiore di Pisa, Italy

Virtual and real in molecular sciences: new bridges across old boundaries

Real or virtual? Experiment or theory? Which one should be trusted more? While a dispute has characterized all scientific fields for decades, the end of the last century witnessed a reconciliation of the first *two pillars* of hard science, thus leading to the widespread employment of integrated experimental-theoretical approaches. Following on from this, a challenging issue arises: *how far can the quantitative prediction of experimental and technological problems be pushed?* This question has puzzled theoretical and computational scientists since the birth of their disciplines, thus originating the never-ending fight between ***feasibility, accuracy and interpretability***. In the last decade, hardware and software developments have led to the birth of the *third pillar* of hard science: computer-based simulation. This is nowadays considered a routine facility in science and has opened the way to an integrated ***experiment/theory/simulation*** approach. This has gone so far that some of the most recent philosophical-scientific theories even state that we are no longer able to know if we live in a 'real world' or in a simulation, thus making the visionary interpretation of reality given by the *MATRIX* movie a little less imaginary. The spontaneous question arising is: *what's next?* The instinctive answer is ***data science***, which is related to the availability of an unprecedented amount of high quality data and represents today the *fourth pillar* of an effective integrated strategy for the investigation of complex phenomena. At the same time, we are witnessing a parallel and fast growth of the ***virtual reality*** (VR) and ***augmented reality*** (AR) paradigms with their promise of a more complex human perception and interaction of the world overcoming our space-time physiological limitations.

On these grounds, we are working on the creation of a new cyber-infrastructure purposely tailored for molecular sciences. In this framework, sets of experimental, computational, data and visualization components will be connected to people by software with the aim of improving research throughput and achieving goals not otherwise possible. This will allow both experimentally- and computationally-oriented researchers to automatically perform all the steps required for the design and analysis of a wide set of experiments and to select the most effective integrated strategy.

The status and perspectives of this project will be illustrated also by means of some case studies.

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