Computational physics (CP) is the study and implementation of numerical algorithms in order to solve problems in physics for which a quantitative theory already exists. CP is maturing as the third leg of the scientific enterprise alongside with experiment and theory. Computer performance, that evolves at an exponential rate, allows new ways of apprehending and solving problems. We are now able to investigate computationally fundamental questions in physics with unprecedented fidelity and level of detail. And that trend will surely continue for many years.

CP implies however more than using simulation to provide insight and interpretation. The IUAP commission on computational physics has broadened the field to include the computational control and data processing of experiments and the physical basis of computer machinery. Thus, CP involves also the acquisition and management of seas of experimental data (as in high energy physics) and new techniques of data acquisition and handling [1].

Computational physics covers a wide range of problems from quantum mechanical calculations to highly complex data processing and it is not easy to pinpoint specific researches in the field. New developments appear mostly as byproducts of other researches made in different fields by groups that rely on computers to perform their works. This inventory of the belgian contributions in CP will thus collect works made by physicists that are heavily involved in developing and improving computer codes and architecture in order to perform their researches.

Software developments

The numerical analysis group in Gent works on the development of numerical methods and software for problems that can be formulated in terms of differential equations, many of which are inspired by physical applications [2]. It Particular attention is paid to Sturm-Liouville problems and to bifurcations of dynamical systems. Among the developed software we mention Matslise [3]) and MatCont [4].

The Condensed Matter Theory (CMT) group belongs to the Department of Physics of the University of Antwerp and makes research in the the area of "Nanostructured semiconductors and superconductors" [5]. A vast amount of computer programs have been developed over the years. Hands-on experience is available on calculations of the strain distribution in self-assembled dots, Hartree-Fock approaches, density functional theory, finite difference techniques e.g. to solve coupled nonlinear differential equations (e.g. the Ginzburg-Landau equations), Monte Carlo simulations, molecular dynamics simulations, variational quantum Monte Carlo simulations, stochastic variational techniques. For its calculations the group

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relies on its own clusters of workstations and on the giant CalcUA (see later).

A toolbox for wavelet manipulations and related signal manipulation, YAWTb (Yet Another Wavelet Toolbox) written for Mathlab, is under development at the Institut de Physique Théorique (FYMA) of the UCL [6].

System simulations & Structure calculations

The ab-initio calculation of the entire structure of a molecule or of an aggregate of atoms (nanostructure) requires a huge amount of calculations. The ABINIT project [7] initiated in Belgium in 1997 and coordinated in Louvain-la-Neuve is aimed at the calculation of such structures and involves a lot a computer code developments. On the technical side the huge code (100000+ lines) relies on modern techniques for its development, and the program itself is continuously improved by more than 50 developers all around the word and has more than 500 registered users. The program is freely available, runs on many platforms, is well documented and adapted for parallel computing. At the UCL, the research mainly focuses on carbon-based systems, high-k dielectrics, and ferroelectrics.

The University of Liège is also active in the the development of ABINIT and has extended the program in different domains [8] (liquid semiconductors, nanodiamonds, silicon clusters or carbon nanotubes, non-linear optical susceptibilities, Raman tensors and electro-optic coefficients).

At the Department of Physics at the University of Antwerp, a group studies the electronic and structural properties of (solid) materials by using first-principles. Electronic structure calculations are carried within the Density Functional Theory formalism. A large part of its work is devoted to the determination of core level electron energy loss spectra, in particular, the "near edge structure" from these bandstructure calculations. The group is mainly interested in carbon materials (e.g. amorphous carbon and nanotubes) and transition metal oxides (e.g. niobiumoxides).

The theoretical study of the interaction of a short laser pulse with an atom or the simulation emerging from "the droplet temperature measurements" technique (UCL, Von Karman) [9] implied also a lot a numerical developments.

The cold atom physics group at the Liège University [10] develops lots of numerical simulations in the field of cavity quantum electrodynamics with cold atoms. The atom-field interaction is modeled in the particular case when the atomic motion must be described quantum mechanically and special algorithms are used and developed to solve the Schrödinger equation. In collaboration with other groups in Germany, numerical simulations are also performed in trapped ion systems interacting with external laser fields. The aim is to predict numerically the non-classical properties of the light emitted by chains of trapped ions.

In the field of atomic physics, and more particularly atomic spectroscopy, substantial progress has been achieved by the Mons Astrophysics group [11] by improving sophisticated computer codes that allow to model, in a more and more realistic way, the atomic structures characterized by very complex electronic configurations.

In the same line, methodological and computational developments are realized by the ULB "Quantum Chemistry and Atomic Physics" group [12], in the ab-initio modelling of electron correlation, many-body relativistic effects and of the relevant interactions in atoms and molecules (neutral, negative and positive ionic species) to allow the calculation of various structural, dynamical and spectroscopic properties.

The physical theoretical chemistry group of the University of Liège is modeling the
properties of different kinds of nanostructures. These models are applied to molecular logic and could lead to the design of nanosensors [13].

An important activity in the Division of Materials Engineering and Process at UCL concerns the development of micromechanics-based hierarchical multiscale models to predict the deformation and fracture of advanced metallic alloys, composites, multilayers and bonded joints [14].

The GeoHydrodynamics and Environment Research group at the Liège University [15] uses 3D models of marine systems to predict circulation patterns, pollution dispersion, ecosystem evolution, thermohaline structures of the ocean and many other marine parameters. To do so, a set of coupled non-linear 3D partial differential equations are solved numerically using finite volume methods. To be able to handle the size of the problem (10^7 state variables advanced in time over 10^4 time steps), parallel computing based on domain decompositions is implemented.

The detailed simulation by Monte-Carlo methods of the experimental signals expected in huge detector systems installed at high energy accelerators, of phenomena predicted by theoretical models, is common practice in experimental particle physics. Software for event simulation and real data reduction is extensively used and developed in the high energy physics groups of the UA [16], IIHE(ULB-VUB) [17], UCL [18], UG [19] and UMH [20].

Astrophysics and Geophysics

The Institut d'astronomie et de géophysique G. Lemaître (UCL) [21] studies the climat evolution on a large time scale. They rely on very complex calculations which are performed by applying different models that are continuously improved. All these calculations involve huge computer power and the development of new algorithms.

The Center for Space Radiation (CSR) [22] of the UCL, in collaboration with the Belgian Institute for Space Aeronomy [23], is simulating (by Monte-Carlo methods) the interactions of energetic particles present in space with matter or gas by using the CERN developed GEANT software toolkit [24].

Computer assisted instrumentation

The Biomedical Physics group of the University of Antwerp is mainly focused on experimental research concerning the middle ear mechanics. For that purpose, the group has developed many specific instruments that are computer controlled [25].

In Liège, the IPNAS laboratory [26] has constructed many new apparatus that use imbedded microprocessors and rely on the virtual instrumentation paradigm [27]. A computerized remote positioning system (developed originally for archaeological measurements) has evolved in a commercial product [28].

Belgian research computer infrastructure

On March 2005 CalCUA [29], the most powerful computer cluster in Belgium (costing 3.8 million euros and provided by Sun Microsystems Belgium), has been installed at the University of Antwerp. The machine, formed by a cluster of 256 nodes, is able to reach a speed of 2 teraflops (10^12 of floating point operations/second). CalCUA is an interdisciplinary project between several departments at the University of Antwerp in which mathematicians, computer scientists, linguistic specialists, biomedical scientists, physicists and chemists are participating. Physicists will use it, a.e. to investigating very small nanostructures such as quantum particles that are applied in lasers and carbon nanotubes.
which are used as components of electronic transmitters at nanometer levels.

The UCL has established since 1991 a center which unifies the computer resources of many groups and gives expertises, technical help and specific formations [30]. This center is also responsible of a mass storage structure. The calculation power is greater than 500 Gflops (milliard of floating point operations/second) and the on-line storage capacity is of 15 terabytes. Among the numerous users (40) using these facilities many are physicists working in the field of ab-initio calculations (a.e. the ABINIT project) or in fluid dynamics (physical oceanography).

Scientists of the Liège University have formed a group called Numerical Intensive Calculation - NIC [31]. They have at their disposal a SGI Origin 3800 computer with a peak power of 48 Gflops (it will be replaced in 2006 by a new and more powerful Linux cluster). This machine is operated under the NIC group supervision and is used by many physicists.

The academic network

In Belgium, the universities, colleges, schools, research centers and government departments are connected by a national research network that provides high-bandwidth Internet connection. This infrastructure, called BELNET, has been initiated in 1989 by the Belgian Science Policy Office’s programming department. The aim was to promote the use of supercomputers by Belgian scientists and to arrive at the installation of a network to enable remote connections between scientists with powerful computers.

Recently, BELNET [32] has decided to initiate a new project called BEgrid [33] that will federate the computing and data resources distributed over several sites. Thanks to the development of fast links and new parallel computing algorithms, this will provide to the users a "virtual structure" able to distribute harmoniously the computer power between computer distributed all over the world. The Vlaamse Gemeenschap has already financed the project to provide "ubiquitous access to distributed heterogeneous resources across the boundaries of administrative and organizational domains” opening the way to the development of BEgrid. This first step has been established as a collaboration between BELNET and different institutions (KUL, UA, UGent, VLIZO, VUB/ULB). A complementary project, supported by 5 french universities (ULB, ULg, UCL, UMH, FUNDP) is also starting and is aimed at developing a computer grid that federates the local computer resources of belgian universities. Again many physicists are associated to the project.

Conclusions

Even if this review is not exhaustive, it proves that computational physics activity in Belgium is important and that a lot of physics groups are active in the field. Computer programs are developed and improved in almost all universities often as byproducts of main researches.

Most of the information given in this paper have been adapted from responses to my request or gathered from the Internet. Many thanks to all of my colleagues and friends that have helped me in realizing this survey.
References

[16] http://hep.ua.ac.be