3rd FLUKA Advanced Course

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Parallelization of Fluka simulations in hadrontherapy
(on CRESCO/ENEA-GRID)

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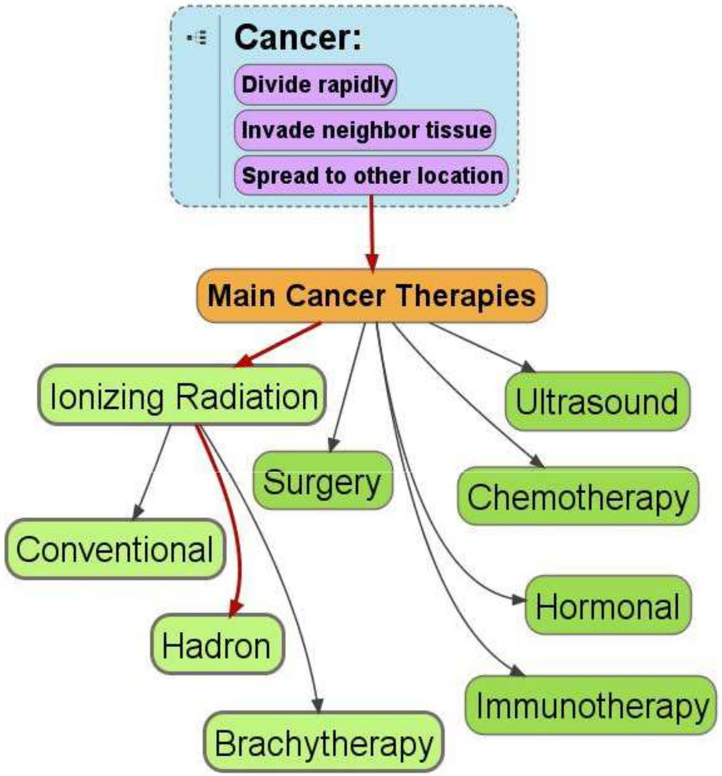
Outline

- ❑ **Introduction to hadrontherapy**
- ❑ Applications:
  1) «Analytical» MC dose evaluation
  2) Online beam monitoring system
- ❑ FLUKA “parallelization”
- ❑ FLUKA simulations and results
- ❑ Conclusions

Radiotherapy



Ionizing radiation kills cells by damaging their reproductive capacity.

Radiotherapy goal is to damage as many cancer cells as possible, while limiting harm to nearby healthy tissue.

Radiotherapy plays a leading role in cancer treatment.

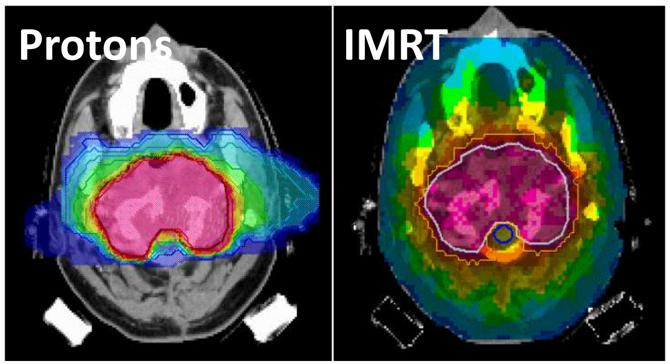
Radiation is not selective, but it is possible to achieve selectivity:

- Tumor cells are more radiosensitive than normal cells
- Reparability of malignant cells is less efficient than normal cells
- Dose delivered can be conformed to diseased tissue

Any additional progress can improve the number of the cured patients and the quality of live: the use of hadrons is presently one of the most promising way in treatment of specific cancers

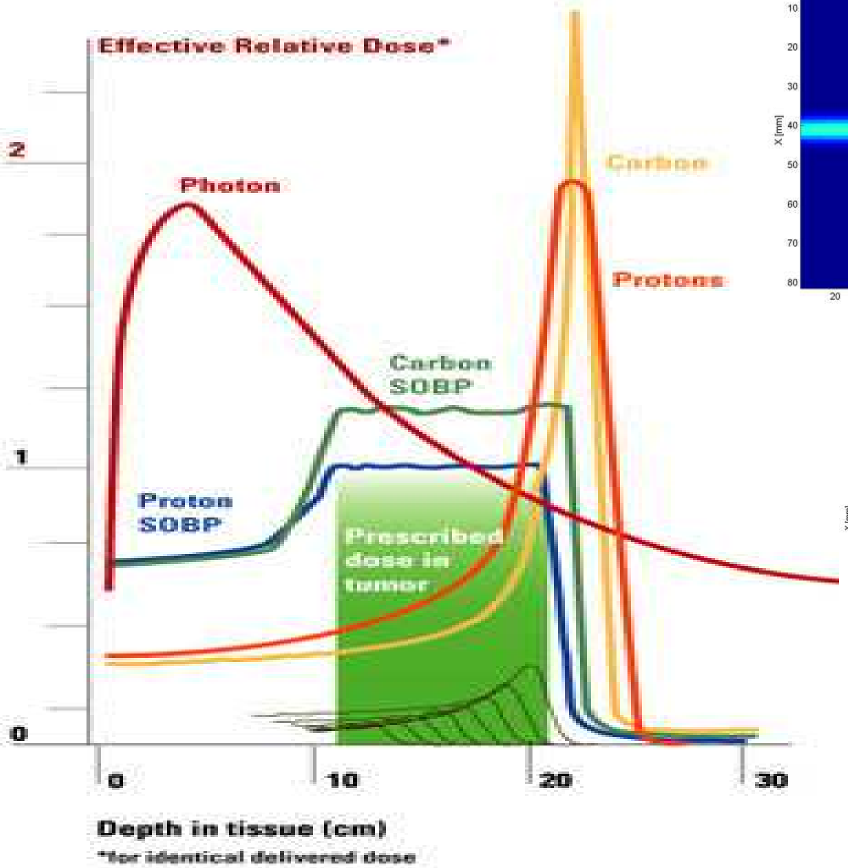
Hadrontherapy physics

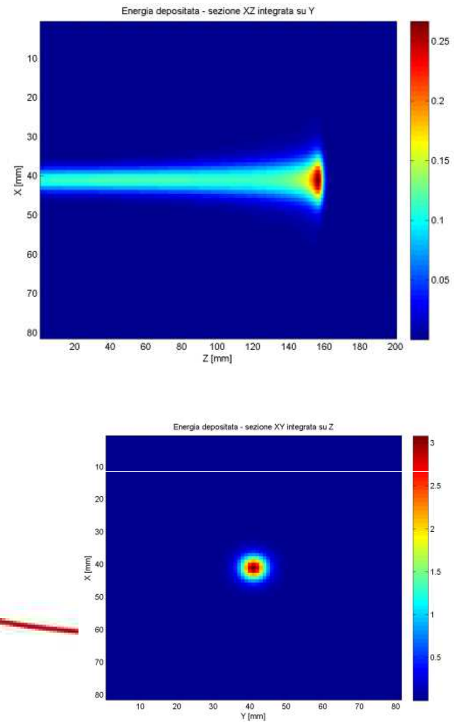
- Hadrons (protons and ions) release almost all of their energy at the end of their range, in the so called **Bragg peak**
- The penetration depth depends on the initial beam energy
- A desired distributed dose is obtained by superimposing beams with different energies (**Spread Out Bragg Peak (SOBP)**)



G. Kraft, GSI, Biophysik, Darmstadt and J. Debus, DKFZ, Heidelberg

Bragg Peak





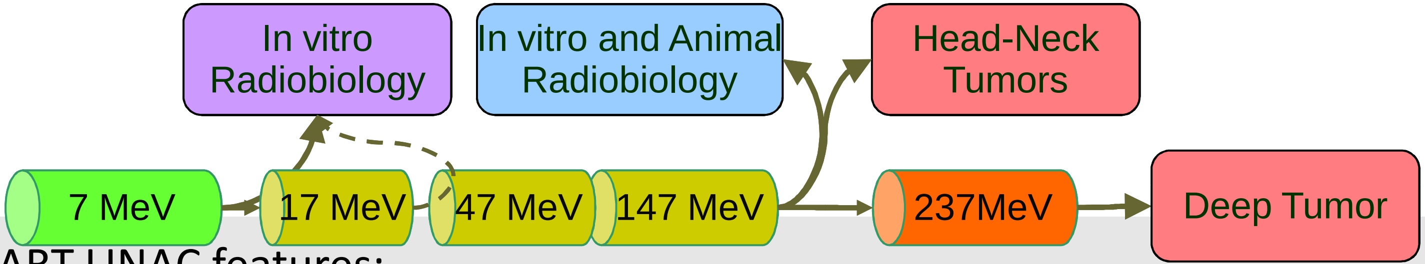
Dose distribution by FLUKA simulations

The hadrontherapy is intrinsically conformational and it is virtually one of the better radiotherapy technique in the cancer treatment.

Protontherapy with LINAC: the TOP-IMPLART project

The TOP IMPLART (*Terapia Oncologica con Protoni - Intensity Modulated Proton Linear Accelerator for Therapy*) project (ENEA - ISS – IFO collaboration) aims to realize an innovative proton therapy facility, based for the first time, on a linear accelerator.

Funding: ISS before 2002, Lazio Region after 2009



TOP-IMPLART LINAC features:

- The **active and fast scanning (3+1D)** in
  - **Intensity** (instantaneous released dose)
  - **Energy** (depth)
  - **Transversal Position** (X/Y)

with **high frequency (100-200 Hz)** allows an highly conformational therapy ⇒**need of:**

- The modular implementation allows a modular/progressive development (based on the financial flow)
- The use of widely diffused (3 GHz) radiofrequency technology reduces realization and maintenance costs

1) **Estimation of dose distribution by optimizing pencil beam directions, energies and intensities**

2) **Accurate monitoring of the beam parameters on a pulse by pulse basis**

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1) Why an «Analytical» MC dose distribution evaluation

Method	Advantages	Disadvantages
Monte Carlo Simulation	the most accurate method for calculating dose distribution	very long computing time
Analytical algorithms (like TPS)	faster	less accurate

Dose distribution evaluation

- is strictly related to the specific facility and adopted delivery technique.
- needs to be promptly available during the development of a new facility to study the dose distribution under specific conditions, using homogeneous phantoms.
- requires to be a system well known and under control.

Use MC results to infer analytical expressions matching the precision of Monte Carlo (MC) simulations and the rapidity of phenomenological or empirical algorithms

1)«Analytical» MC dose distribution implementation

FLUKA MC simulations → analytical expressions for the dose distribution in a heterogeneous material

Study in different configurations (right table):

1) Bragg curve in heterogeneous media (reproduction of Bragg curve in materials other than water)
2) Multiple Coulomb scattering (fit of the distribution in the transversal plane)
3) Beam incidence not orthogonal to surface

Material	Energy	Angle (for each energy)
Water	100 150 200 230	0° 2° 5° 10° 15°
Bone	100 150 200 230	0° 2° 5° 10° 15°
“Lung”	100 150 200 230	0° 2° 5° 10° 15°
Composited material “WLB”	100 150 200 230	0° 2° 5° 10° 15°

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2)Beam monitoring system for the TOP-IMPLART LINAC

The beam monitor (for online indirect estimation of the delivered dose) must provide:

- Real-time measure of beam parameters (position, intensity profile, direction/emittance)
- Quick response (faster than beam pulse period)
- Feedback information to correct small deviation from the planned therapeutic treatment
- Fast shutdown in case of large (not recoverable) deviation from planned parameters
- High reliability

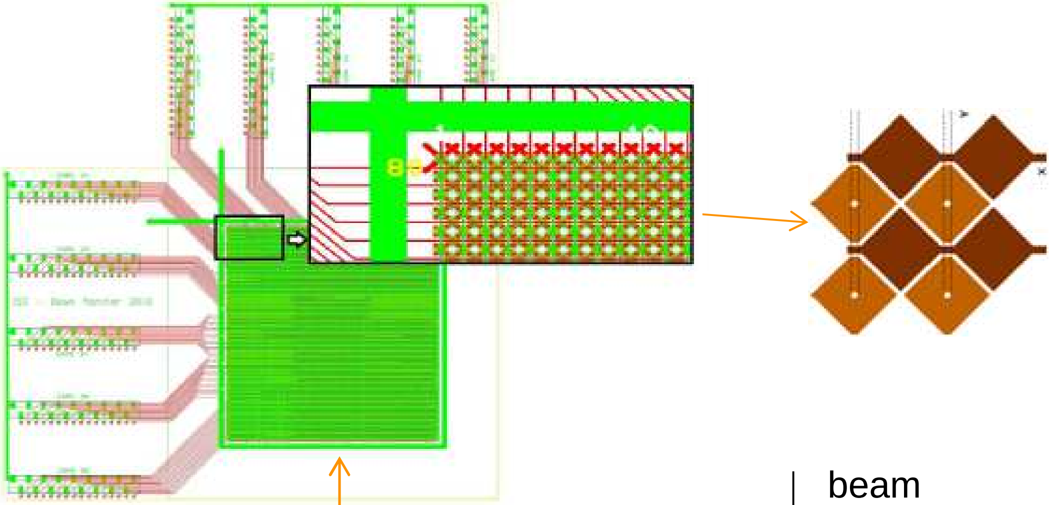
Pulsed beam characteristics		Beam monitoring system specifications
Energy in the range	130-250 MeV	Light compact chamber
Beam cross section	1-10 mm	Good spatial resolution (~1/10 mm) ⇨ **MPGD**
Beam current	0.1-10 μA	Wide dynamic range (10^4 at least) } **Dedicated Electronics**
Average current:	3.5 nA	Good sensitivity (~100 fC) } **Dedicated Electronics**
Pulse period	1-3.5 μs	Zero dead time (or near zero)
Pulse frequency (fast dose repainting)	10-100 Hz	Rapid response (< 1ms)
		Typical number of channels: few 100

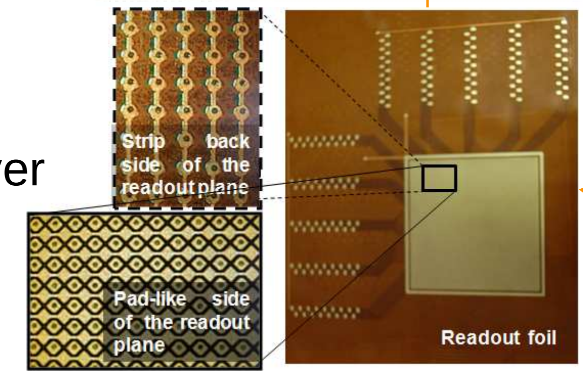
2) Beam monitor implemented

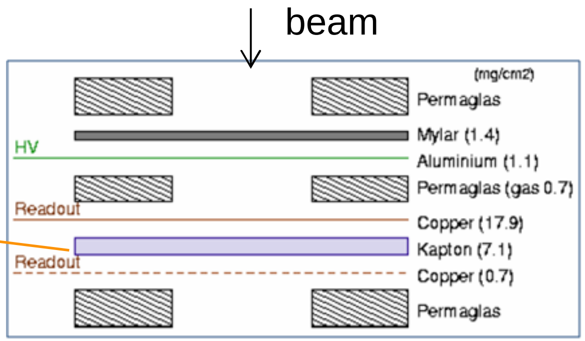
The TOP-IMPLART monitor system is based on 2D segmented ionization chamber built with Micro-Pattern Gaseus Detector (MPGD) technology and it is driven by a dedicated front end electronics, with a multi range logic

✓Suitable for the monitoring of proton (or electron) beam in other facilities

- the prototype consists of 2 planes separated by a gas gap
- the anode is a Kapton foil sandwiched between two Copper layers engraved so to obtain a pads-like map
- alternate pads are connected along a given direction
- dedicated electronics
- active surface able to cover the beam scan

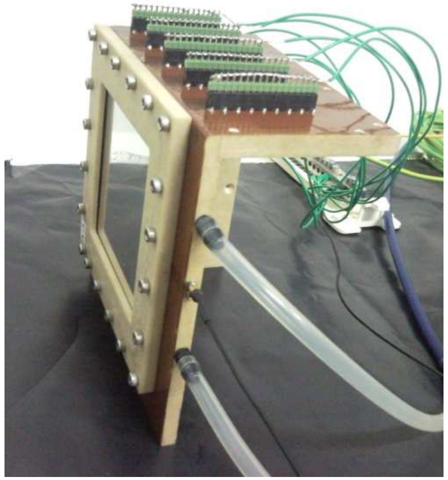


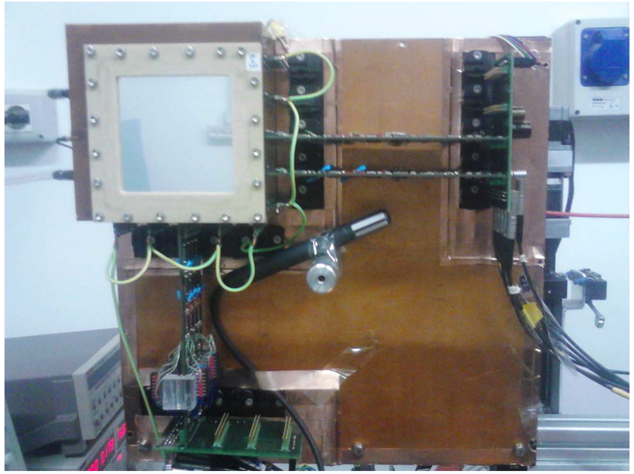


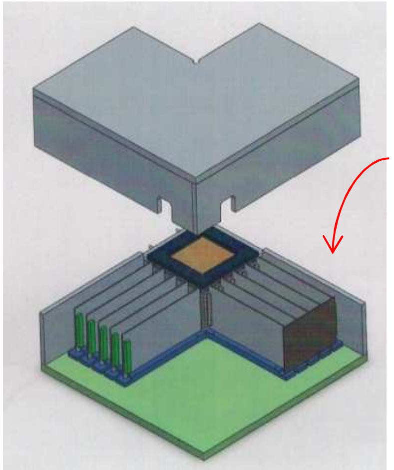


Chamber xsection

2) TOP-IMPLART beam monitoring system simulation needs







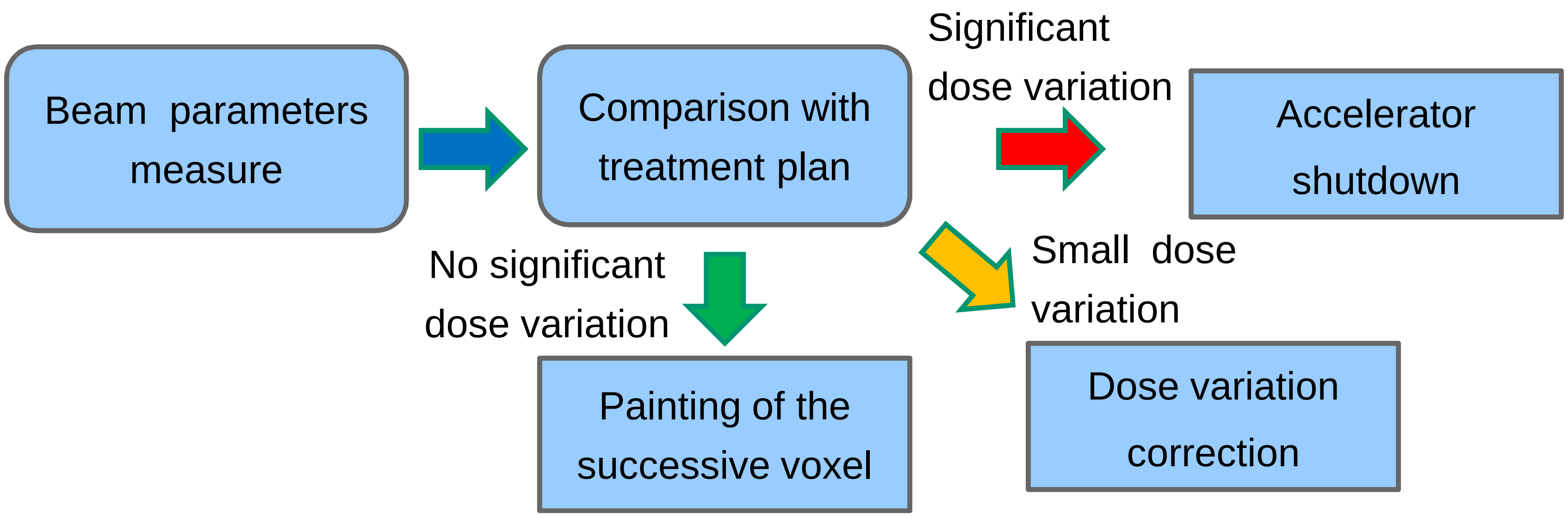
Readout Electronics

The chamber is interposed between the beam exit and the patient, so it has to perturb the beam as little as possible → simulations required for estimation of:

- Beam energy loss in the detector
- Amount of secondary particles produced
- Transversal and longitudinal beam spread variation

Linking online beam monitoring system and «Analytical» MC dose evaluation

- The monitoring system must check the consistency of the assessed dose with the planned dose in real time to provide the proper feedback:



- A feedback system + patient monitor (e.g. movement) + a fast dose evaluation (using an «analytical» MC formulation of the dose distribution):
  - evaluate, in real-time, the actual delivered dose,
  - calculate in real time, the dose correction (if any) for the next pass

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Simulation time: need of "parallelization"

- The work needs about 100 simulations with 10^8-10^9 events each to get reasonable statistics

Architecture	Number of total primary particles	Number of primary particles per run	Number of parallel run	Number of cycles per parallel run	Cpu time (h)	Real time (h)
Intel Dual Core	100.000.000	100.000.000			~12.300	~12.300
ENEA GRID	100.000.000	100.000	100	10	1.700	17

- parallel simulation REQUIRED!

- *100 simulations* on CRESCO system of ENEA-GRID run in about 70 days (for an equivalent CPU total time of about *20 years)*.

Without a cluster of processing nodes the simulation work cannot be carried on with good statistics.

CRESCO system of ENEA-GRID (in 2010)

• **ENEA-GRID** computational resources are distributed in six centers

• **CRESCO** is a Portici center project and it make available many processors. There were three sections, cresco1, cresco2 and a third section, with fronted servers and more than 300 calculation nodes having Linux OS and the following features:

– multi core architecture up to 48 core for node (standard: 16 core Xeon cresco1 and 8 core Xeon on cresco2)

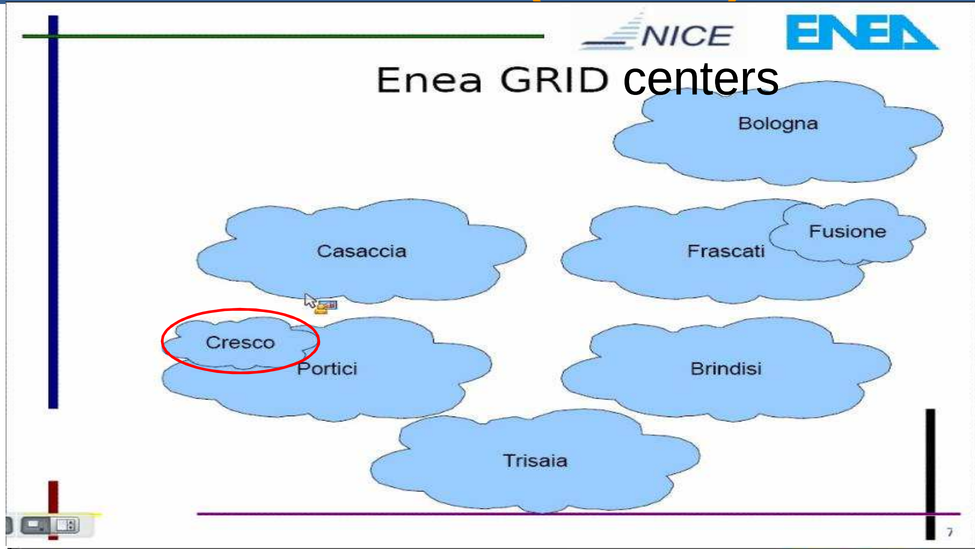
– memory standard: 16, 32 or 64 GB for socket

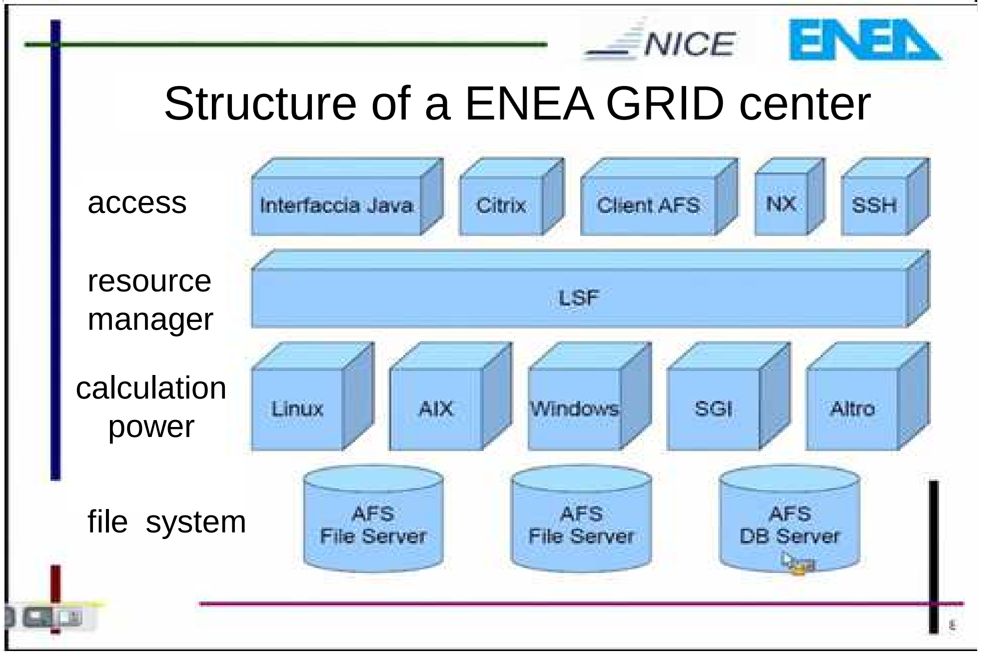
• Additional CRESCO functionality are:

– Infiniband: interconnection net between nodes, allows obtaining high data exchange velocity between processes.

– GPFS: high performance parallel file system

Today the system is more powerful, see http://www.cresco.enea.it/





CRESCO system of ENEA-GRID software

•The CRESCO system of ENEA-GRID allows access to computational resources by AFS, Citrix or SSH connection.

• A **job** is a command submitted to LSF (Load Share Facility) for execution.

•A **queue** is a clusterwide container for jobs. All jobs wait in queues until they are scheduled and dispatched to hosts. LSF dispatches the job to the best available execution host in the cluster to run that job.

Several **LSF queues** are available for running jobs on the CRESCO system.

Several LSF commands allow the user to choose the queue and submit and monitor a job. For example the command bqueues allows viewing available queues and job slot limits for queues. For running FLUKA on a single processor:

bsub <*para_bsub*> $FLUPRO/flutil/rfluka -N*x* -M*y* *input_file_name &*

FLUKA “parallelization” for running on GRID

Some considerations about FLUKA simulations:

In FLUKA there are:

- Independent particle interactions
- Independent radiation histories

Embarrassingly parallel approach:

- many short simulations treating a reduced number of histories in parallel on many processors.

The "short simulation" number depends on job slot limits for available queues

FLUKA “parallelization” step by step

a) Different and independent random number sequences are initialized by introducing a variable (__DACAM__) in WHAT(2) of RANDOMIZE card in FLUKA input file:

```
KEYWORD   WHAT(1)    WHAT(2)    WHAT(3)    WHAT(4)    WHAT(5)    WHAT(6)    SDUM
*23456789 123456789 123456789 123456789 123456789 123456789 123456789 123456789
RANDOMIZE    1.0      __DACAM__
```

b) bsub -q <serial_queue_name> -J '<*job_name*>[*1-N*]' -o out.%J.%I <*path*>/par_submit.sh <*input_file_name_without.inp*>

command calls the *par_submit.sh* **bash script** and submits a job on N processors in Cresco. The *par_submit.sh* script:

- defines the environmental variable FLUPRO
- creates a folder identified by the jobid and in this folder creates N folders identified by the jobindex
- in each of this N folder assigns random value to __DACAM__ variable and run the input file for M cycles

```
infile=$1
infilepath=<path>/${infile}.inp
sed s/__DACAM__/${RANDOM}./ ${infilepath} >${infile}.inp
```

1. *sumUSRBINmatr.sh* and *sumUSRBDX.sh* **(bash scripts)**, combine the output files from different processing nodes, calling FLUKA post-processing routines (usbsuw, usbrea, usxsuw).

Running FLUKA on ENEA-GRID

Write **FLUKA Input file**

Connect to ENEA-GRID

Connect to CRESCO system

Copy Input file in remote system

Check the queues load

Eventually modify ***par_submit.sh*** script for running many cycles on the same processor

Submit a job array choosing a queue and running ***par_submit.sh***

par_submit.sh allows creating as many folder as is the job array size specified. In each folder as many output file groups as are the submitted cycles will be generated

Create or modify **bash script** needed for combining the thousands of output files generated

Copy the sum file to local pc

Create a **Matlab** or **ROOT** file for data analysis

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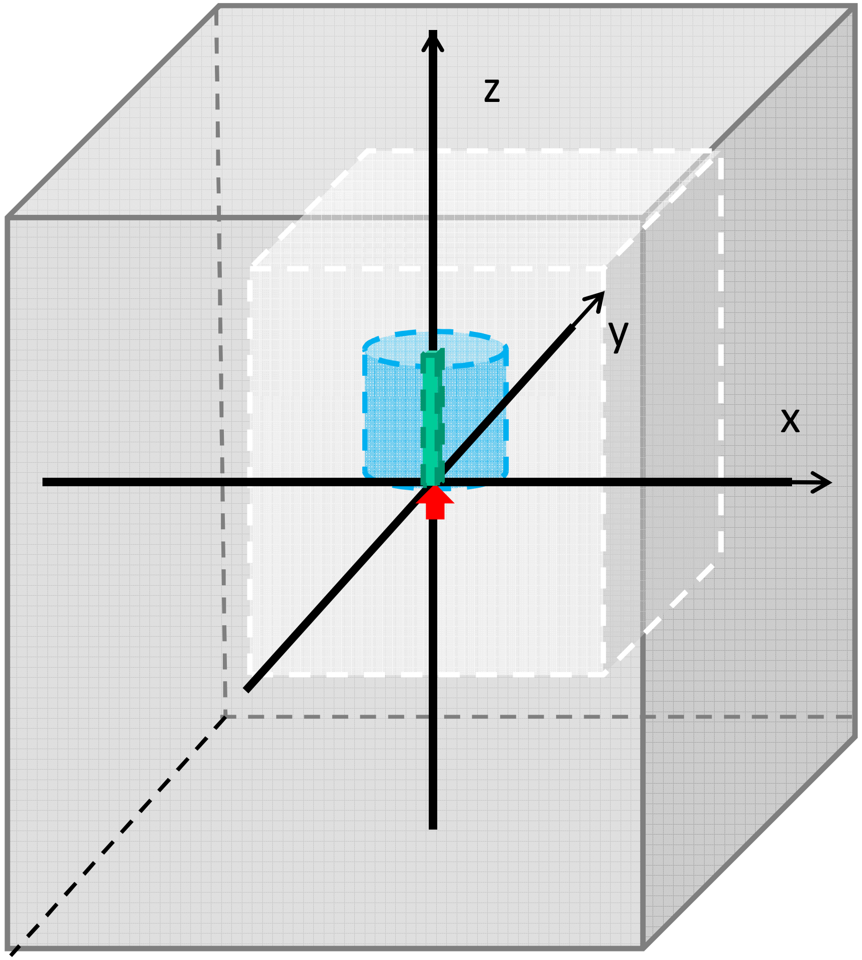
1)Simulation in homogeneous target
- Proton beam - Configuration details

- The proton beam is injected at (0,0,-0.1) and is directed along z axis with:
  - Gaussian momentum distribution: FWHM=0,72*10^{-03} GeV/c
  - Gaussian angular distribution: FWHM=0.35325 mrad
  - Gaussian profile in x and y: $FWHM_x$=$FWHM_y$=0,471 cm
- A circular cylinder of height parallel to the z axis, with base centered at (0,0,0), is inside a vacuum box, contained within the external black hole region.
- Materials assigned to cylinder are water, bone or lung depending on simulation.
- By the USRBIN card the energy density is requested in a Cartesian mesh.
- By the USRBDX card double differential proton beam "current" distribution in energy and solid angle is requested at several penetration depth



1)Steps for reproducing Bragg peak

- Plot of integrated deposited energy versus mass depth;
- evaluation of the mean residual proton energy from USRBDX detector;
- interpolation of the Mass Integrated Deposited Energy (MIDE) in lung and in bone versus the mean residual proton energy at the same depth;
- fit of the interpolated MIDE in lung and in bone versus the MIDE in water;
- interpolation of the depth in lung and in bone versus the mean residual proton energy;
- fit of the interpolated depth in lung and in bone versus the depth in water;
- check of the results and the generalization to any energy

Dose distribution in water from simulation

↓

Generalized analytical formula

↓

Dose distribution in other materials

1)Generalized formula

MIDE=Mass Integrated Deposited Energy

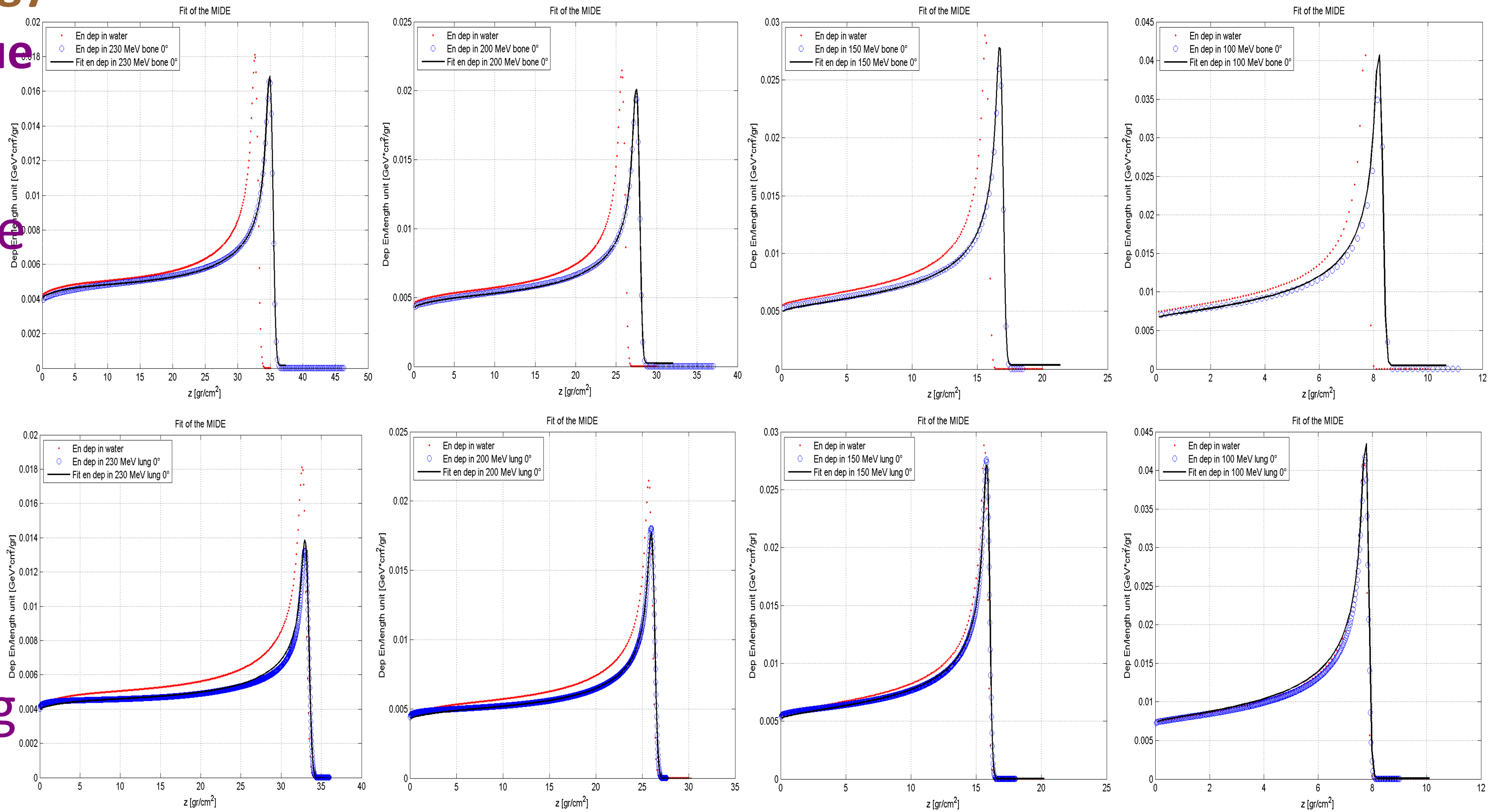
- ○ Fluka simulation in tissue
- • Fluka simulation in water
- — Analytical MC evaluation

Energy 230 MeV 200 MeV 150 MeV 100 MeV

Tissue

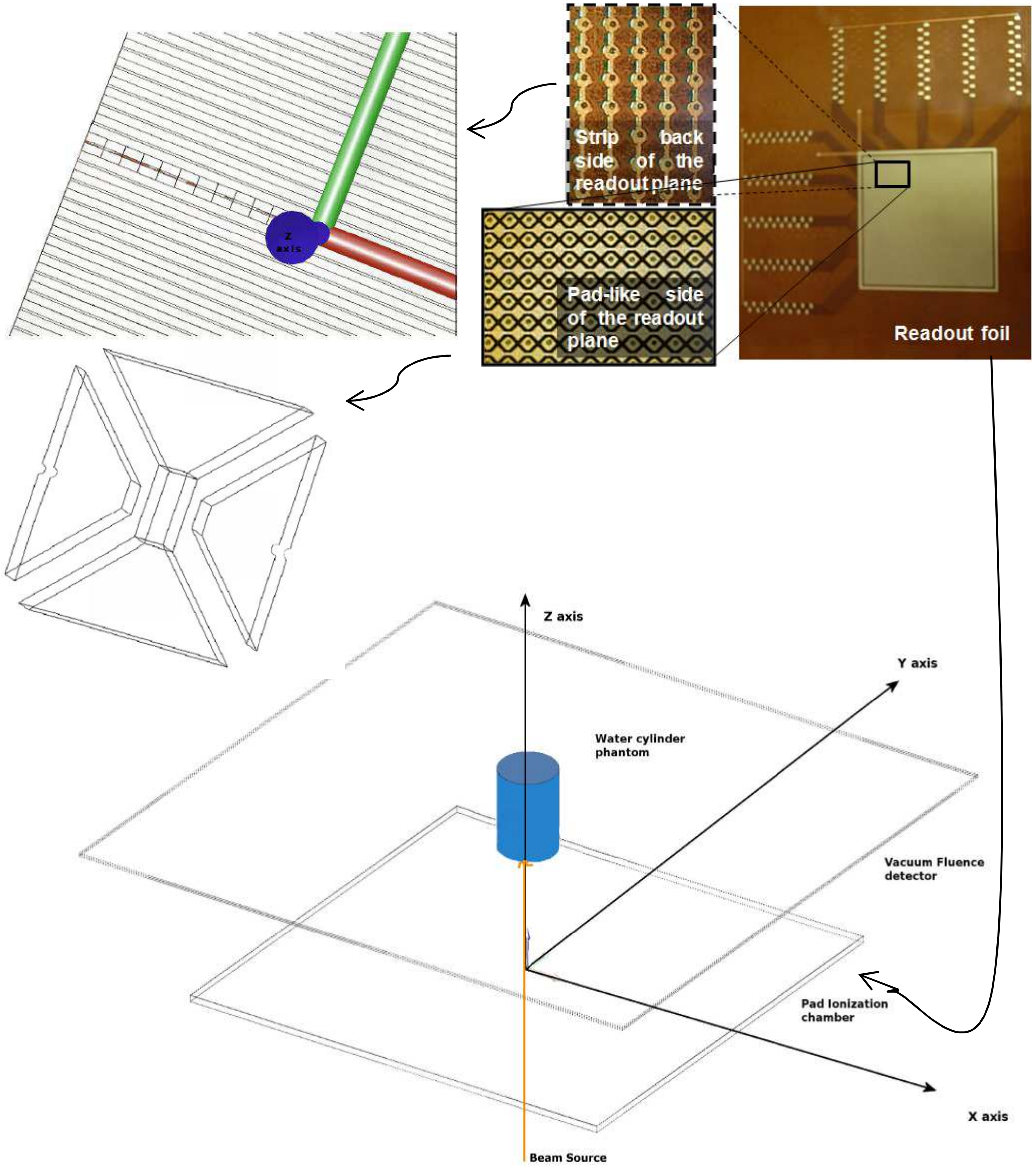
Bone

Lung

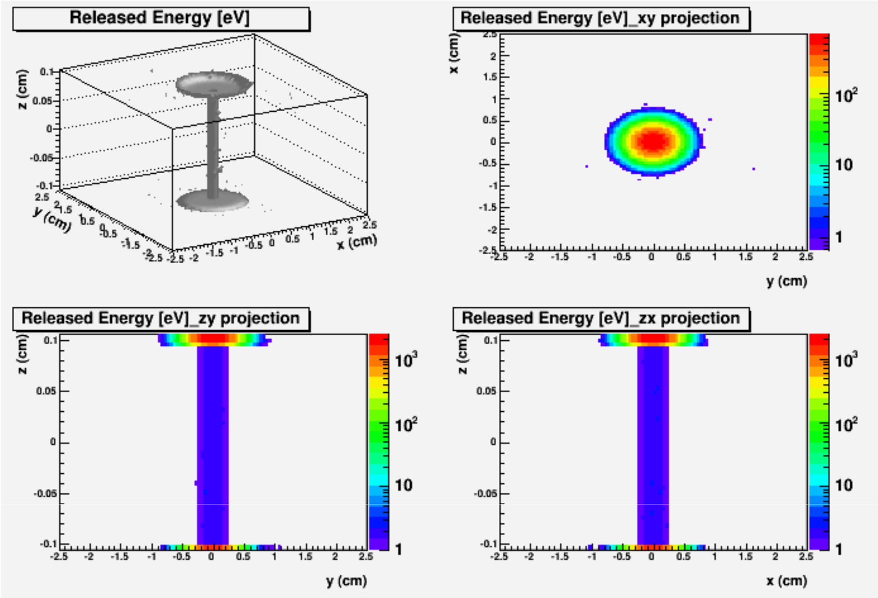


2)Geometry for beam monitoring system study

- The **proton beam** is directed along z. It has a Gaussian profile with FWHM of 0.2, 0.5 or 1.0 cm depending on simulation.
- The centre of the beam spot is (0,0,-5)
- The **chamber** is interposed between the beam injection point and a **water phantom,** represented as a circular cylinder coaxial with the beam line.
- The **readout foil** of the ionization chamber is simulated using the LATTICE card to replicate the **"pad basic region“** (a set of four geometry regions created by the intersection of planes and solid figures) and the **strips** connecting the pads on the back of kapton foil.
- The cylinder and the chamber are inside a vacuum box, contained within the external black hole region.

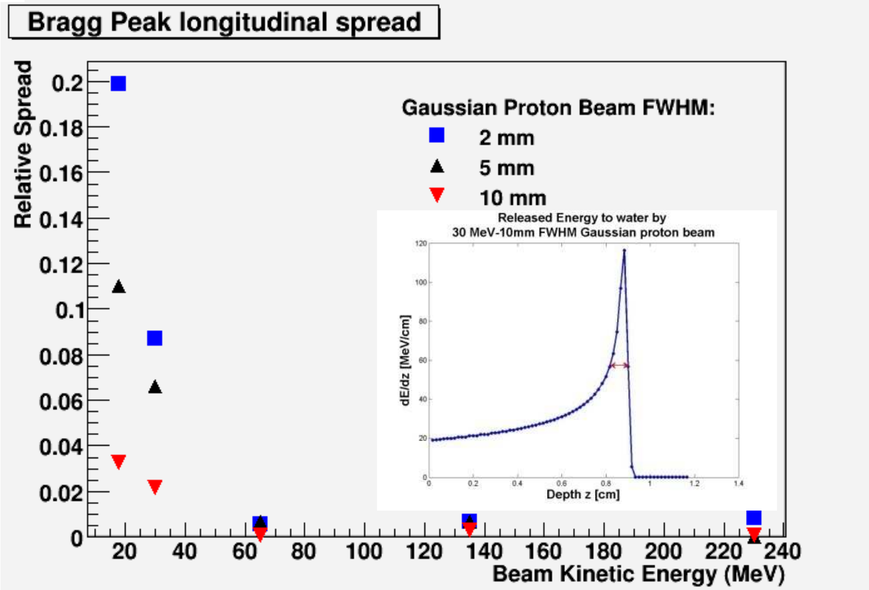


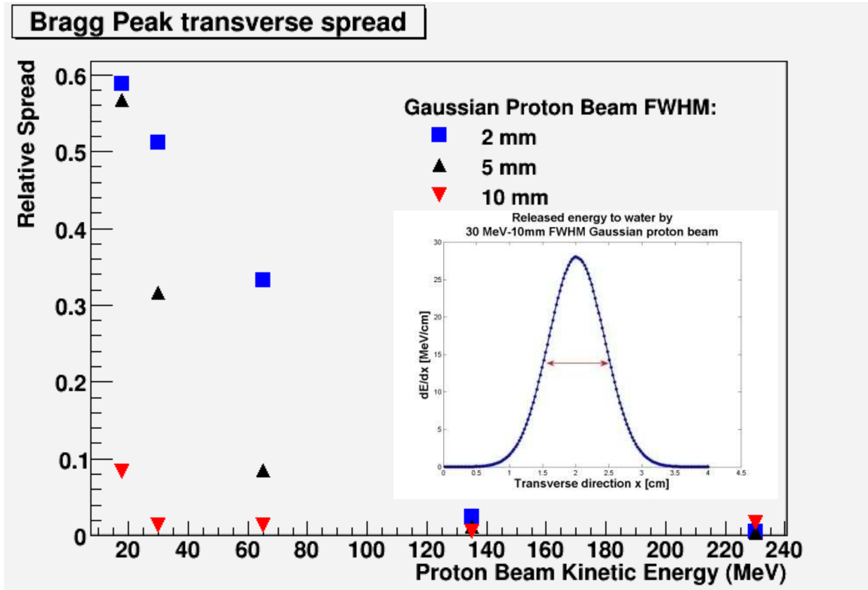
2)The perturbation effect induced by the chamber on the dose delivery



Fluka Simulation on water phantom.

- Longitudinal relative variation of the Bragg peak spread less than 1% above 65 MeV
- Transverse relative variation of the Bragg peak spread less than 3% above 135 MeV



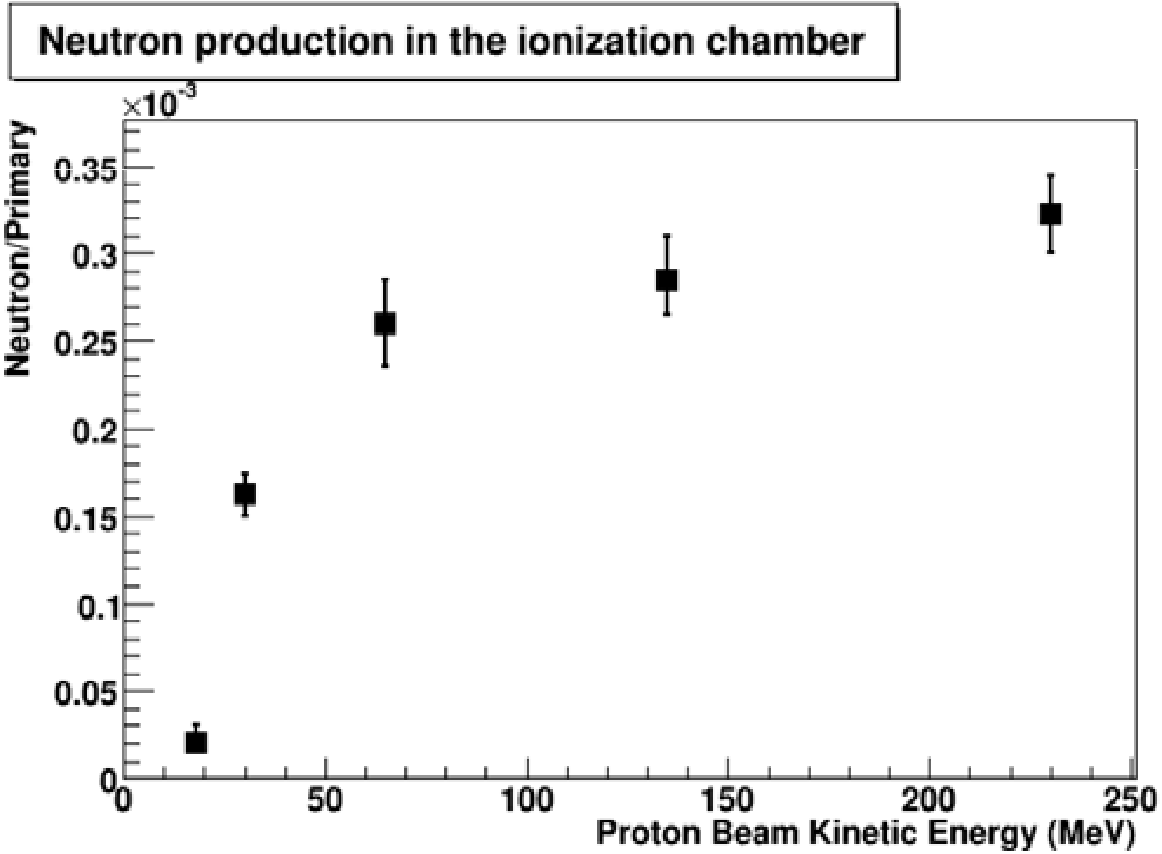


2)Neutron produced in the chamber

• Neutrons seem to be the main secondaries that can release unwanted dose to the patient.

• Evaluation of the neutron number produced in the chamber is important

• This number should be compared with the neutron number produced in the patient body



Noticeable production

To be validated!

Conclusions

- Without (parallelization + CRESCO/ENEA-GRID) this work could not be done
- Jobs have been parallelized by "simple" shell scripts on CRESCO/ENEA-GRID
- Simulations of the deposited energy in homogeneous and heterogeneous phantoms have been carried out to develop an «Analytical» MC dose evaluation.
- Simulations of the ionization chamber and of a water phantom have been carried out to estimate the impact of the monitoring system on dose delivery.

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