Published on *BSC-CNS* (https://www.bsc.es)

ScalaLife: Scalable Software Services for Life Science

Description

Life Science developed into one of the largest e-Infrastructure users in Europe, in part due to the ever-growing amount of biological data. At the time of the project, modern drug design typically included both sequence bioinformatics, in silico virtual screening, and free energy calculations, e.g. of drug binding. This development has accelerated tremendously, and has put high demands on simulation software and support services.

e-Infrastructure projects such as PRACE/DEISA have made important advances on hardware and scalability, but have largely been focused on theoretical scalability for large systems, while typical life science applications rather concern small-to-medium size molecules. This project addressed this by implementing new techniques for efficient small-system parallelization combined with throughput and ensemble computing to enable the life science community to exploit the largest next-generation e-Infrastructures. We will also build a new cross-disciplinary Competence Network for all of life science, to position Europe as the world-leading community for development and maintenance of this software e-Infrastructure.

Specifically, the outputs were to:

1. develop new hierarchical parallelization approaches explicitly based on ensemble and high-throughput computing for new multi-core and streaming/GPU architectures, and establish open software standards for data storage and exchange.
2. implement, document, and maintain such techniques in pilot European open-source codes such as the widely used GROMACS & DALTON, a new application for ensemble simulation (DISCRETE), and large-scale bioinformatics protein annotation.
3. create a Competence Centre for scalable life science software to strengthen Europe as a major software provider and to enable the community to exploit e-Infrastructures to their full extent. This Competence Network provided training and support infrastructure, and established a long-term framework for maintenance and optimization of life science codes.

Source URL (retrieved on *18 Dic 2024 - 09:46*): https://www.bsc.es/es/research-and-development/projects/scalalife-scalable-software-services-life-science