



DEISA Extreme Computing Initiative LIFE SCIENCES

The main objective of the DEISA Research Infrastructure is to advance computational sciences in Europe. Enabling and operating new challenging supercomputing applications is a central part. The DEISA Extreme Computing Initiative (DECI) has been launched in May 2005 by the DEISA Consortium, as a way to enhance its impact on science and technology. The main purpose of this initiative is to enable a number of “grand challenge” applications in all areas of science and technology. These leading, ground breaking applications must deal with complex, demanding and innovative simulations that would not be possible without the DEISA infrastructure, and which benefit from the exceptional resources provided by the Consortium. The DEISA applications are expected to have requirements that cannot be fulfilled by the national services alone. In this fact sheet three current DECI projects in life sciences are described.

TASEC – Towards Atomistic Simulations of Eucariotic Chromatine: the nucleosome

Scientific Discipline: Bioinformatics
Principal Investigator: Modesto Orozco
Institutions: Instituto Nacional de Bioinformática

TASEC project uses DEISA resources to perform a land-mark molecular dynamics study of the structure of two nucleosomes: a highly positioned nucleosome for which a crystal

structure is available, and an artificial nucleosome created by substituting the DNA sequence in the crystal structure of Richmond and co-workers by a AATT rich sequence that is known to largely disfavour nucleosome formation. These extremely time consuming simulations enable the scientists to gain insight into the complex rules that guide the nucleosome positioning in the cromatine.

BET – First-Principles and Mixed quantum classical QM/MM Simulations of Biological Electron Transfer

Scientific Discipline: Computational Biophysics
Principal Investigator: Paolo Carloni
Institutions SISSA, Trieste, Italy, Swiss Federal Institute of Technology EPF, Lausanne, Switzerland

BET uses state-of-the-art first-principles techniques to investigate electron transfer in the context of iron- and copper-based proteins. The project considers a small iron-protein (Rubredoxin), which is for its size well suited for a full quantum calculation, and medium size copper protein (Azurin). In Rubredoxin the metal spin delocalization in the presence of the full quantum field of the environment will be studied combining classical multi-nanoseconds molecular dynamics simulations and full *ab initio* electronic structure calculations of the protein in its crystalline phase within the density functional theory framework. The *ab initio* calculations will be carried out

using an innovative hybrid Gaussian and plane waves (GPW) method (5) as implemented in the QuickStep module (6) in the CP2K code.

SNARE – Membrane Fusion

Scientific Discipline: Computational Chemistry/Biology
Principal Investigator: Marc Baaden
Institutions: Labo de Biochimie Theorique, CNRS UPR9080

The SNARE protein complex is central to membrane fusion, a ubiquitous process in biology. Modeling this complex in order to better understand its guiding principles is a challenging task. This is mainly due to the complexity of the environment: two adjacent membranes and a central complex of four helices made up by v- and t-SNARE proteins. Not only the size of the actual system but also the computing time required to equilibrate it render this a demanding task requiring exceptional computing resources. The project suggests the use of the innovative replica exchange method where several simulations simultaneously run in parallel to enhance sampling in order to establish a realistic microscopic view of the membrane-embedded SNARE complex. This model will be a starting point for further investigations related to membrane fusion, and will provide detailed insight into one of the key steps bringing the two membranes together.