



UNIVERSITAT POLITÈCNICA DE CATALUNYA

BARCELONATECH

PROJECT DESCRIPTION

Title: Predictive models and simulations in nano- and biomolecular mechanics: a multiscale approach

Project description:

The predictive ability of current simulations of interesting systems in nano- and biomolecular mechanics is questionable due to (1) uncertainties in material behavior of continuum models, (2) severe limitations of atomistic simulations in the computationally accessible length and time scales in relation with the scales of scientific and technological interest, and (3) the limited understanding gained from terabytes of data produced in supercomputing platforms. These difficulties seriously undermine the credibility of computer simulations, as well as their real impact in scientific and technological endeavors. Examples include fundamental challenges in materials science (structure-property relations), molecular biology (sequence-structure-function of proteins), or product engineering (virtual testing for analysis, optimization, control). This project addresses three important topics in nano- and biomolecular mechanics, whose full understanding and technological exploitation require predictive models and simulations: (1) Mechanics of carbon nanotubes at engineering scales, (2) Mechanics of fluid membranes in eukaryotic cells and bio-inspired technologies and (3) Local-to-global conformational space exploration and free energy calculations for biomolecules. We follow a multiscale approach, which seeks to incorporate the net effect of the small-scale phenomena described by fundamental models of physics into the coarser (computable) scales at which the system or device operates. In addition to specific impact in these applications, the proposed research is expected to exemplify the potential of multiscale approaches towards predictive and quantitative science and technology, as well as contribute to the credibility and utility of large investments in supercomputing.

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OTHER INFORMATION

Funding: between 25.000 €/year and 33.000 €/year

Duration: 4 years for PhD, 2 years renewable for post-docs

Facilities: Computational lab with personal workstations and high-performance servers.