



Belgian research institutions involved in grid projects

Grid Press Meeting 30/05/2005

BEgrid:

BELNET (10 CPUs)

CETIC (not yet operational) (100 CPUs)

Facultés Polytechniques de Mons (not yet operational) (20 CPUs)

KULeuven (22)

Université Libre de Bruxelles and Vrije Universiteit Brussel (60)

Universiteit Antwerpen (24)

Universiteit Gent (74)

Vlaams Instituut voor de Zee (5)

BEgrid is a multidisciplinary computing/storage grid for research and is open for participation to all institutions affiliated with BELNET.

The five Flemish institutions involved in BEgrid have received a subsidy from the Flemish Government for the purchase of grid equipment. This subsidy amounts to € 741,000, spread over a 4-year period. A first tranche was provided for the linking of some 200 CPUs and for 3 Tbytes of storage capacity.

In addition, the participant departments involved are connecting their own existing equipment to the grid: approximately 50 CPUs; this number will increase during 2005.

The two participants that are not yet operational will add 20 and 100 CPUs respectively to BEgrid.

All concerned will contribute between 0.5 and 1 FTE to allow the grid to function, for both middleware and applications.

Applications being tested or already operational on BEgrid

Within the Numerical Analysis and Applied Mathematics section (NATW) of the department of Computer Science of the K.U. Leuven, a Monte Carlo algorithm was chosen as case study due to its very high level of parallelisability and the simplicity of the algorithm. Since Monte Carlo is principally used for functions that are difficult to integrate, the variance of this function is not easy to calculate. This makes it difficult to predict how many points will be required to obtain a specific level of accuracy. The grid experiment then consists of running a number of these Monte Carlo simulations on the grid, independently of each other. The implementation of the Monte Carlo algorithm is done in FORTRAN 95. The programme was statically linked so that it does not require the availability of the FORTRAN libraries on the grid. A control process then collects all individual approximations, combines these and, based upon this combined result, decides whether further simulations are required to increase the accuracy.

The **Centre for Plasma-Astrophysics (CPA)** will study among others coronal loops on the sun. The GRID application is used to formulate a mathematical model in order to model coronal loops. The model contains a large number of parameters; based upon these parameters, a virtual photo can be made of the loop as it would be seen from the earth. The hope is that by using a large number of parameters and then comparing these with the observations made, the usability of the model can be demonstrated and that the parameters that generate a realistic loop can be detected.

The **Nuclear Solid State Physics (NVSF)** section of the Institute for Nuclear and Radiation Physics of the K.U. Leuven makes intensive use of quantum chemical simulations of solids. WIEN2k is a software package that is able to predict the characteristics of solids based on quantum mechanical calculations, without needing to input experimental data. Like most such software packages, WIEN2k is based on the density functional theory (DFT, Nobel Prize Walter Kohn 1998). WIEN2k uses a very precise method to solve the DFT equations (APW+lo). Because of this, the code is not especially fast, but it is well suited to applications in which accuracy is important. WIEN2k is used by several hundreds of research groups worldwide. Depending on the nature of the solid being calculated, the time required for a serial calculation varies from a few minutes to a number of years. Such large problems are of course parallelised, which still results in calculation times of several months. To date, good scaling has been obtained with simple parallelisation strategies: a typical problem can be divided to a certain degree into independent subtasks that can be run on different computers (diagonalisation of a series of large matrices that can be formulated independently of each other).

This is insufficient for very large problems and further parallelisation of these serial components is required with the assistance, for example, of MPI (distribution of the diagonalisation of one matrix over multiple CPUs).

WIEN2k is in many ways suitable code to be implemented on a GRID:

In the Hydraulics Laboratory of the Department of Civil Engineering of the K.U. Leuven, a directional second-order wave model was used to generate unidirectional

and multidirectional waves. To generate stable statistics, a minimum of 250 17-minute random time series are required. Each realisation requires a 2D spectrum as input with 2048 frequencies and 31 directions. To obtain a precise description of the water surface, a sample frequency of 4 Hz (4096 time steps) is imposed. The code was written in Matlab. With the input as described above, there are 108 loops per realisation in the final programme. To put this in perspective, this means a simulation time of approximately 40 days per time series on a Windows machine with a 1.8 Ghz processor. The simulation of a large number of random time series can easily be distributed across several processors. The GRID facilities of BEgrid were then used.

At the Structural Mechanics section of the K.U. Leuven, numeric models are being developed for the study of vibrations in the built environment such as those caused by traffic or construction activities. Modelling ground wave propagation is a critical component of these models. Presently, probabilistic models are being developed that allow verification of the influence of uncertainties in the dynamic ground characteristics on the predictions. To accomplish this, use is made of Monte Carlo (MC) methods. The new GRID infrastructure of BEgrid was used in the realisation of MC simulations. The same calculation was repeated many times with different parameters, with the number of simulations established beforehand.

The Elementary Particle Physics section (ELEM) of the Vrije Universiteit Brussel is participating in the building of the Large Hadron Collider (LHC) at CERN and especially in the construction of the CMS (Compact Muon Solenoid) detector. This machine, which studies proton-proton interactions, will be operational in 2007. In the meantime, contributions have also been made to the simulations in multiple physics channels. Simulation software was developed in an international collaborative effort (use was often made of Monte Carlo). The CMS simulation software is already being used on the LCG grid and the scripts required to run on BEgrid have been written. This software is now ready to go into production on BEgrid.

The ELEM department of the Vrije Universiteit Brussel is participating in the AMANDA project, which is observing high energy neutrinos from astrophysical sources in the northern hemisphere. The detector is located at the Geographic South Pole. Part of the analysis of the data coming from this detector is being performed in Brussels. This analysis software now also makes use of the grid.

At the Vrije Universiteit Brussel, an application in the area of medical imaging has used grid computing for the first time. This application is capable of comparing medical images in order to recognise changes in a disorder's symptoms. The software written makes use of MPI (Message Passing Interface) to take advantage of the possibility of parallelisation on BEgrid.

The Department of Hydrology of the Vrije Universiteit Brussel has gridified software for the flood management in river basins. This application is currently in a test phase.

BELGRID

Facultés Universitaires Notre Dame de la Paix

UCL

ULB

UMH

ULG

70 CPUs, sponsored by the National Fund for Scientific Research (FNRS), are evenly distributed throughout these institutions with the intent to start a multidisciplinary grid.

Involvement in projects at European level

The Vrije Universiteit Brussel and the Université Libre de Bruxelles are participating in the European project Enabling Grids for E-science (EGEE).

The Facultés Polytechniques de Mons and CETIC are partners in COREgrid.