Monte Carlo in radiotherapy: experience in a distributed computational environment

B Caccia[1], M Mattia[1], G. Amati[3], C Andenna[2], M Benassi[4], A d'Angelo[4], G Frustagli[1], G Iaccarino[4], A Occhigrossi[1], S Valentini[1]

[1] Istituto Superiore di Sanità (ISS) and Istituto Nazionale di Fisica Nucleare (INFN), Rome, Italy

[2] Istituto Superiore Prevenzione e Sicurezza del Lavoro (ISPESL), Rome, Italy

[3] Inter-University Consortium for the Application of Super-Computing for Universities and Research (CASPUR), Rome, Italy

[4] Medical Physics Department, Istituto Regina Elena, Rome, Italy

Abstract. New technologies in cancer radiotherapy need a more accurate computation of the dose delivered in the radiotherapeutical treatment plan, and it is important to integrate sophisticated mathematical models and advanced computing knowledge into the treatment planning (TP) process. We present some results about using Monte Carlo (MC) codes in dose calculation for treatment planning. A distributed computing resource located in the Technologies and Health Department of the Italian National Institute of Health (ISS) along with other computer facilities (CASPUR - Inter-University Consortium for the Application of Super-Computing for Universities and Research) has been used to perform a fully complete MC simulation to compute dose distribution on phantoms irradiated with a radiotherapy accelerator. Using BEAMnrc and GEANT4 MC based codes we calculated dose distributions on a plain water phantom and air/water phantom. Experimental and calculated dose values below ±2% (for depth between 5 mm and 130 mm) were in agreement both in PDD (Percentage Depth Dose) and transversal sections of the phantom. We consider these results a first step towards a system suitable for medical physics departments to simulate a complete treatment plan using remote computing facilities for MC simulations .

E-mail: caccia@iss.it

1. Introduction

In recent years the accuracy of dose calculation has improved together with the computing power available in Radiotherapy departments and new mathematical approaches to dose calculation and optimization have been introduced in the clinical practice. Owing to their better accuracy, Monte Carlo (MC) methods have been considered as an alternative to analytical methods for treatment planning in cancer radiotherapy [1, 2]. MC-based treatment planning systems (TPS) model radiation transport with great accuracy so that a more realistic dose distribution is obtained in inhomogeneous media. Unfortunately MC methods require a large amount of computational resources often unavailable in hospitals. To speed up the dose computation, the modelling of matter-radiation interaction has to be simplified, but this may lead to incorrect results, so these codes need to be benchmarked. We believe it

is important that clinical physicists have some insight into MC methods, before to operate in a clinical environment, even because vendors of commercial TPS have recently started to offer MC based systems. Considerable work is required to set up MC codes and to organize and manage the necessary computing resources. It is therefore important for clinical physicists to share knowledge and computing resources to introduce, in the best possible way, the use of MC codes in the clinical practice.

This work is a first step towards a web-like system for the remote access to computing resources for Radiotherapy in order to make MC-based treatment planning available in any Radiotherapy department, at least as a quality assurance tool.

2. Computing facilities

A Beowulf cluster (*BeoCluster*) of 30 computers has been used (Figure 1) to distribute the histories simulated by the MC codes, actually without any parallelization of the codes (i.e. farming). With farming we had a fault tolerant computing system, where every single task was independent from the other.We chose a Beowulf cluster because it is a general purpose architecture and it represented a cheap and simple solution for this first approach.

For computational tasks requiring almost no communications among nodes, as in our MC simulations, adding more nodes to the *BeoCluster* results in a quasi-linear increase in computation performance with a small amount of extra synchronization processing (cluster turns out to be linearly scalable). *BeoCluster* runs the Linux SUSE 9.2 distribution and is configured with 30 nodes (slaves) and 1 master server connected via a private LAN (1 Gb/s) through two switches *3Com Baseline 2816* with 16 programmable ports. Each node is a Pentium IV (3.2 GHz) equipped with a 1GB memory and an integrated Ethernet card. All the processors use Hyper-Threading technology: theoretically every CPU supports two processes.

Figure 1. BeoCluster at the Technologies and Health Department of the Italian National Institute of Health (ISS).

The master shares its disk space via NFS (Network File System). The master acts as a firewall between Internet and the cluster private subnet, such that it is the only entry-point to the cluster for the user. Only secure and encrypted connections are allowed.

For some simulations we have also used other computer clusters (from CASPUR) using different types of CPU (single and dual core AMD Opteron, Intel Xeon, for details see http://www.caspur.it).

3. Monte Carlo simulations and experimental data validation

A Varian Clinac 2100 C/D linear accelerator has been simulated at nominal accelerating potential of 6MV, equipped with a dynamic multileaves collimator (MLC) Millennium 120. A full simulation of

the accelerator geometry has been performed: Figure 2a shows the component modules used for the MC simulation.
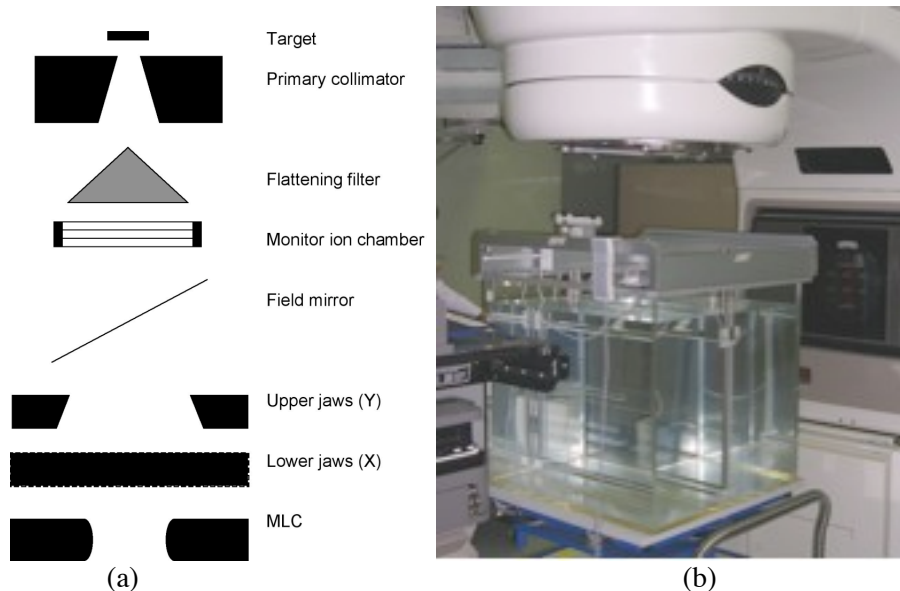

Figure 2. Simulations and experimental measurements: (a) a schematic representation of the component modules used for the MC simulations; (b) experimental measurements equipment

All the materials and geometric data about the accelerator were acquired from the manufacturer (Varian) and from measurements made during commissioning of the accelerator.

Following a standard procedure [1, 10, 11] the parameters of the primary electron beam hitting the target, as its energy, angular distribution and spatial distribution, were chosen in order to minimize the discrepancies between simulation results and measured data. Both for GEANT4 and BEAM codes we chose a parallel electron beam hitting the target with a gaussian energy distribution (σ=0.127 MeV, E=6.0 MeV).

In some cases the energy differs from its nominal value up to 0.5 MV. According to the usual procedure followed for modeling photons beams, a depth–dose curve from MC simulations for a mono-energetic beam was calculated and then compared with the corresponding measured curve.

To evaluate MC simulations, results were compared with experimental measurements on two phantom geometries (Figure 2b). One (see figure 3a) is a simple homogeneous water phantom PTW mP3-S (50 cm per side). The other geometry (Figure 3b) is a heterogeneous phantom, half water and half air inside a PMMA (PolyMethylMethAcrylate) box.

Experimental measurements were made with both Farmer PTW 30013 and diode based probes. Square fields of 6, 10, 20, 30 and 40 cm per side were investigated. The accelerator and the phantom geometries were simulated by two different MC codes: GEANT4 [3] and EGSnrc [4]. We did not reprogram the MC codes to run in parallel on the cluster, but we distributed the histories among the nodes of the used clusters. We chose a voxel dimension of 5x5x1 mm^3.
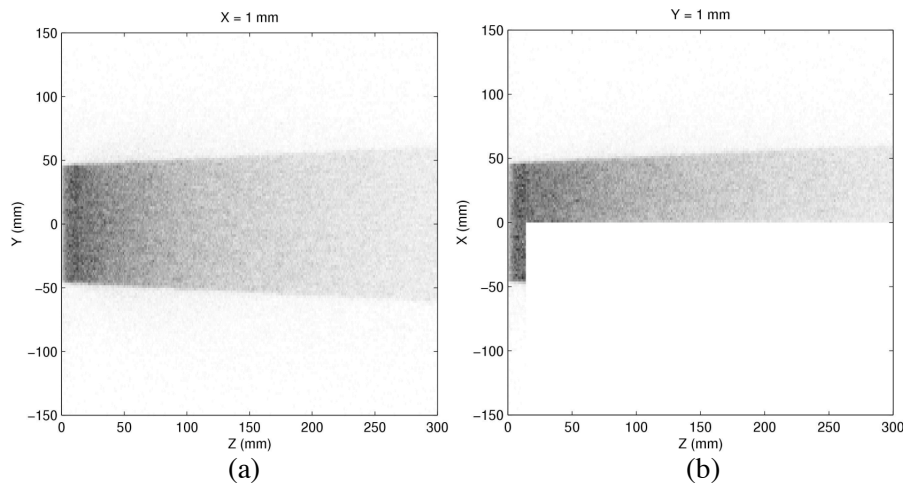
Figure 3. Phantom dose profiles: the sum of the absorbed dose along one of the transverse directions (X or Y) is shown for a homogeneous water phantom (a) and a heterogeneous water/air phantom (b). The darker is the shading the higher is the total absorbed dose.

GEANT4 (GEometry ANd Tracking 4) is an object-oriented MC simulation toolkit. The best fitting model of the medical accelerator is a modified version of the *Medical Linac*, an advanced example of GEANT4 [5].

DOSXYZ [6] and the BEAM code [7] were used to model the linear accelerator and the phantoms in the second MC code. BEAMnrc is an EGS-based code developed for the modelling of a linear accelerator. DOSXYZ allows to import and translate Computing Tomography (CT) data in voxels, and simulates the interaction between the phantom and the radiation. BEAMnrc and DOSXYZnrc are widely used by medical physicists. In all simulations the energy cutoffs were 0.7 MeV per electrons and 0.01MeV per photon. The EGSnrc transport parameters were taken as BCA = EXACT, electron step algorithm = PRESTA-II, NIST cross section for bremsstrahlung, and Koch and Motz cross sections for bremsstrahlung angular sampling. Bound Compton scattering, Rayleigh scattering, photoelectron angular sampling, and atomic relaxations were switched on. No variance reduction techniques were employed.

3.1. Distributed application: GEANT4
We wrote a dedicated program in C++ language using GEANT4 libraries. The program reads the values of some parameters from an external file to allow the flexibility necessary for our *BeoCluster*.

Since the desired accuracy could be achieved only through a high number of primary histories, several tasks have to be run for a single simulation. Consequently each node of the cluster runs some instances of the program, and different seeds for the random generator have to be provided for each instance. Seeds, the number of the primary histories and other parameters are specified in a launch file. Several hundreds of instances are generally run for each simulation and the same number of launch files have to be generated with different seed number. A dedicated bashscript program generates all the required files. Simulations performed at CASPUR were executed using the Sun Grid Engine (SGE http://gridengine.sunsource.net/) queuing system in order to check the amenability of this approach to Grid computing. Energy of 6 MV and a square field of 20cm per side was used to compare the computing time on BeoCluster and the simulations performed at CASPUR. The voxel dimension is 5x5x1 mm^3.

CPU	Clock	Estimated time (hour)	Number of CPU	Elapsed time (hour)
Intel Xeon	2.4 Ghz	500	20	25
Intel Pentium IV	3.2 Ghz (with hyper-threading)	300	30	10
AMD Opteron	2.0 Ghz	320	48	7
AMD Opteron	2.4 Ghz	280	48	6
AMD Opteron	2.4 Ghz (dual core)	150	48	3

Table 1. Computing time on different processing units available at CASPUR. Simulation is referred to a square field of 20cm per side and the absorbed dose is calculated for a voxel size of 5x5x1 mm^3. First two columns describe the processing units type while the first estimated time column refers to the time needed to simulate 10^9 primary events trough the accelerator model described in Fig. 2 using GEANT4 MC on a single processor architecture. Last column lists the time needed for the same task using all the CPU available by the parallel computers hosted by CASPUR.

In Tab. 1 the total time to perform a 10^9 primary histories is shown using both only one CPU and all the processing units available by the computer clusters at CASPUR. The improvement due to dual core CPU is apparent. It is apparent that even using a mid-size cluster (i.e. 48 CPU rack-mounted) it is possible to perform all the simulation in few hours: a computational time compatible with the clinic requirements.

3.2. Distributed application: BEAM
In the case of BEAMnrc two launching configuration files per task are required, one for the BEAMnrc compiled program computing the phase space, and the other for the DOSXYZnrc program to calculate dose distribution in the phantom. As with GEANT4, several instances of each program have to be run in order to obtain the necessary statistics and, consequently, an adequate number of launch files have to be generated. To automatize file generation, two prototype files have been produced by modifying those created with the dedicated GUI interfaces. A script takes these prototype files as input and generates all the launch files required, changing the parameters to differentiate each instance. In particular, each launch file is characterised by specific random seed numbers and, in the case of dose calculation, by a phase space file. As with GEANT4, the same bashscript program generates a second bashscript program that specifies the sequence in which the BEAMnrc programs have to be run. We used the same processes-delivering approach we had used for the GEANT4 application.

In both cases, once all the configuration files have been generated, a queue manager program on the master server distributes the jobs to the nodes.

4. Simulation results and discussion
The GEANT4 MC code was validated on square fields, from 6 to 30 cm × side (Fig. 4), while a 40 cm side field was used to compute with BEAMnrc code the dose distributions (Fig. 5) in the homogeneous water phantom. As expected, in order to obtain similar standard errors the number of primary events needed for field with larger size is smaller than for narrow fields: 30×10^9 primary electrons for the 6×6 cm^2 field; 10×10^9 electrons for 10×10 cm^2 and 4×10^9 primary electrons for the 30×30 cm^2 field. Indeed, being simulated the whole linear accelerator, the histories contributing in delivering dose to the water phantom is a small fraction: for the 20×20 cm^2 field only about 4% of them are effective.

Both beam profiles at different depth and depth dose curves are evaluated from the MC calculations and compared to the ones measured. Discrepancies of the PDDs between MC data and experimental measures are with 2% within a depth interval between 5 mm and 130 mm, while is not larger than 4% for depths greater than 130 mm. This is mainly due to having kept constant the size of the voxels (1 mm size in depth): lower doses may correspond to lower number of hits in the water phantom increasing the statistical uncertainty.
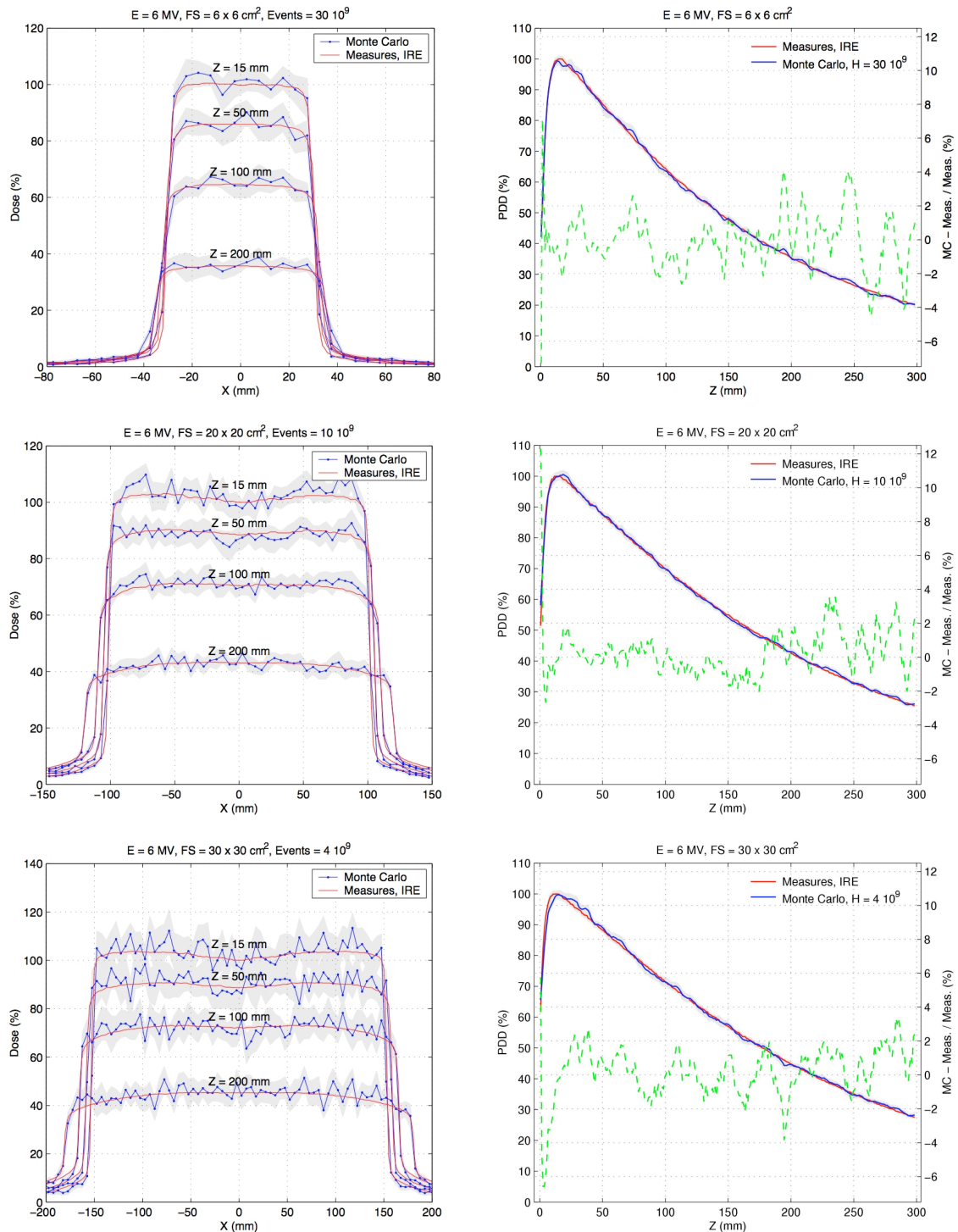
Figure 4. Match between GEANT4 MC results and measured doses for the 6 × 6 cm² (top), 20 × 20 cm² (middle) and 30 × 30 cm² (bottom) fields in water phantom. Red lines refer to measured data; blue lines, to GEANT4 MC data and the gray strips are the confidence intervals related to 1 st. dev. for the MC results green dashed line on the right plots shows the percent difference between measured and calculated local doses. The values are normalized to have the same mean dose on the central axis within a depth range from 50 mm to 250 mm. Left panels: cross profiles at 15, 50, 100, and 200 mm depth; Right panels: PDDs and relative difference between MC and measured data.

If a strategy similar to the one reported in [11] is adopted, such that larger voxels at larger depths are considered an invariant standard error may be recovered.

In Fig. 5 the depth dose curve for the 40 x 40 cm^2 field the agreement between BEAM MC simulations and measured data has a comparable statistical uncertainty to the one reported for GEANT4 in Fig. 4, with the exception of a significant difference for depth larger than 25 cm. Such failure is due to a modeled phantom with depth of 30 cm, which is shorter than the one used in the experimental set up (50 cm) and modeled in GEANT4.
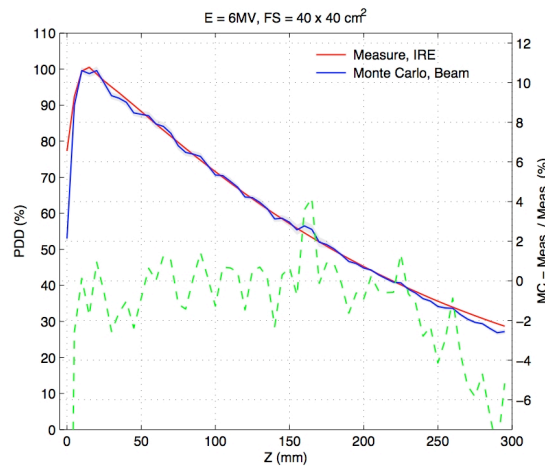

Figure 5. Depth dose profile in water phantom for a 40×40 cm^2 field. The red line refers to measured data while the blue line refers to EGSR/BEAMnrc MC results. Green dashed line is the percent difference between measured and calculated local doses.

It has to be pointed out that the number of histories of the two MC codes cannot be directly compared. The GEANT4-based code primary histories refer to the whole set of electrons hitting the target, most of which are lost and do not contribute to the dose in the phantom. On the other hand the number of histories for the BEAMnrc code refers to the number of particles of the phase space used by the dose tool calculation.

An acceptable agreement between calculated and measured data was also obtained along the transversal sections, as shown in the left panels of Fig. 4. Large errors are visible in the PDD plots at distances close to the build up region as usual.

As for computing time, the BEAMnrc-based code showed the best performance, but this was probably due to the fact that it was better optimized than the GEANT4-based code. Code optimizations, such as the use of the phase space, are scheduled.
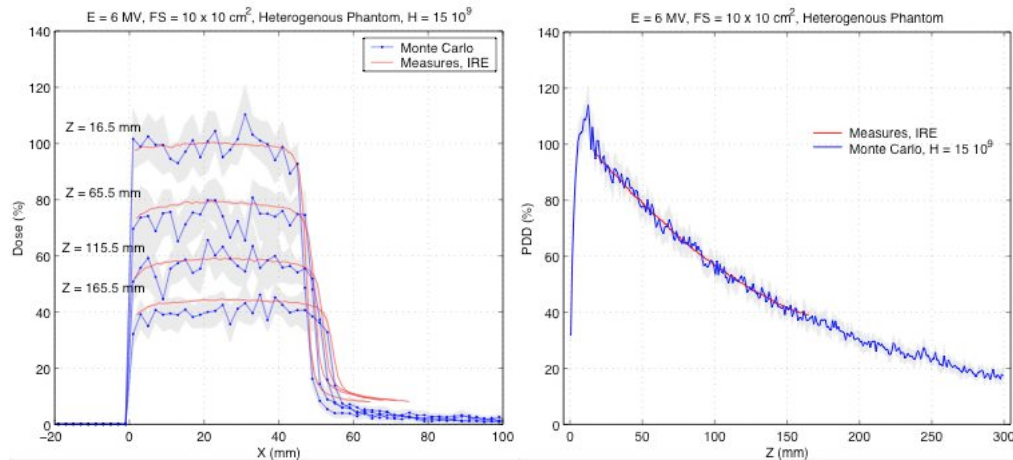
Figure 6. Results for the $10 \times 10 \ cm^2$ field in a heterogeneous phantom (air/water). The red lines refer to measured data; blue lines, to GEANT4 MC data. The values are normalized to the dose on the central axis at 16.5 mm depth. Left panel: Cross profiles at 16.5, 65.5, 115.5, and 165.5 mm depth. Right panel: PDD.

The C++ GEANT4-based model was also applied to a heterogeneous phantom, half water and half air inside a PMMA box. The water surface is parallel to central axis of the beam as shown in Fig. 3. In Fig. 6 both the dose profiles and the depth dose curve inside water are reported: a quite good agreement between experimental data and MC simulations appears at least for not too large depths (< 10 cm), even if a deeper investigation makes apparent a significant discrepancy at the penumbra zones of the cross profiles. Further analyses are scheduled to investigate this behavior.

5. Conclusions

The comparison between the performances of GEANT4 and BEAMnrc-based MC codes showed it was necessary to optimize our C++ GEANT4-based code in order to speed it up. Some tests on the heterogeneous phantom are still in progress. The first results show that the agreement with the experimental data is within the standard acceptability range (2% for Z between 5 mm and 130 mm for a PDD sampled every 1 mm). Some code optimizations are being implemented.

The possibility to run jobs in a remote fashion has been implemented. As a first approach GEANT4 and BEAMnrc-based MC codes were developed and tested on a simple water phantom.

We consider our results as a first step towards a system suitable for medical physics departments to simulate a complete treatment plan based on MC computation using a remote computing facility. We believe that in this way it is possible to encourage and develop the usage of MC codes in dose calculation for treatment planning. We are working on a project to provide a generic MC service as a Web-like service. Furthermore we believe it would be important to create a repository of phase space data for external beam Radiotherapy [8, 9] and hope to contribute to the construction of such a database in the near future.

References
[1]   Verhaegen F and Seuntjens V 2003 Monte Carlo modelling of external radiotherapy photons beams *Phys. Med Biol*. **48** R107-R164.
[2]   Nederlandse Commissie Voor Stralingsdosimetrie 2006 Monte Carlo Treatment Planning: An introduction *NCS Delft* The Netherlands, Report 16.
[3]   Agostinelli S et al. 2003 GEANT4 – a simulation toolkit *Nucl. Instrum. Methods Phys Res* A **506**, 250-303
[4]   Nelson W R, Hirayama H and Rogers W O 1985 The EGS4 code system *Stanford Linear Accelerator Publications*

[5]   Guatelli S, Moshicki J, Pia M G, Piergentili M 2005 Monte Carlo simulation for radiotherapy in a distributed computing environment The Monte Carlo Method: versatility Unbounded in a dynamic computing world, Tennessee, April 17-21, 2005, on CD-ROM, American Society, LaGrange Park, IL (2005)

[6]   Ma C M, Reckwerdt P, Holmes M, Rogers D W O and Geiser B 1995 DOSXYZ User manual, NRC Report *PIRS* 509, b

[7]   Rogers D W O, Feddegon B A, Ding G X, Ma C M, We J and Mackie T R 1995 BEAM: a Monte Carlo code to simulate radiotherapy treatment units *Med. Phys.* **22**, 504-524

[8]   IAEA - INDC International Nuclear Data Committee Phase-space database for External Beam Radiotherapy – December 2005

[9]   Capote R 2006 Monte Carlo IMRT dosimetry First European Workshop on Monte Carlo Treatment of the European Workgroup on MCTP, 22-25 october 2006, Gent, Belgium.

[10]   Ding G X 2002 Energy spectra, angular spread, fluence profiles and dose distributions of 6 and 18 MV photon beams: results of Monte Carlo simulations for a Varian 2100EX accelerator *Phys.Med.Biol.* **47**, 1025-1046.

[11]   Cho S H, Vassiliev O N, Lee S, Liu H H, Ibbott G S and Mohan R 2005 Reference photon dosimetry data and reference phase space data for the 6 MV photon beam from Varian Clinac 2100 series linear accelerators *Med. Phys.* **32**(1), 137-148