# BIOMEDICAL APPLICATIONS

Biomedicine is a major application area for the EGEE project. With 23 applications deployed and being ported, it is subdivided into three areas: medical image processing, biomedicine, and drug discovery, all of which already have many individual applications deployed on the EGEE infrastructure.

These applications stress the middleware with specific requirements, especially related to security (sensitivity of data), data management (complex data structures and distribution), and execution of large numbers of small jobs with data intensive needs. The biomedicine applications are now established as regular users of the infrastructure (with approximately 15000 jobs executed per month) and a computationally-intensive molecular docking analysis aimed at drug discovery that required 80 CPU-years was completed within one month.

Below is an overview of the biomedical applications currently deployed on the EGEE infrastructure.

The **medical imaging** sector targets the computerised analysis of digital medical images. It includes medical data federation, compute-intensive medical procedures, processing large data sets and statistical studies over large populations.

- **GATE** is a Monte Carlo-based simulator for planning radiotherapy treatments based on patient images. It uses the EGEE Grid infrastructure to reduce the time to needed complete Monte Carlo simulations to a value reasonable for clinical use.
- The Clinical Decision Support System (**CDSS**) uses image classification based on expert knowledge to aid clinical decisions. The Grid is exploited both for collecting large data sets and for efficiently training classification software over these large data sets.
- The **Pharmacokinetics** application studies the diffusion of a contrast agent in the liver from sequences of magnetic resonance images. Artefacts due to the movement of the patient make images directly incomparable. However the parallelised image co-registration computations running on the Grid allow analysis of the sequence in a reasonable time.
- **SiMRI3D** is a Magnetic Resonance Imaging simulation for the production of artificial but realistic 3D Magnetic Resonance (MR) images to analyse images from perfectly known sources, study artefacts, and further develop and optimise MR sequences.
- The **gPTM3D** application allows interactive reconstruction of 3D medical images, e.g. for the volume reconstruction of large or complex organs. The quality-of-service required for interactivity means that some sites on the Grid have to define a high-priority for this class of jobs.
- The **Bronze Standard** is an application to evaluate medical image registration algorithms. The amount of data to manipulate and the cost of computations are out of reach for standard computers, yet the application can easily be distributed over a Grid.
- The **SPM** software package is used by the neurological research community for the early diagnosis of Alzheimer's disease. It is based on the comparison of the candidate case to a large set of normal cases. Grid technologies allow easy access to distributed data as well as to distributed computational resources.

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The **bioinformatics** sector targets gene sequences analysis. It includes genomics, proteomics and phylogeny.

- Grid Protein Sequence Analysis, **GPS@**, is a Web portal that provides a user-friendly interface to these bioinformatics resources on the EGEE Grid. A prototype of the GPS@ portal is online, interfacing 13 Grid-enabled programs out of the 46 on the original portal.
- **xmipp_MLrefine** is used for the 3D structural analysis of large macromolecular complexes. Many electron microscopy images corresponding to different views of the specimen are combined in the reconstruction process. However, the recorded images typically suffer from large amounts of noise, and as a result many iterations are needed to find the most likely model that describes the experimental data.
- Images obtained from with an electron microscope are affected by many forms of aberration. Mathematically, the difference between a theoretical projection and the actual experimental projection is modeled by the contrast transfer function (CTF). To determine the actual shape of the CTF affecting the experimental images, a simulation method, **Xmipp_assign_multiple_CTFs**, is needed.
- **SPLATCHE** (SPatiaL And Temporal Coalescences in Heterogeneous Environment) is a cellular tool for genome evolution modeling. It allows the reconstruction of the global spread of past humans in a genographically realistic landscape, and to generate the molecular diversity of different human populations.

The **drug discovery** sector aims to help speed up the process of finding new drugs through *in silico* simulations of protein structures and dynamics.

- The **WISDOM** application runs large-scale computations for the *in silico* drug discovery against emerging and neglected diseases. These molecular docking calculations determine how well certain drugs attach to specific sites on the target virus – those which dock are more likely to be active against the virus. It has been successfully deployed against malaria and avian influenza, and other targets are planned for the future.
- **GridGRAMM** is a simple interface to do molecular docking on the Web. Results include a quality score and various access methods to the 3D structure of the complex. Molecular docking can be used for the study of molecular interactions, to analyze enzyme-substrate interactions, for drug design and to understand morbid mutant behaviour.
- The goal of **GROCK** (Grid Dock) is to provide an easy way to conduct mass screenings of molecular interactions using the Web by allowing users to screen one molecule against a whole database of known structures.

EGEE is keen to consider other applications. For further information on how to participate, as well as more information about the applications running on EGEE, visit the User and Application Portal at http://egeena4.lal.in2p3.fr/.

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