iSGTW Image of the week - Molecular dynamics simulation on DEISA infrastructure

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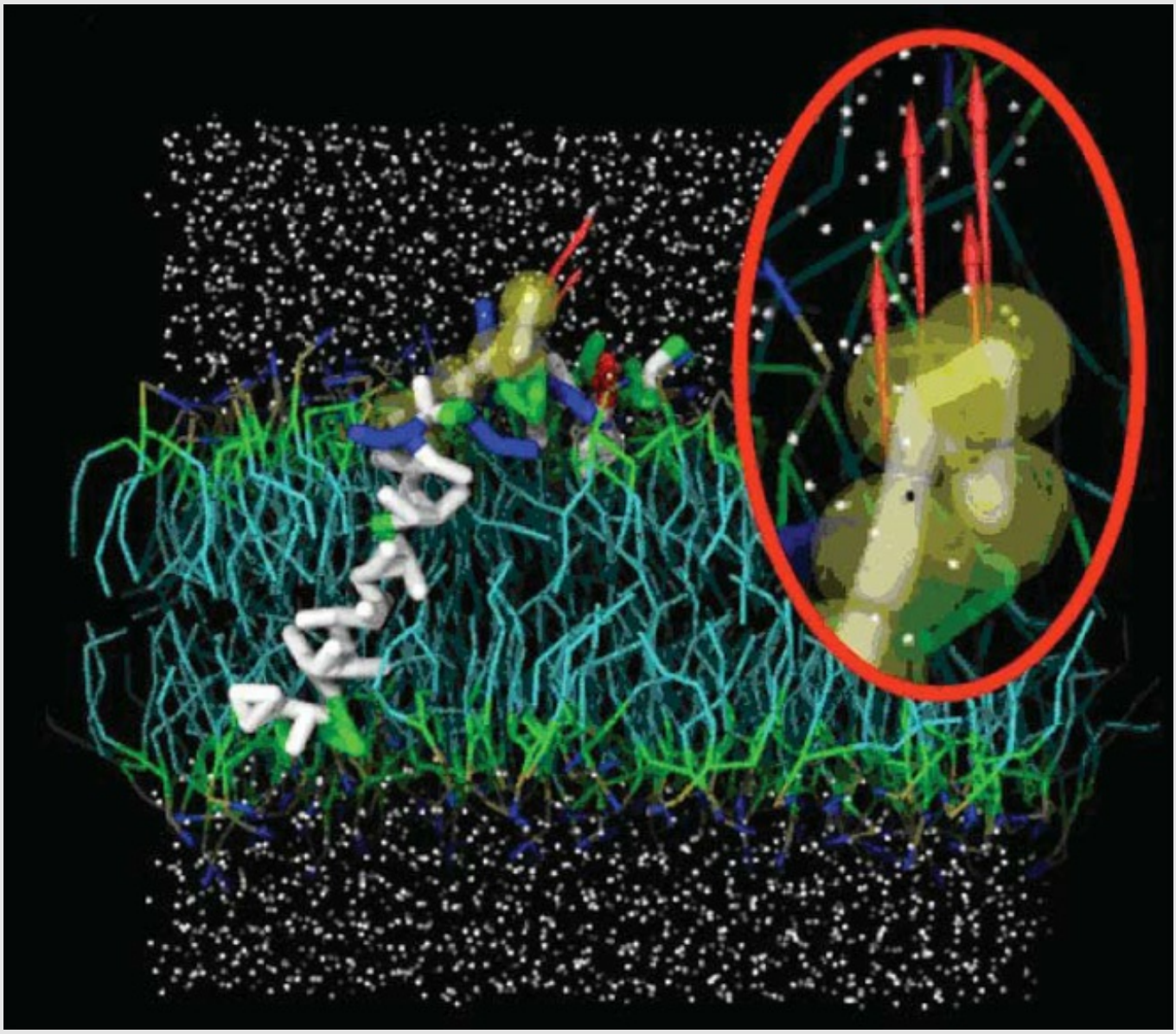

A single snapshot of a coarse-grained molecular dynamics simulation of a protein (Synaptobrevin transmembrane domain) in a lipid bilayer. The protein is shown as licorice, lipids as lines and water as points. The red arrows show the user external forces applied interactively in the simulation. Here, the membrane anchoring of protein is probed by pulling on one particular side (on tryptophane residues).

Image courtesy of deisa.eu.

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Coupled applications

Many complex systems can be viewed as sets of components that obey their own physical laws and interact weakly with one another. Code-coupling, which deals with multi-physics, multi-models and multi-scale numerical simulations, is well-suited for inter-disciplinary research projects in which different legacy codes cooperate within the whole coupled application.

Generally, due to the complexity of these applications, coupled codes run with a moderate efficiency on parallel machines such as the DEISA infrastructure. A Joint Research Activity team within DEISA has enhanced the coupled applications to work on DEISA resources so that research teams can tackle new classes of numerical investigations.

As an example, large-scale computer simulations of biological systems provide valuable insight into molecular processes as diverse as enzymatic catalysis and membrane fusion.

Researchers at the theoretical biochemistry laboratory at the Institut de Biologie Physico-Chimique in Paris have used the visualization tool VMD to drive their GROMACS molecular dynamics simulations that examine the mechanical properties of (macro) molecules and their assemblies.