



ICT e supercalcolo al servizio di Ricerca e Imprese | Risultati e prospettive

Applicazioni dei Codici di Calcolo Nucleari ed agli Elementi Finiti nelle Attività di Ricerca dell'Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti

Lina Quintieri, ENEA

ENEA, Rome, 17 March 2015

Outlook

- ❖ Introduction to INMRI: Metrological National Institute of Ionising Radiation
- ❖ Monte Carlo Applications: particle detector design, dosimetric calculations,
- ❖ Finite Element method Applications: multiphysics analysis (structural/thermal/electromagnetic coupling)

ENEA INMRI Institute

It is charged with the responsibility of developing and maintaining the Italian standards in the field of ionizing radiation measurement.

Metrological activities:

- ❖ Therapy level and industrial radiation processing dosimetry
- ❖ Protection level dosimetry standards
- ❖ Radionuclide standards
- ❖ Neutron standards

ENEA-INMRI Bldg. T-11: Laboratory of Metrology for Therapy-Level Dosimetry



ENEA-INMRI Bldg. T-5

Laboratories of Metrology for Protection-Level Dosimetry and Radionuclide Measurement



ENEA-INMRI Bldg. T-2Bis: Laboratory of Radon Metrology



ENEA-INMRI Bldg. T-17: Laboratory of Neutron Metrology



INMRI Simulation Activities

- ❖ Extensive use of several among the main Monte Carlo codes for dosimetric and metrology characterisation of radiation beams, mainly from accelerator driven particle sources
- ❖ MC for radiation detector development and response characterisation (both electron/gamma and neutron fields)
- ❖ Finite element codes as support for thermal detector response and accelerator component design (particle dump)

MC Methods: General Remarks

- ❖ Deterministic methods provide more exact solutions of approximate models, whereas **Monte Carlo methods provide approximate solutions of more exact models (stochastic events)**
- ❖ MC method is **eminently suited to study stochastic processes**, particularly radiation transport, such as motion of photons and neutrons and charged particles through matter.
- ❖ Monte Carlo simulations play an important role in the optimisation particle detector design..The method uses **probabilities distribution functions** and **random sampling** instead to give an accurate picture of what can happen. Statistically the random samplings will most often demonstrate the most likely possibilities
- ❖ **The accuracy and reliability of a Monte Carlo predictions depends on the models or evaluated data libraries** on which the probability distribution functions are based
- ❖ **Statistical precision of results** depends on the number of "histories"(in analogue mode: **$1/\sqrt{N}$**)
- ❖ Track of a large number of histories require a big computational resources and large CPU time
- ❖ Often variance reduction techniques are required to improve the result accuracy and accelerate the statistical convergence(increasing statistics using weight for secondaries, in order to not affect the physics)

MC code used in INMRI:

Fluka, Geant4, MCNP(X), EGS

They are general-purpose Monte Carlo code that can reproduce geometric 3D configurations of materials and simulate particle transport through them

General	GEANT4	FLUKA	MCNP(X)	EGS
UPDATE VERSION	Geant4.10	Fluka 2011.2c	MCNP6	EGSnrc
LANGUAGE	C++	Fortran 77	Fortran 90/C	C++
RELEASE FORMAT	Source & binary	Binary	Source & binary	Source & binary
INPUT FORMAT	N/A	~85 cards	~120 cards	N/A
PARALLEL EXECUTION	YES	YES	YES	YES

Finite Elements Codes used in IMRI:

General Remarks

General	ANSYS	COMSOL Multiphysics
UPDATE VERSION	Ansys14.5	version 5.0
LANGUAGE	N/A	N/A
RELEASE FORMAT	Binary	Binary
INPUT FORMAT	Well structured predefined command	User interface or by script
PARALLEL EXECUTION	YES	YES

Overview of Some Representative Application Cases of MC Codes:

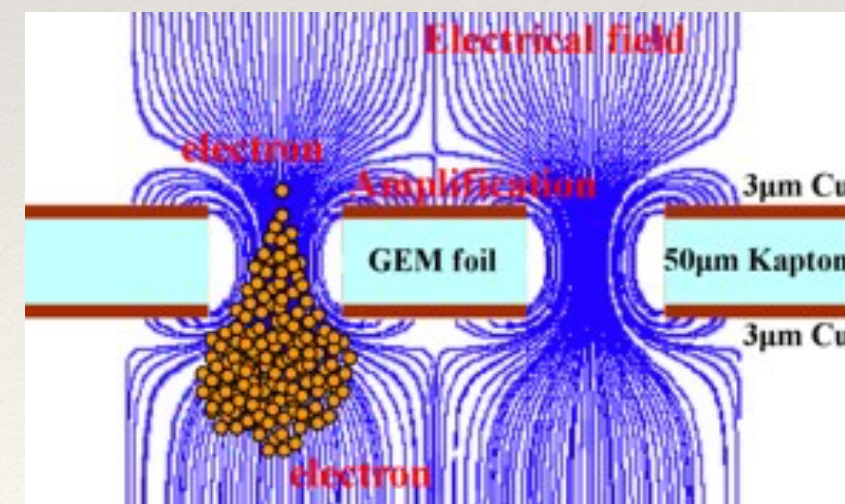
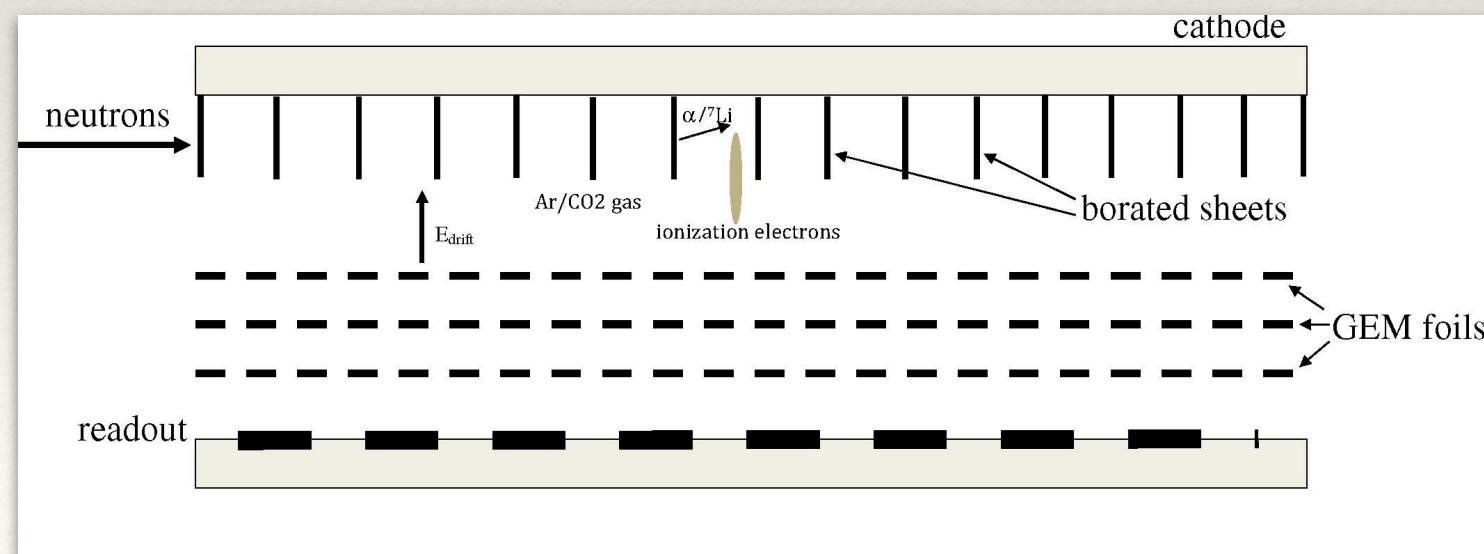
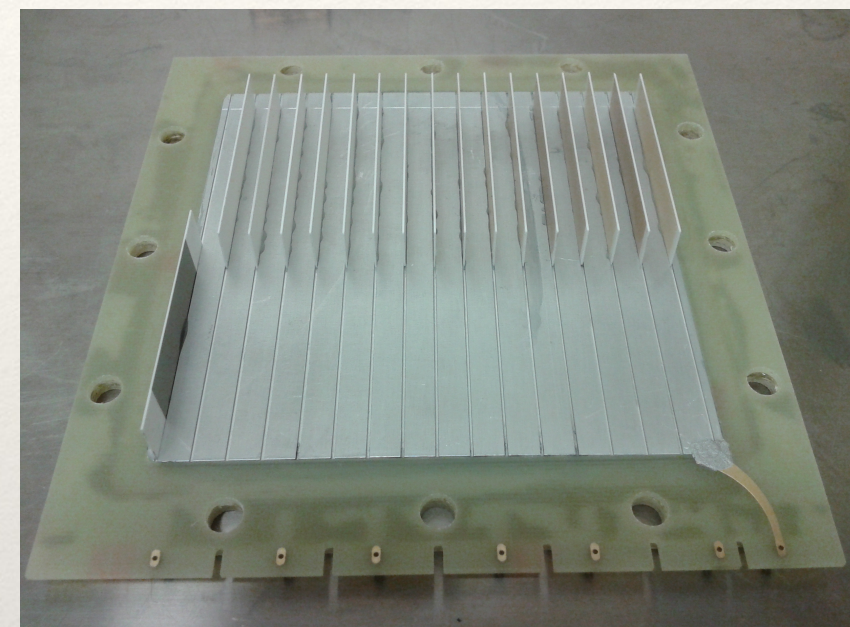
Neutron R&D Activities:

Design and Optimisation of Innovative Neutron Detectors

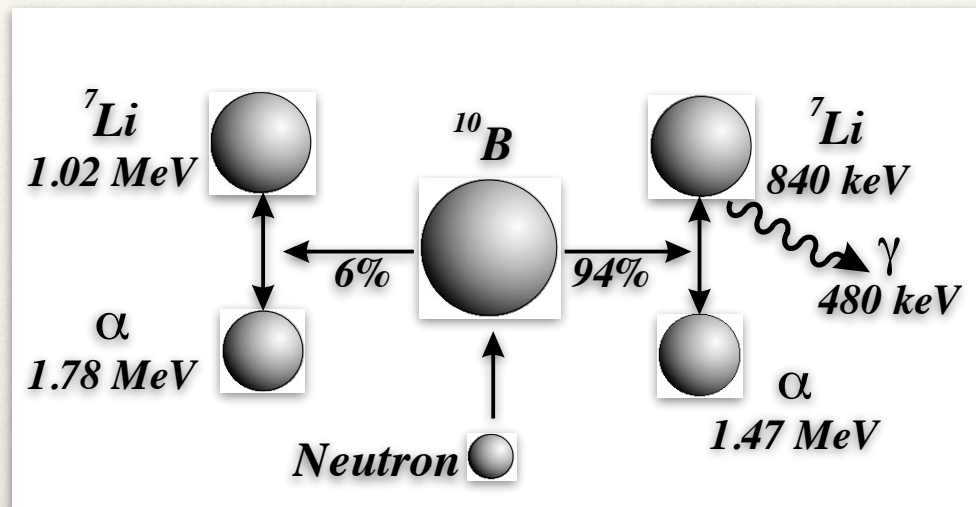
In collaboration with INFN (Laboratori Nazionali di Frascati) and CERN within European project (BEAM4Fusion, INFN -E)

- ❖ He-3 is obtained from Tritium production for use in nuclear weapons by Tritium β -decay into He with a half life of 12.3 years.
- ❖ Only the US and Russia are providing significant amounts of He-3. With the end of the Cold War He production from Tritium decay has been reduced significantly and since September 2001 the demand of He has increased drastically due to security program launched in US and other countries.
- ❖ **Severe depletion** of the existing ³He stockpile and shortage

In this frame it is easy to understand the strong importance of MC simulations as a valuable and "costless" tool to address the research toward new neutron valuable detector in alternative to the He-3.

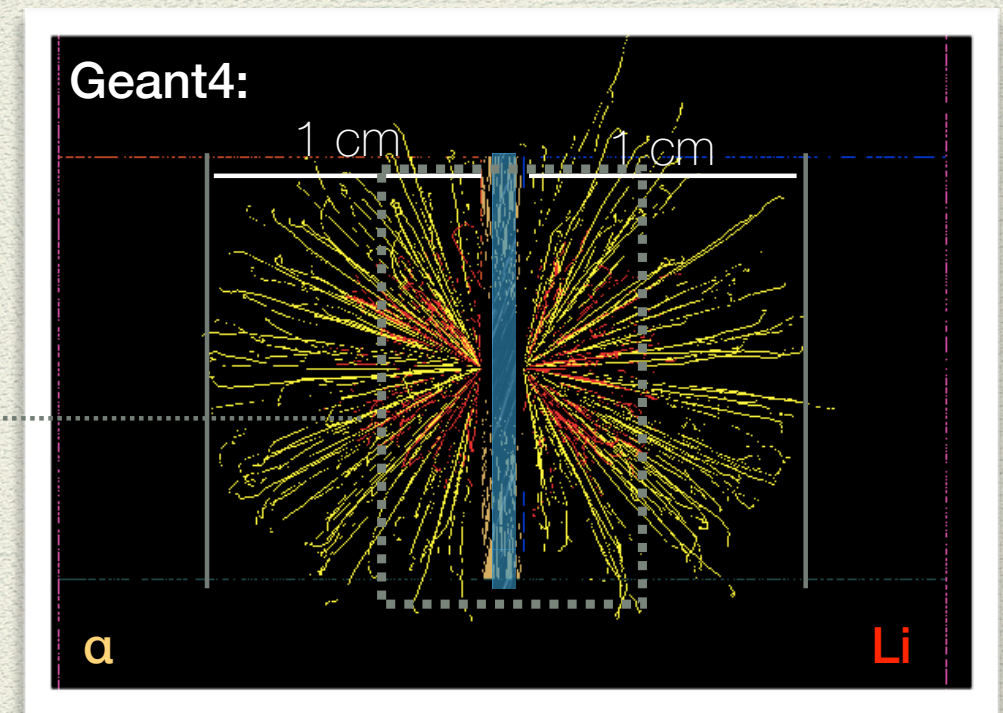
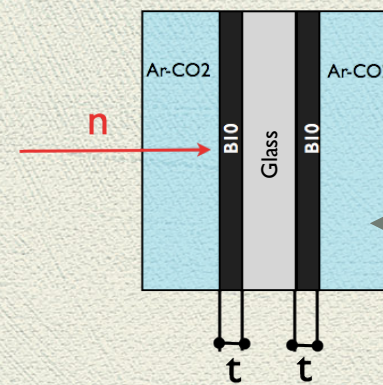


B-10 Cathode: MC Optimisation of "Gem SideOn" Detector Design



The reaction products are released in opposite direction when thermal neutrons are absorbed by B-10.

After the absorption 94% of the reactions leave ^7Li in its first excited state, which rapidly de-excites to the ground (10^{-13}s) by releasing a 480 keV gamma).



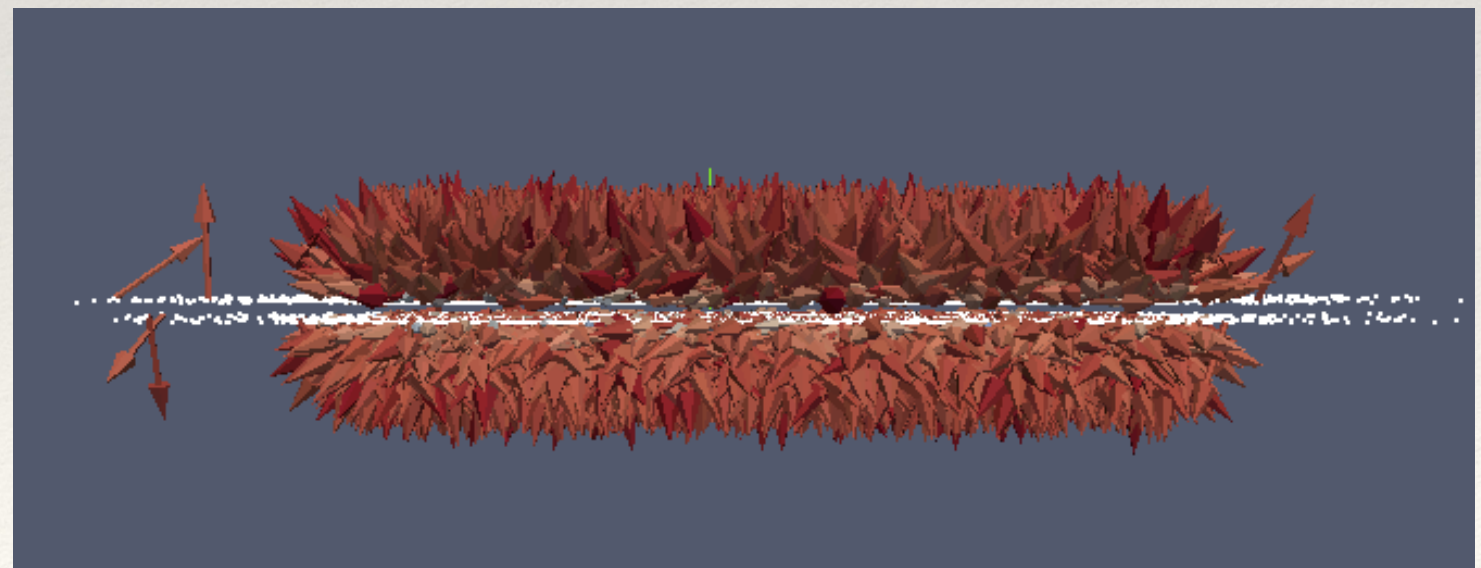
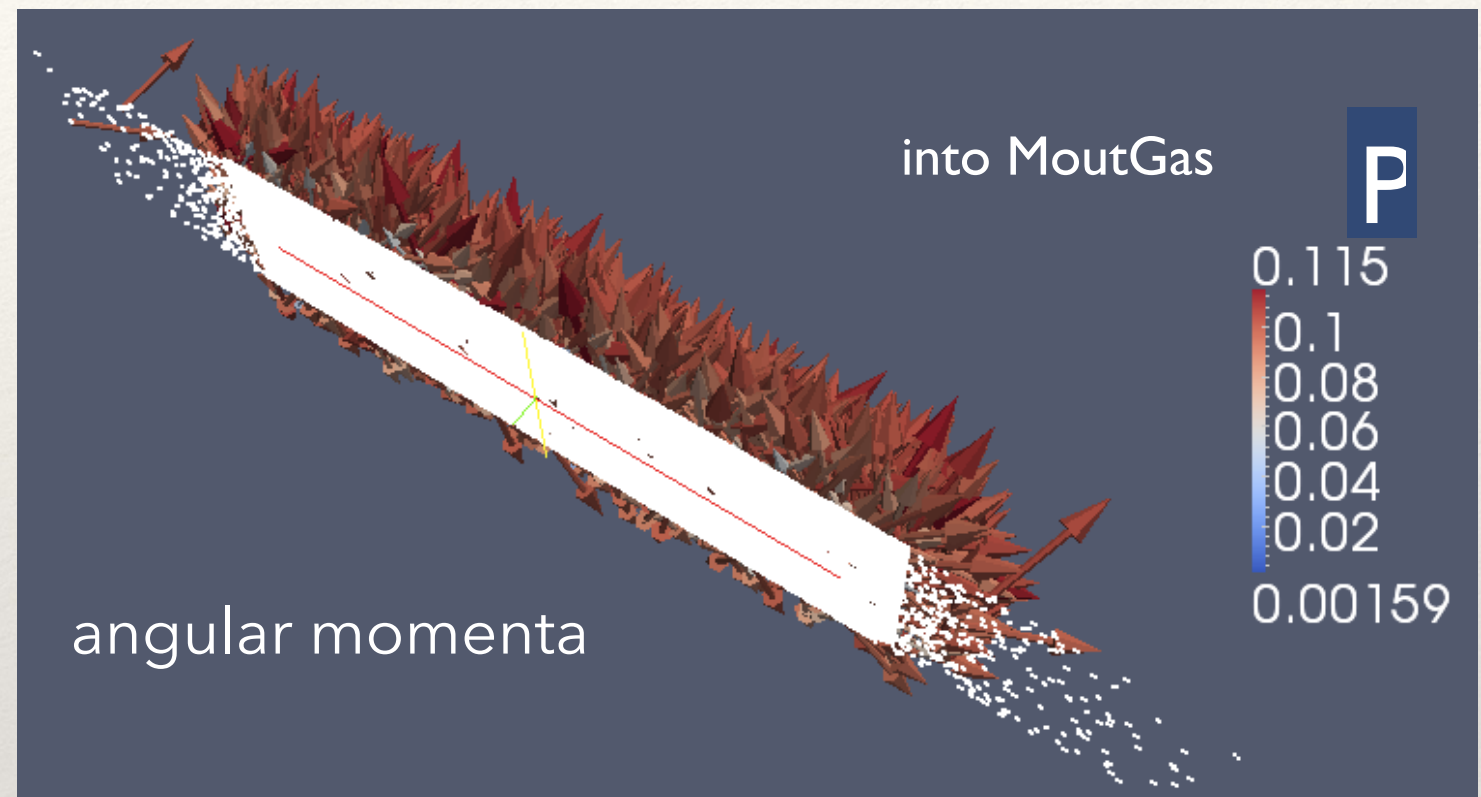
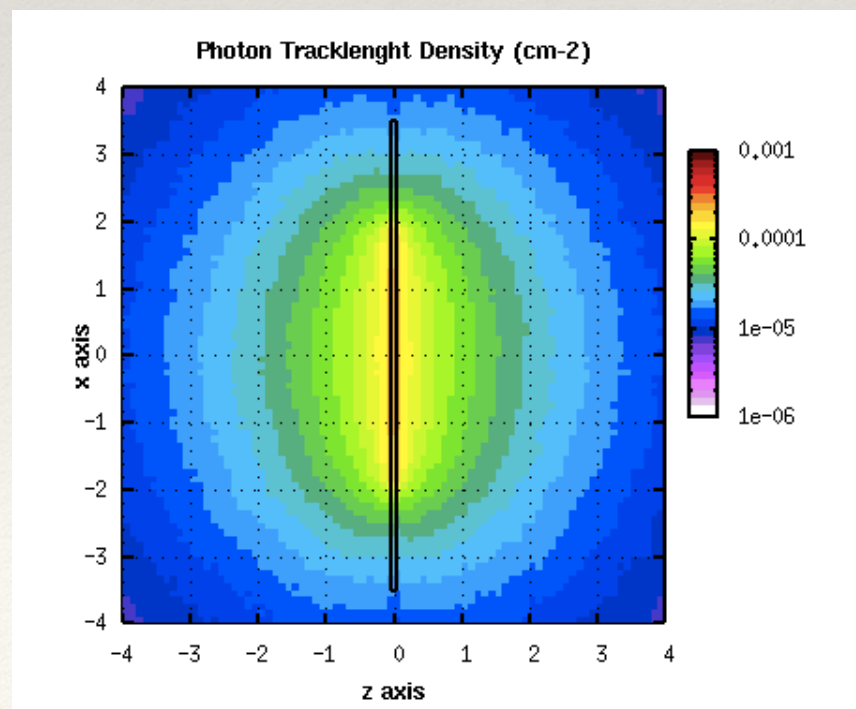
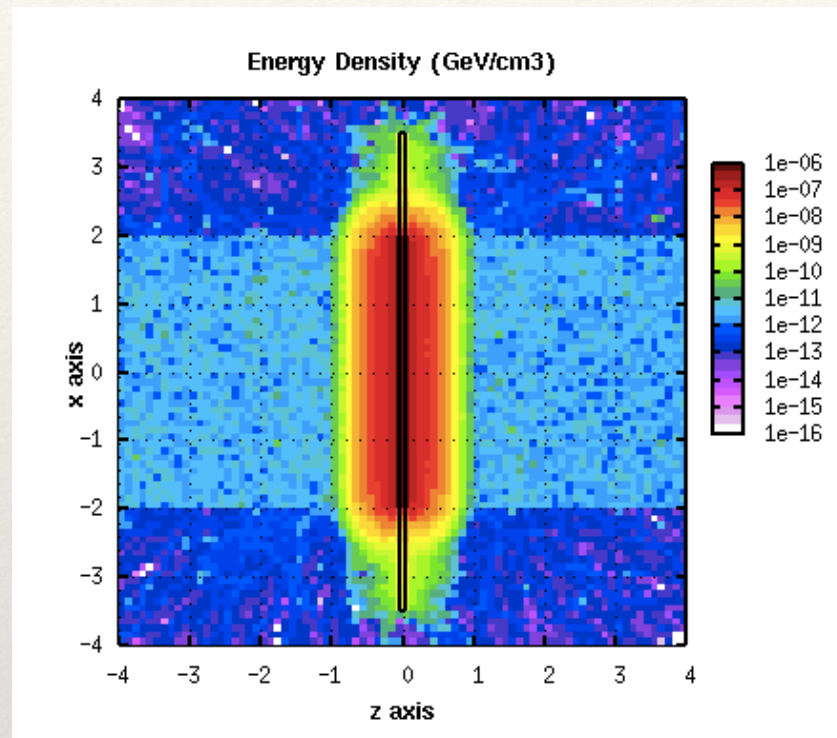
Results of simulations, shown in figure, refer to Al_2O_3 plate coated (on both sides) with B-10 uniform layers in ArCO_2 hit by thermal neutron.

A primary (25 meV) neutron beam impinges perpendicular to the wider sheet surface, (zero divergence)

The simulations intended to help in seeking the optimal geometrical set-up and material thickness (converter layer, gas gap, sheet substrate) to improve the final detector design in terms of achieving the best detector efficiency possible.

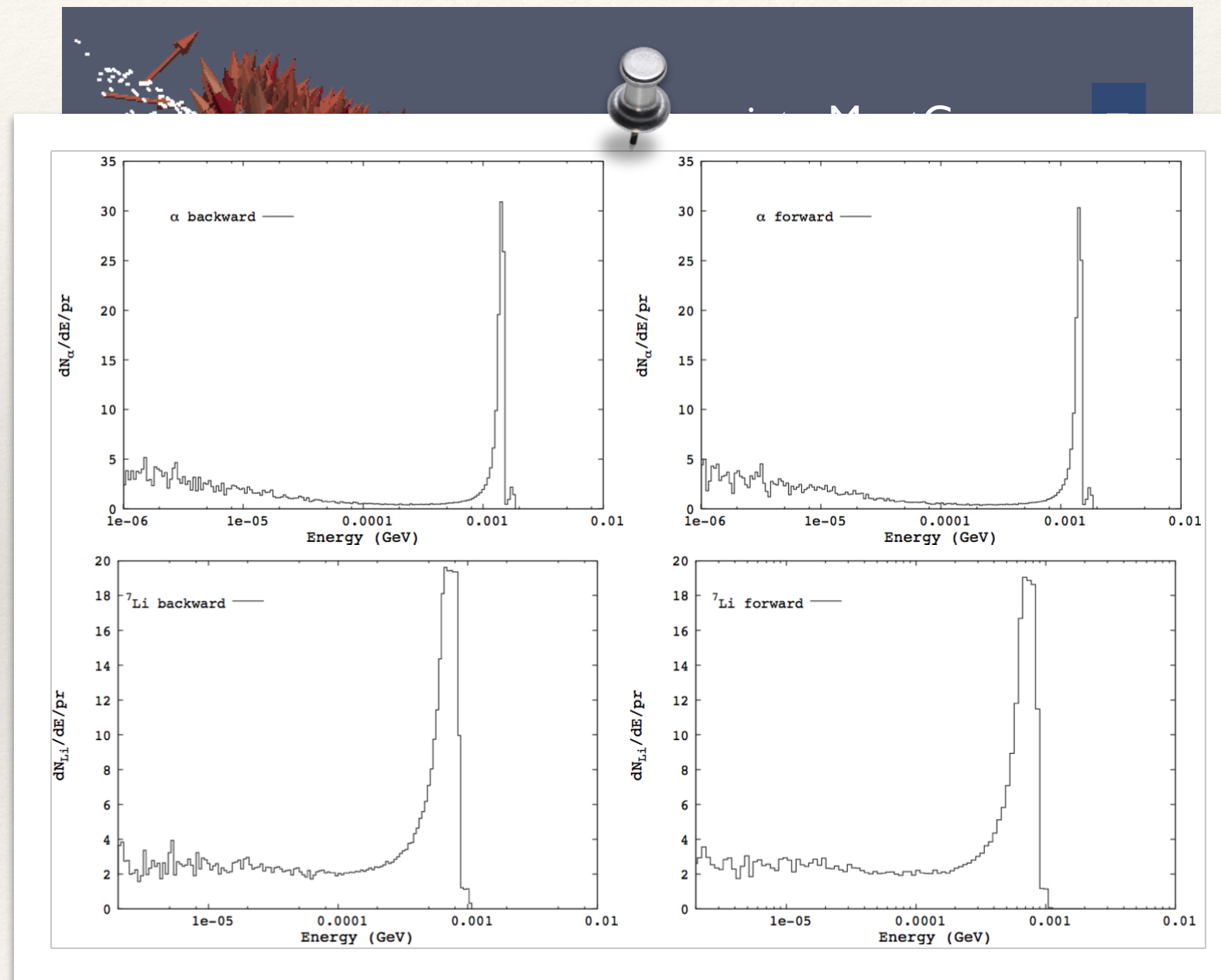
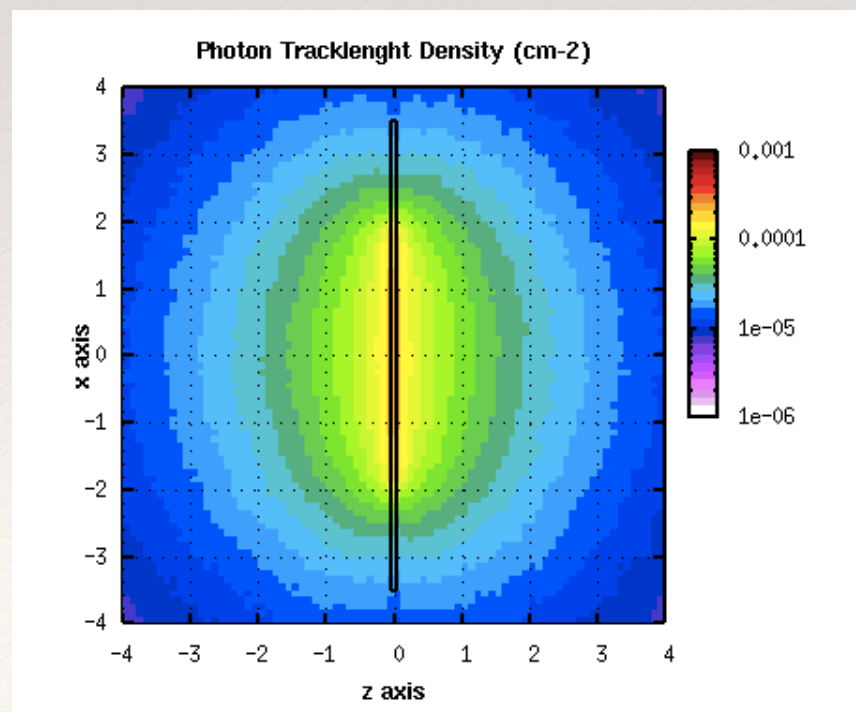
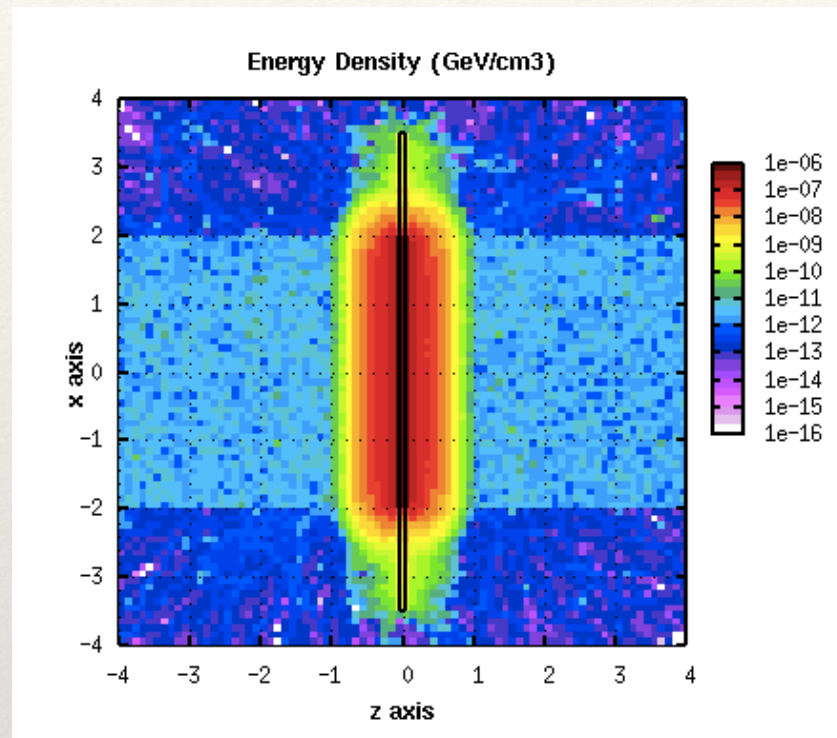
$\propto$ 3D scatter plots: Particle Entering into the Gas

These plots refer to the case of a double coated plate with 300nm Boron film. The angular contribution to efficiency attenuation become an issue for value of the convert thickness above 1000nm, as shown in the following slides



α 3D scatter plots: Particle Entering into the Gas

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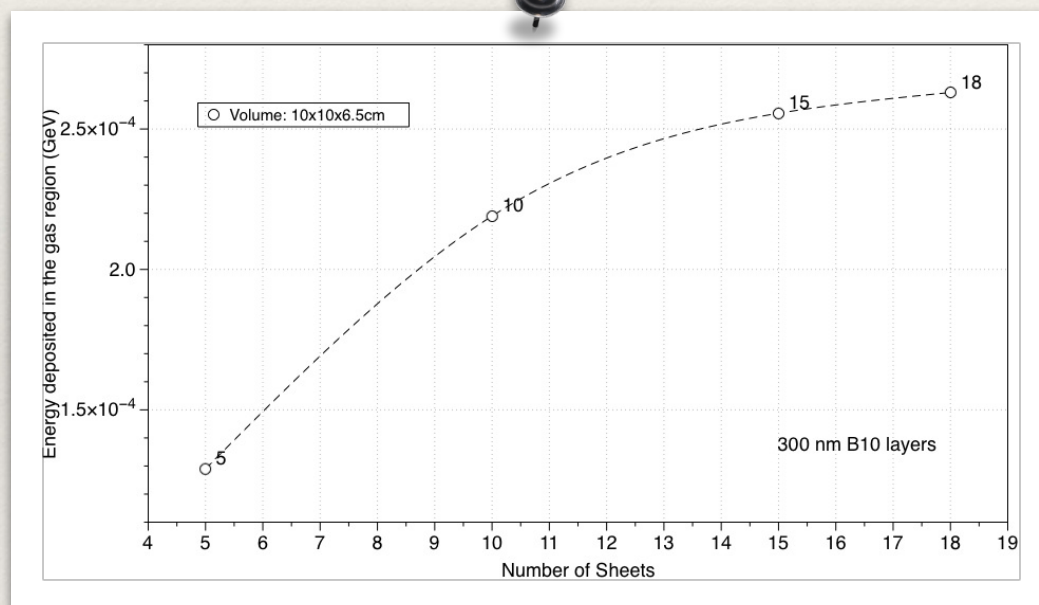


Multiple Sheet Detector Geometric Configuration Optimization

Optimal configuration with respect to maximize the number of charged particles that can ionise the gas region

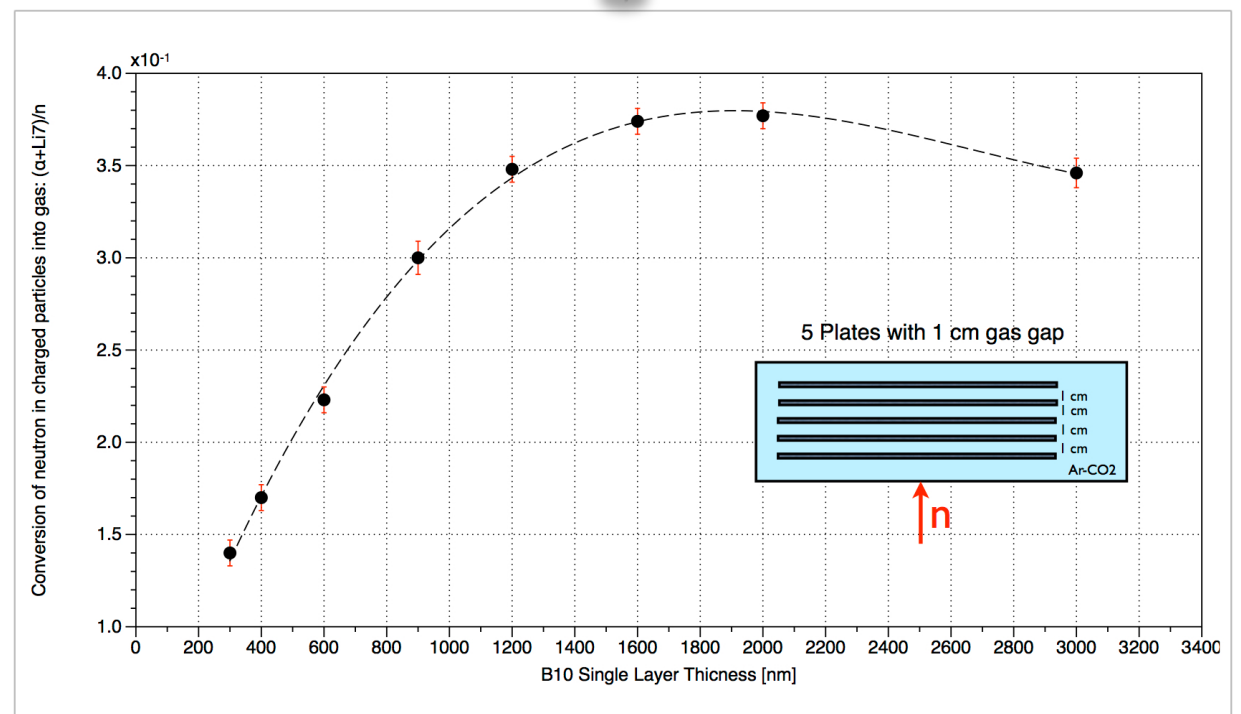
A. Optimal distance among stacked plates (coating thickness and the volume fixed)

Energy deposited by the charged particles in the gas as a function of the **number of sheets** in a fixed volume with two-side 300nm B-10 thickness. Four cases have been simulated: 5, 10, 15, 18 (gas gap, respectively, 1cm, 0.5cm, 0.3125cm and 0.25cm)



A detailed estimation of the energy deposited in each gas region in between two adjacent sheets indicates that more than 95% of the total kinetic energy of all alphas and ⁷Li ions is deposited within 0.5 cm from the sheet 10B external surface. **An optimum gap of 6 mm has been assessed**

B. Optimal thickness of the coating (fixing the number of sheets and the relative distance)

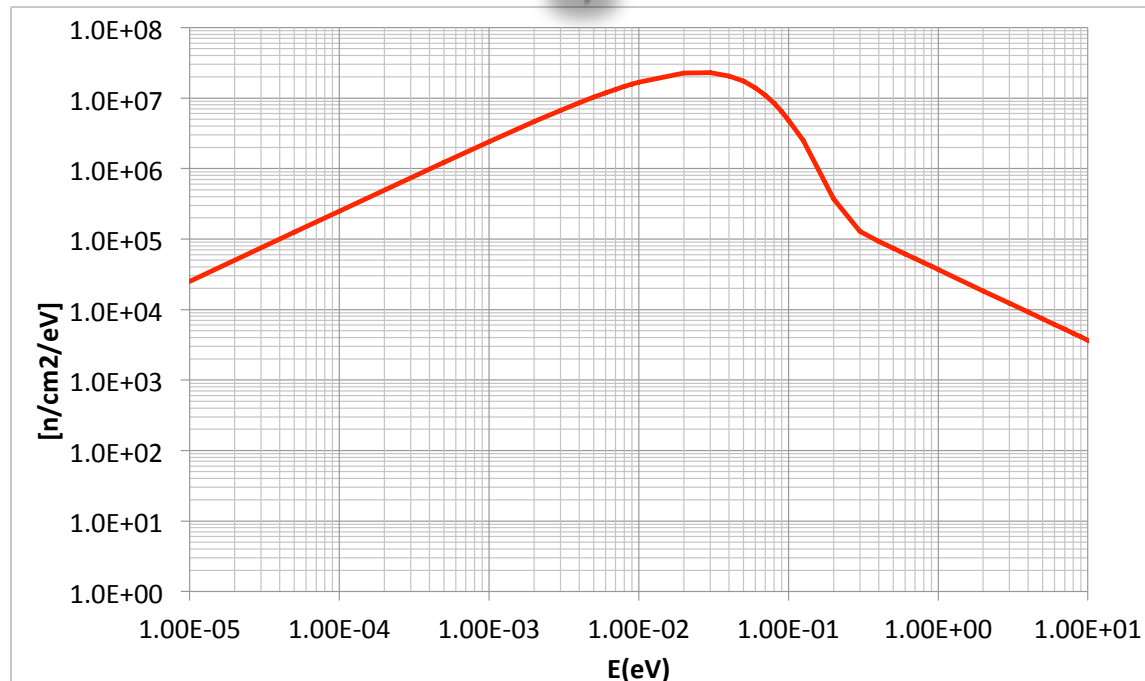
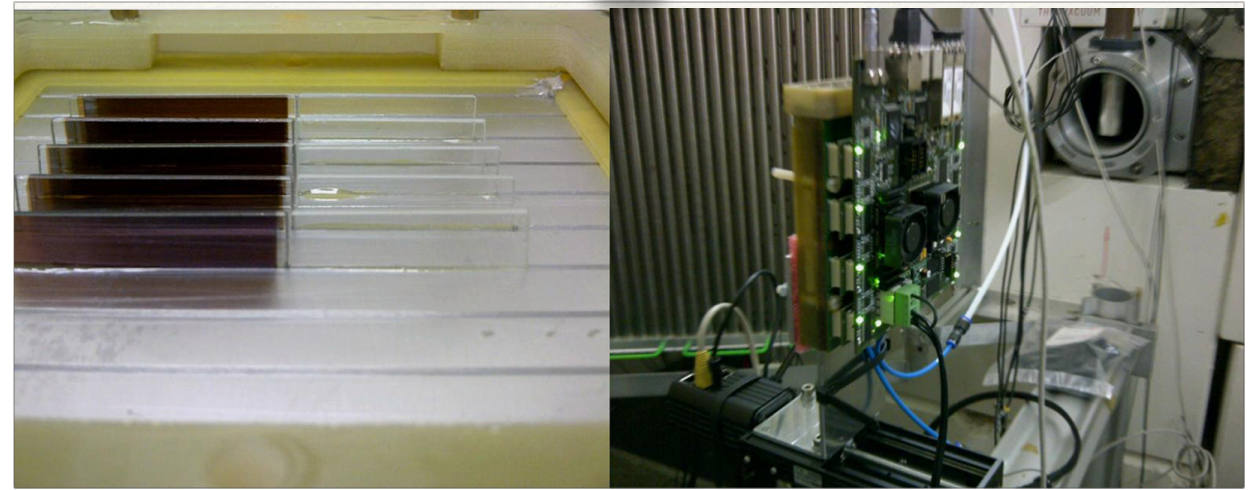


This analysis shows that an **optimum B-10 thickness** exists for a given volume and number of sheets: **in case of 5 sheets it is around 1800 nm.**

The optimisation process has required parametric calculations (i.e changing the layer converter thickness) and since each case is high cpu demanding, this kind of analysis has been possible in a reasonable time tanks to the high level computational resources of CRESCO4

MC Predictions and Experimental Results: Comparison for 5 Sheets 300 nm B-10 Detector at ENEA TRIGA

- ❖ TRIGA reactor at the ENEA-Centro Ricerche Casaccia (Rome):
- ❖ The reactor can be operated at different powers from a few Watt to 1 MW with a neutron flux of about 2×10^6 n/cm²/s at the maximum power, whose spectrum is shown in the picture



Conv. Efficiency

ϵ [%]

MC

7.4 ± 0.6

Exp

4.6 ± 0.5

- Difference between MC prediction and the measurement likely due to:
- ❖ the overall **charge production/amplification/threshold in the detector stages**, that is not included in the MC model;
 - ❖ a **possible contamination of B₂O₃** and the reduced density of the films with respect to the bulk value in the conversion film (importance of the spectrometric analysis of the layer)
 - ❖ The **experimental contribution of the external face of the first sheet** is lost, whilst it has been taken into account in the simulation

MC Predictions and Experimental Results: Comparison for 5 Stages of the TRIGA Reactor

- ❖ TRIGA reactor at Casaccia (Rome):
- ❖ The reactor can produce powers from a neutron flux of maximum power to the picture



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A new ^3He -free thermal neutrons detector concept based on the GEM technology

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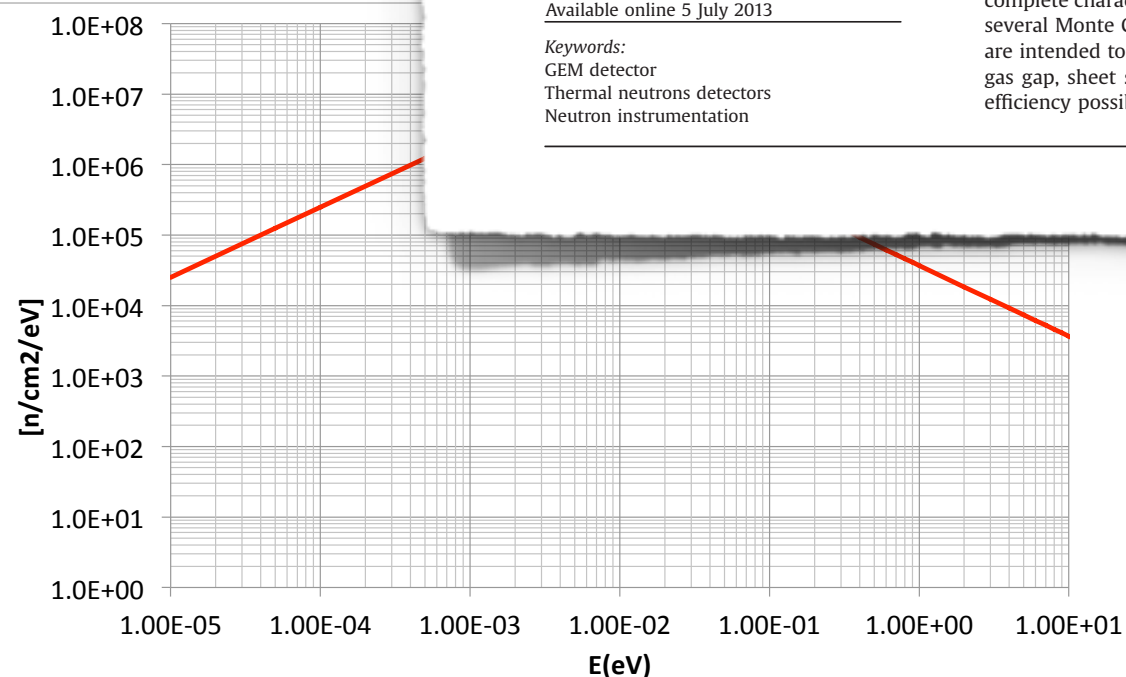
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GEM detector
Thermal neutrons detectors
Neutron instrumentation

ABSTRACT

A thermal neutron detector based on the Gas Electron Multiplier technology is presented. It is configured to let a neutron beam interact with a series of borated glass layers placed in sequence along the neutron path inside the device. The detector has been tested on beam both at the ISIS (UK) spallation neutron source and at the TRIGA reactor of ENEA, at the Casaccia Research Center, near Rome in Italy. For a complete characterization and description of the physical mechanism underlying the detector operation, several Monte Carlo simulations were performed using both Fluka and Geant4 code. These simulations are intended to help in seeking the optimal geometrical set-up and material thickness (converter layer, gas gap, sheet substrate) to improve the final detector design in terms of achieving the best detector efficiency possible.

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MC	Exp
0.6	4.6 ± 0.5

Measurement likely due to:

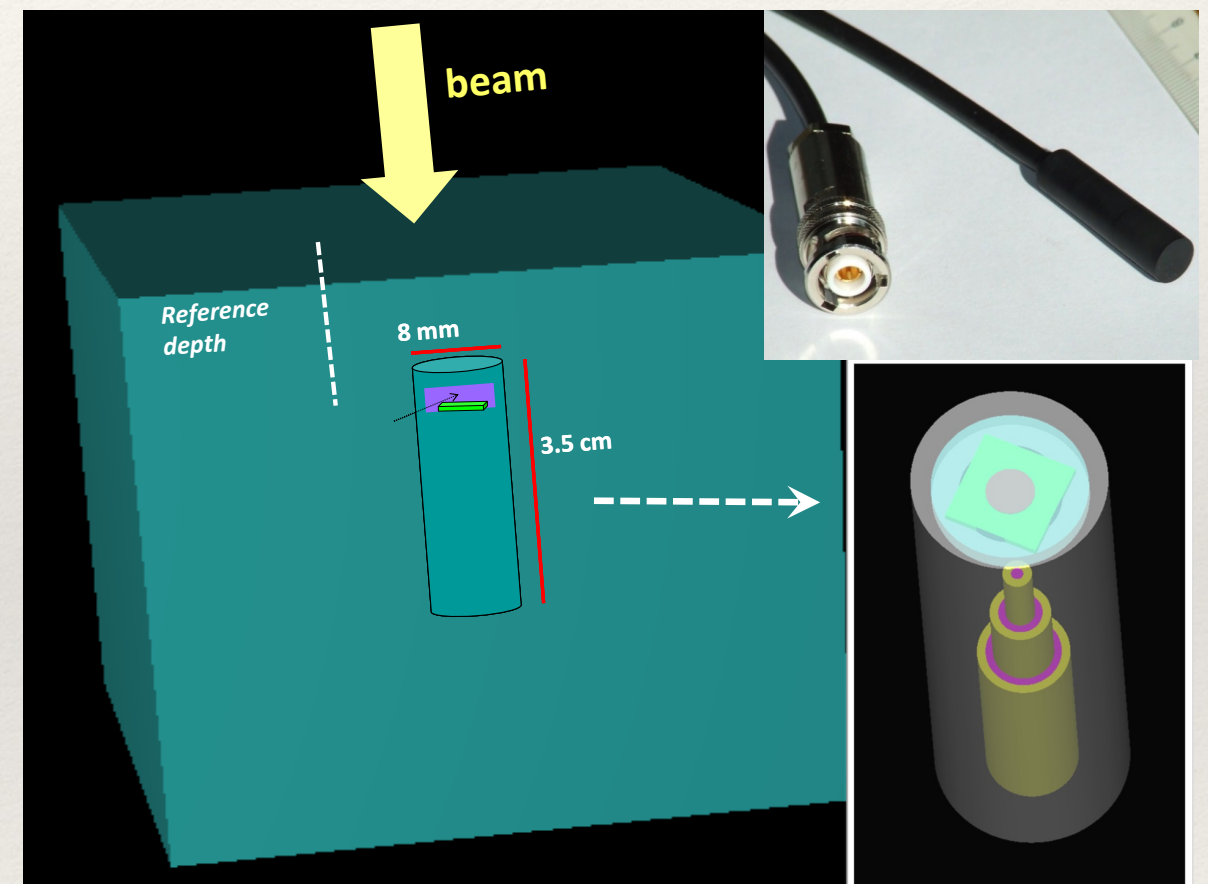
- ❖ the overall **charge production/amplification/threshold** in the **detector stages**, that is not included in the MC model;
- ❖ a **possible contamination of B_2O_3** and the reduced density of the films with respect to the bulk value in the conversion film (importance of the spectrometric analysis of the layer)
- ❖ The **experimental contribution of the external face of the first sheet** is lost, whilst it has been taken into account in the simulation

Development and Characterisation of Diamond Detectors for Dosimetry for Hadrotherapy

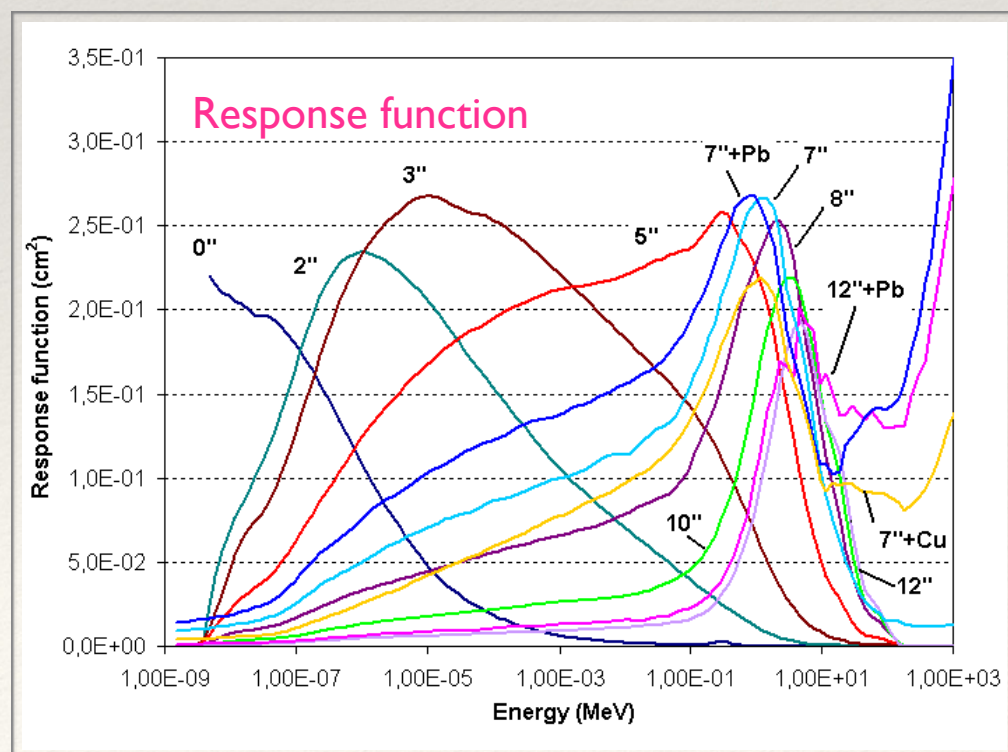
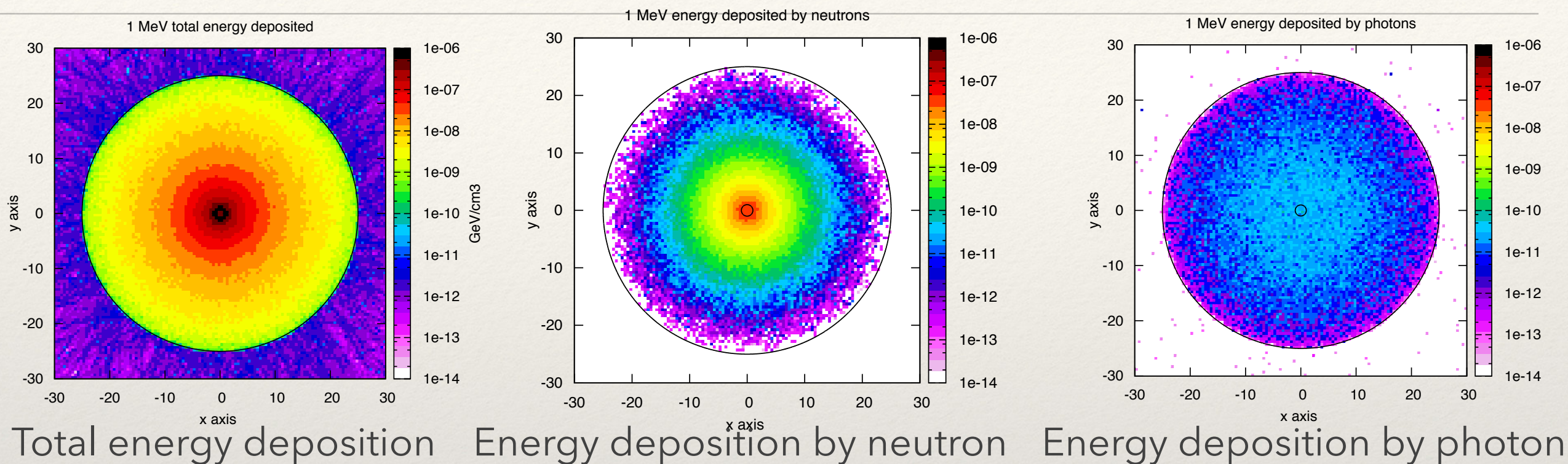
(M.Pimpinella, L.Silvi and C.Caporali)

In collaboration with University of Tor Vergata and CNAO within collaboration for Metrological European Project

- ❖ MC simulations are used for developing and characterizing new devices for challenging dosimetry required by modern radiotherapy modalities
- ❖ At ENEA diamond detector prototypes fabricated at Rome Tor Vergata University have been characterised in terms of absorbed dose to water response by MC simulations performed on CRESCO 4
- ❖ Correction factors for dosimetry in small photon beams have been calculated for prototypes as well as for the commercially available detector by PTW, Freiburg, Germany
- ❖ **Due to the very small detector sensitive volume (0.004 mm^3) in a large medium (water 30 cm^3), MC calculations are very time consuming taking hundreds of CPU hours to reach the required statistical uncertainty (about 0.1% on absorbed dose in the 0.004 mm^3 scoring region)**



Neutron Survey Meter Particle Sensitivity Estimations and Response Function of Bonner Sphere Spectrometers



Scientific Publications related to the R&D

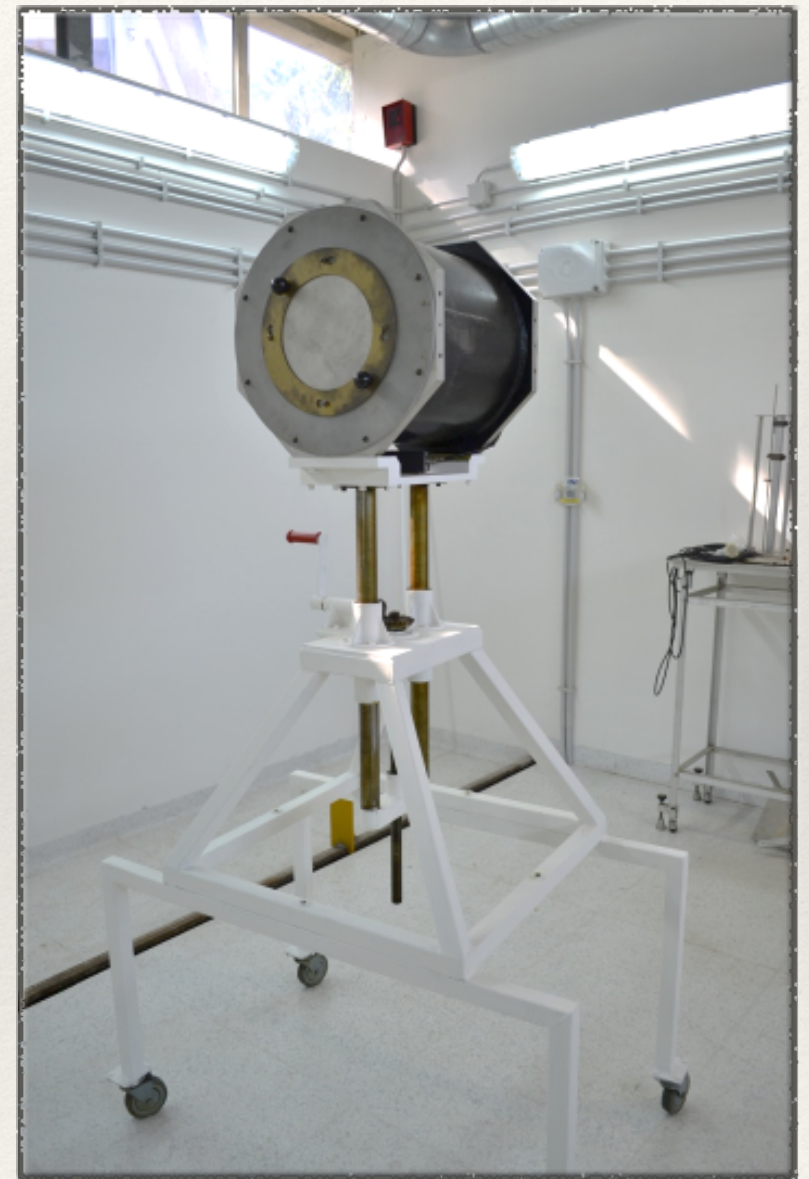
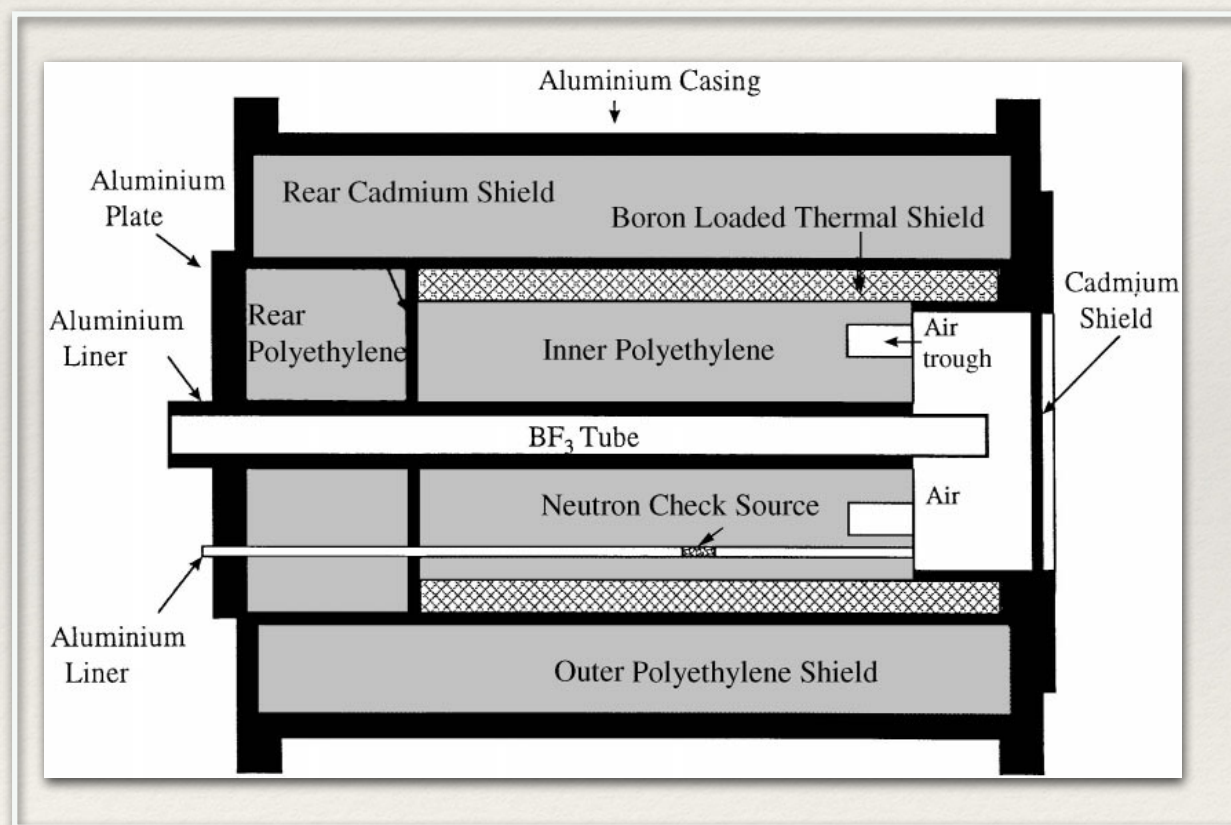
- ❖ 1) A.Pietropaolo, F.Murtas, G.Claps, **L.Quintieri**, D.Raspino, G.Celentano, A.Vannozzi, O.Frasciello, A new ^3He -free thermal neutrons detector concept based on the GEM technology, *Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment* (Impact Factor: 1.32). 07/2013; 729:117. DOI: 10.1016/j.nima.2013.06.058
- ❖ 2) M.Ferrario,**L.Quintieri** et al., IRIDE: Interdisciplinary research infrastructure based on dual electron linacs and lasers, *Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment* (Impact Factor: 1.32). 03/2014; 740:138-146. DOI: 10.1016/j.nima.2013.11.040
- ❖ 3) A. Pietropaolo a,n, F. Murtas b, G. Claps b, **L. Quintieri** ,1 D. Raspino, G. Celentano, A. Vannozzi , O. Frasciello, A new ^3He -free thermal neutrons detector concept based on the GEM technology , *Nuclear Instruments and Methods in Physics Research A* 729 (2013) 117–126
- ❖ 3) G.Claps, F.Murtas, A.Pietropaolo, G.Celentano, A.Vannozzi, A.Santoni, **L.Quintieri**, L.A.Riedele, ^3He -free triple GEM thermal neutron detector, *EPL (Europhysics Letters)* (Impact Factor: 2.27). 12/2013; 105(2). DOI: 10.1209/0295-5075/105/22002
- ❖ 4) R. Bedogni, J.M.Gómez Ros, A.Pola, M.V.Introini, D.Bortot, A.Gentile A.Esposito, G. Mazzitelli, B.Buonomo, **L.Quintieri**, L.Foggetta, Testing a newly developed single-sphere neutron spectrometer in reference monochromatic fields from 147 keV to 14.8 MeV, *Nuclear Instruments and Methods in Physics Research Section A Accelerators Spectrometers Detectors and Associated Equipment* (Impact Factor: 1.32). 01/2013; 714(110):114.
- ❖ 5) M. Prata, D. Alloni, **P. De Felice**, M. Palomba, A. Pietropaolo, M. Pillon, **L. Quintieri**, A. Santagata, P. Valente, Italian neutron sources, *The European Physical Journal Plus*, November 2014, 129:255

Highlight on Simulation

Activities in progress

On-going Activity: Calibration and Monte Carlo Modelling of Neutron Long Counter

- ❖ The long counters ("De Pangher") will be put in operation as a transfer standard for neutron fluence measurements. This represents one of the main goals to reach before the end of 2015.

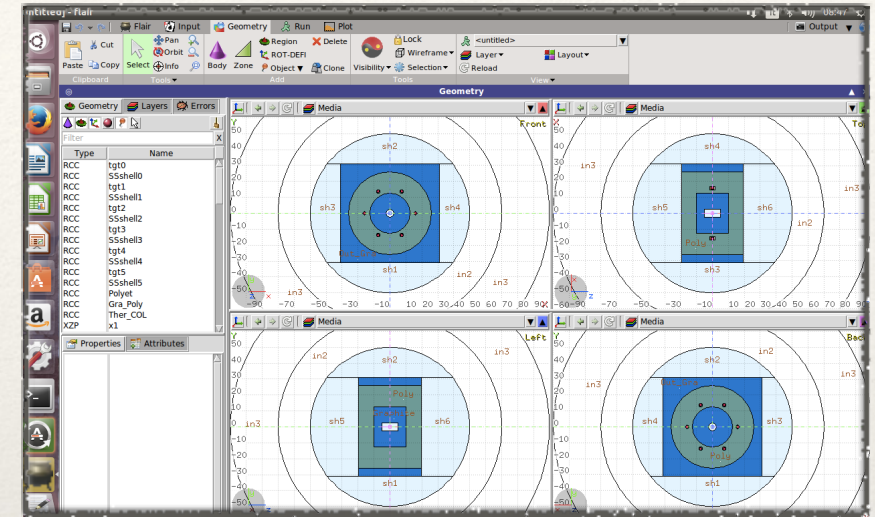


Schematic of transversal cross section of the "De Pangher" Long counter

Feasibility Study of a Thermal Neutron Irradiation System for Calibration of Personal Dosimeters in Terms of Hp (10)

Monte Carlo estimations to optimise shape, material thickness, source distribution in order to maximise the thermal flux density inside the column.

- ❖ Goal: 35 cm diameter cylindrical air cavity (to allow the uniform irradiation of 30cm x30cm x15 cm water slab phantom, according to what stated on Hp(10) by International Standard ISO 8529-3)
- ❖ It is foreseen to use AmBe sources to reach in the cavity at least a neutron fluence rate around $5 \cdot 10^{+4} \text{ cm}^{-2} \text{ s}^{-1}$
- ❖ 2 m³ reactor grade graphite; Polyethylene shell in addition and other suitably chosen materials
- ❖ Thermal fluence homogeneity should be guaranteed within few percent (the design of suitable flattening filters are also considered)

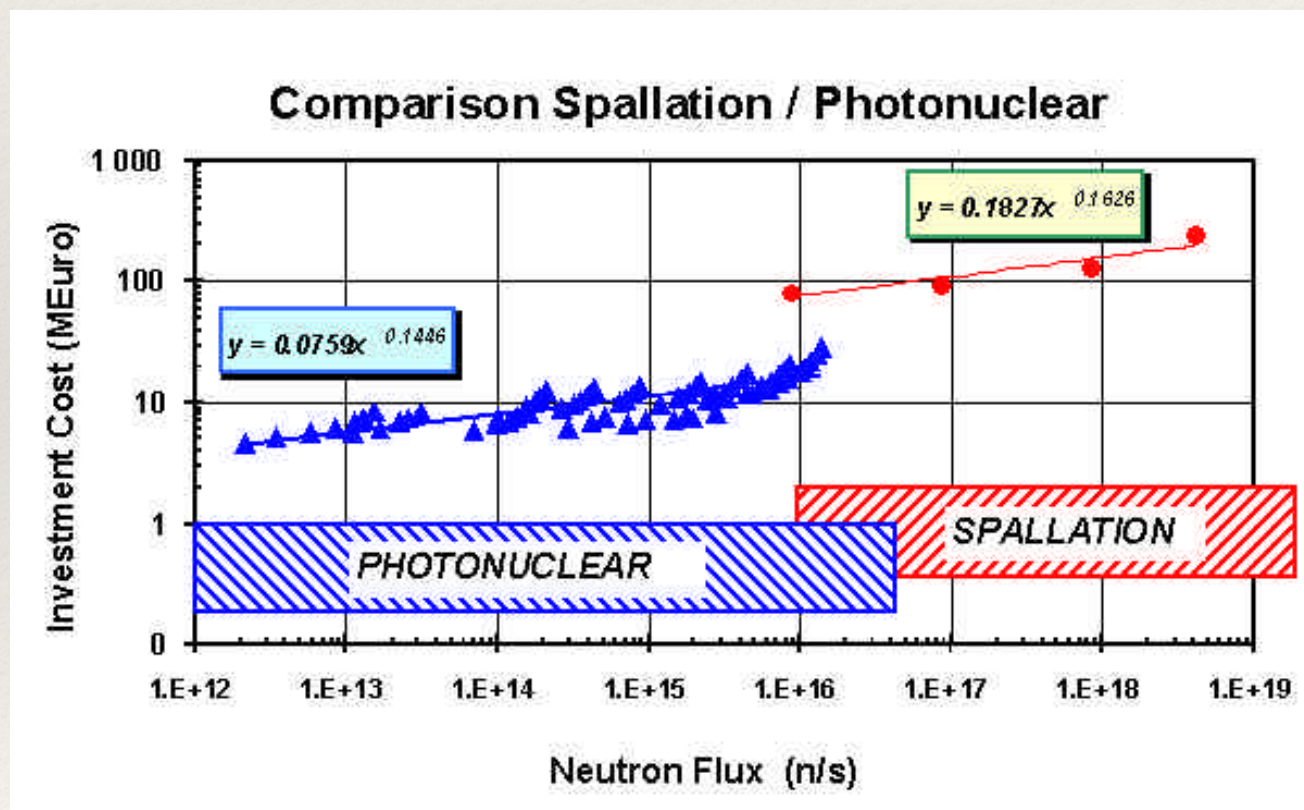


High purity reactor grade graphite already available

Characterisation of Accelerator Driven Source for Metrological Purposes by MC Codes

Simulations of Photo-neutron Accelerator Driven Sources: IRIDE Case

- ❖ Spallation source are very effective in producing neutrons, but are large and expensive
- ❖ Electron drivers although are much less effective in neutron production are rather cheap and compact machine that might also bring advantages in terms of reliability



- ❖ Above a given neutron flux (10^{16} n/s) the spallation will be preferred while for the lower fluxes, the photonuclear process will tend to be more convenient

IRIDE_V4_17/07/2013

IRIDE

An Interdisciplinary Research Infrastructure based on Dual Electron linacs&lasers

A WHITE BOOK



Astract

This report describes the scientific aims and potentials as well as the preliminary technical design of IRIDE, an innovative tool for multi-disciplinary investigations in a wide field of scientific, technological and industrial applications. IRIDE will be a high intensity “particle factory”, based on a combination of a high duty cycle radio-frequency superconducting electron linac and of high energy lasers. Conceived to provide unique research possibilities for particle physics, for condensed matter physics, chemistry and material science, for structural biology and industrial applications, IRIDE will open completely new research possibilities and advance our knowledge in many branches of science and technology. IRIDE will contribute to open new avenues of discoveries and to address most important riddles: What does matter consist of? What is the structure of proteins that have a fundamental role in life processes? What can we learn from protein structure to improve the treatment of diseases and to design more efficient drugs? But also how does an electronic chip behave under the effect of radiations? How can the heat flow in a large heat exchanger be optimized?

The scientific potential of IRIDE is far reaching and justifies the construction of such a large facility in Italy in synergy with the national research institutes and companies and in the framework of the European and international research. It will impact also on R&D work for ILC, FEL, and will be complementarity to other large scale accelerator projects. IRIDE is also intended to be realized in subsequent stages of development depending on the assigned priorities.

Iride Collaboration

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IRIDE: Interdisciplinary research infrastructure based on dual electron linacs and lasers

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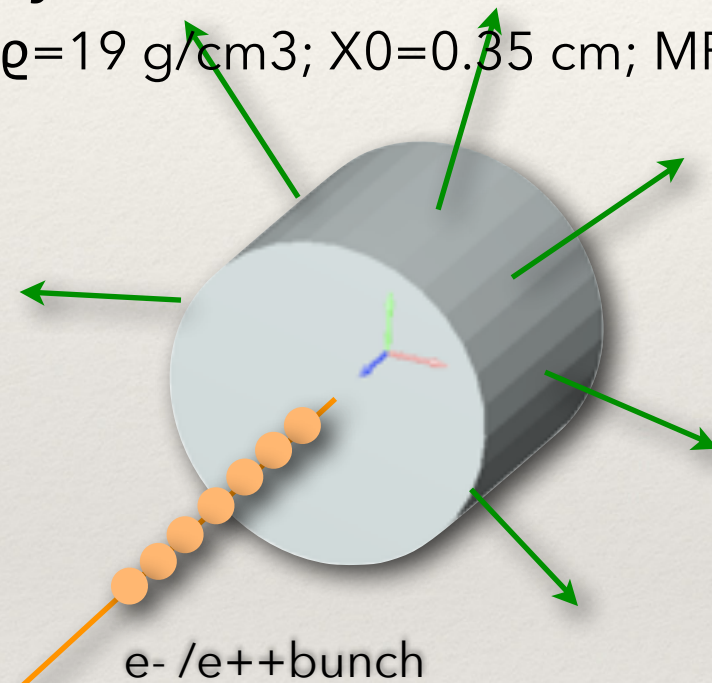
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W Target Optimisation for Neutron Yield as a Function of Primary Electron Energy

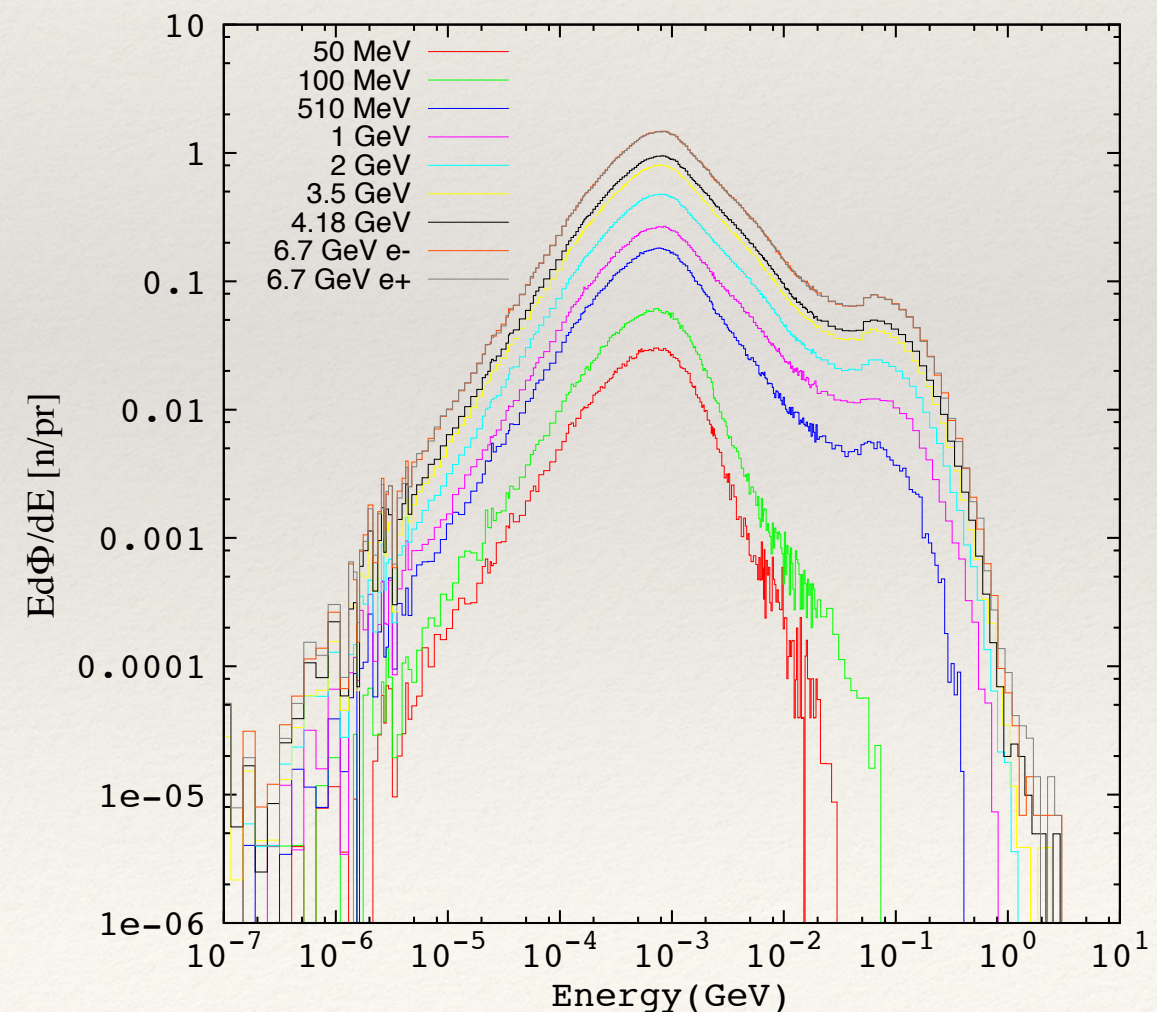
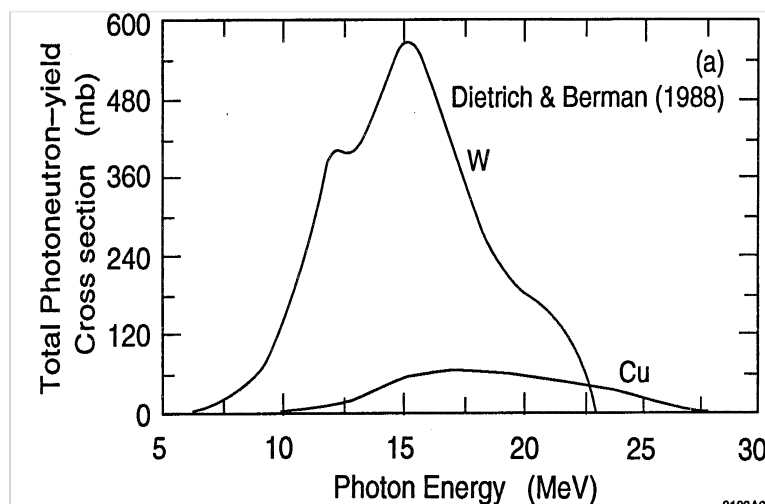
Optimized target as designed exploiting MC parametric simulation results

W cylinder R=35 mm L=60 mm

(Z=74; $\rho=19 \text{ g/cm}^3$; $X_0=0.35 \text{ cm}$; $MR=0.9 \text{ cm}$)

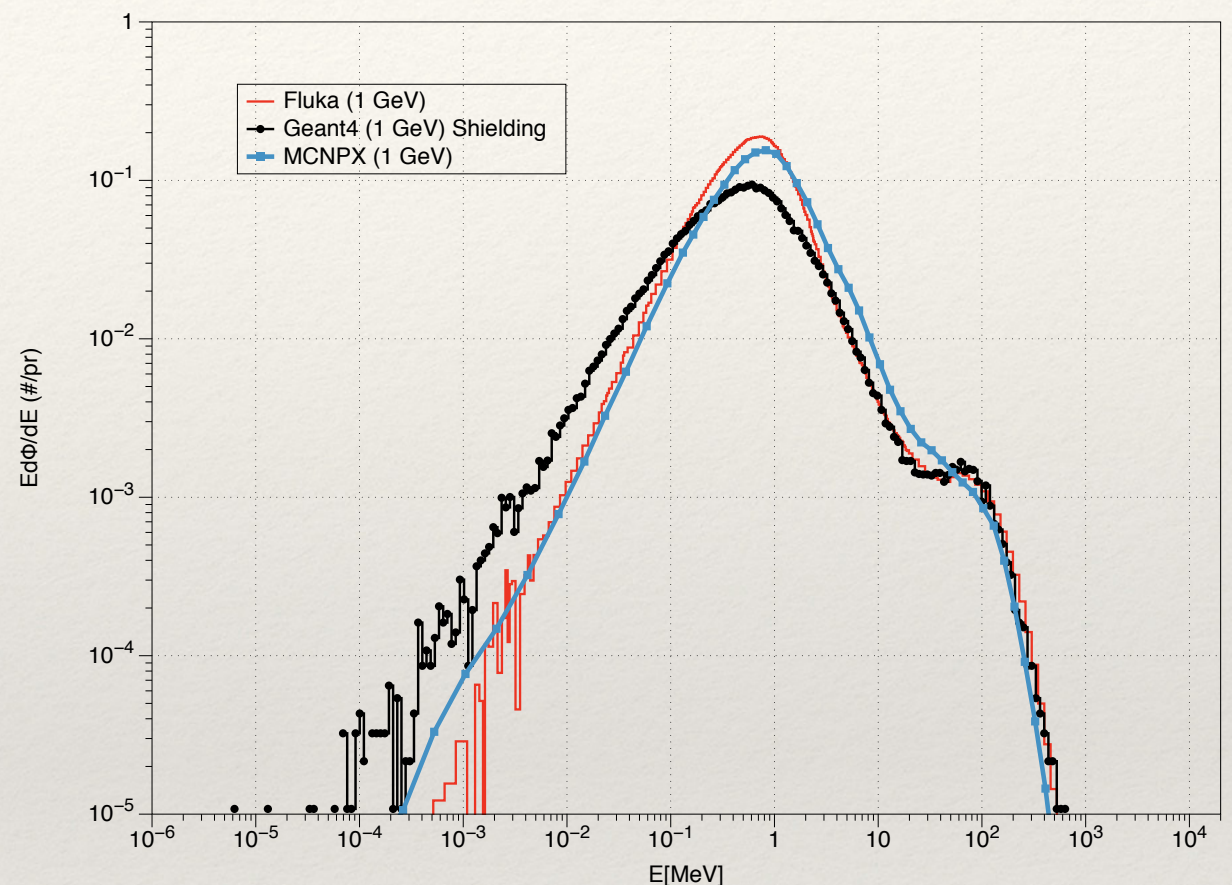


Facility Parameters	nElbe	Gelina	nToF	ISIS	IRIDE
Source		e-Linac	p spallation	p spallation	SC e- Linac
Part E (MeV)	40	120	20000	800	1000 (2000)
Max Power (kW)	18	11	45	160	32/1000 (pulsed/continuous)
Neutrons/s	3.4E+13	3.2E+13	8.1E+14	1E+16	7E+14/3E+15



Computational issues of photo-nuclear physics in particle transport codes

- ❖ For a long time photonuclear processes were neglected mainly due to the lack of complete evaluated data for applications
- ❖ Photonuclear data are isotopic in nature, the cross sections showing irregular dependence on atomic number (Z) and atomic mass (A). Thus while photoatomic data are readily tabulated by element photonuclear data must be tabulated for each isotope of an element
- ❖ A relatively complete photonuclear data file in ENDF format for 164 isotopes became available only “recently”, in 2000 (ENDF-6 formatted files containing complete interaction descriptions, i.e., double differential cross sections, suitable for use in transport calculations)

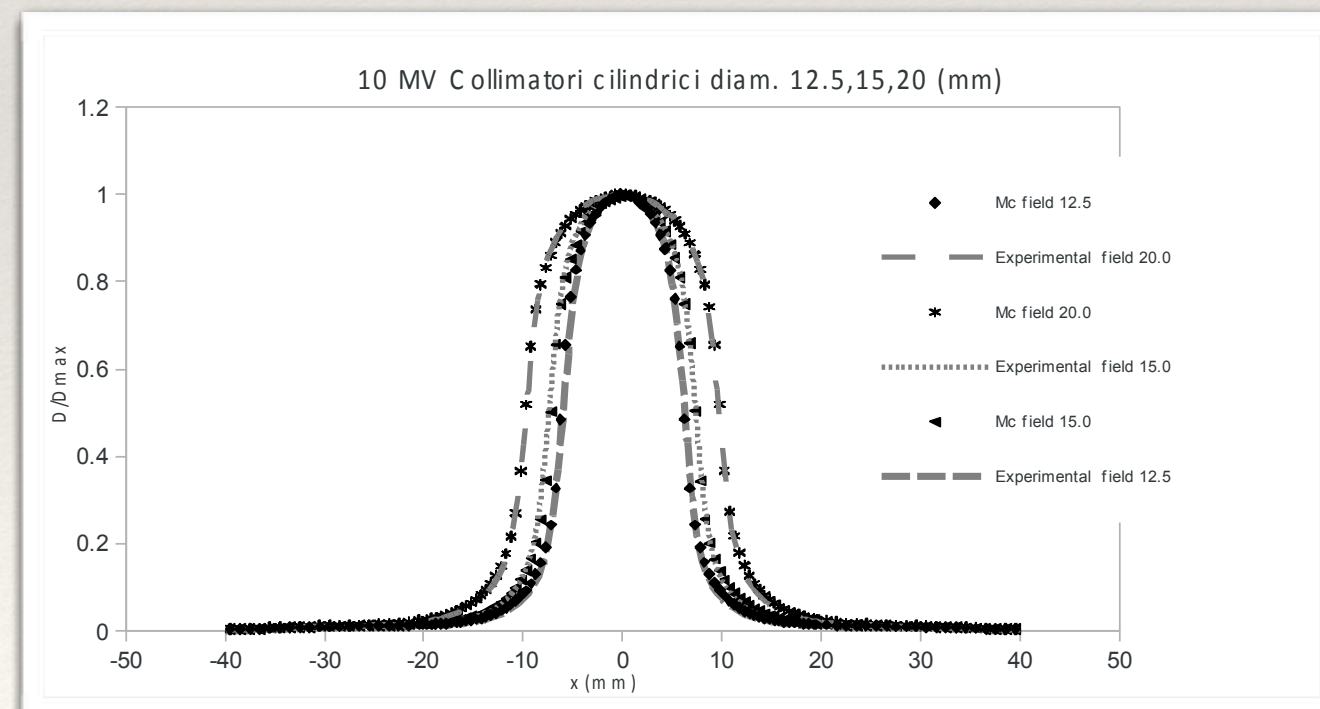
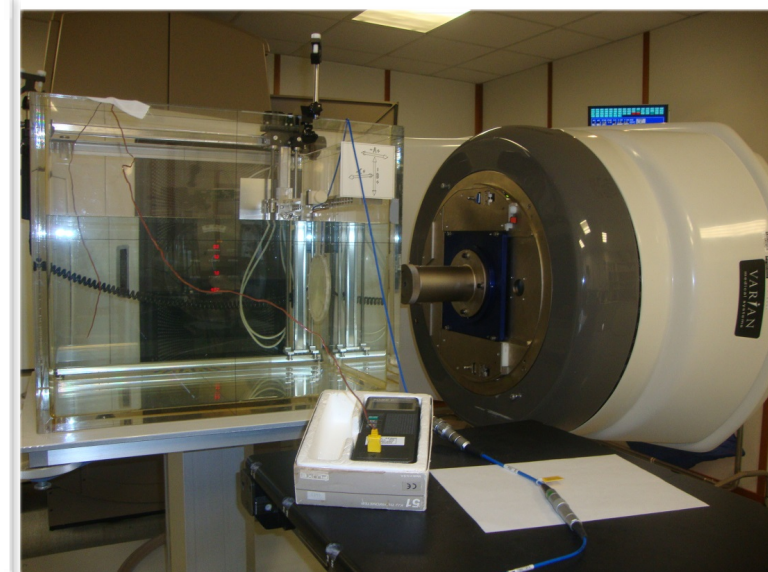
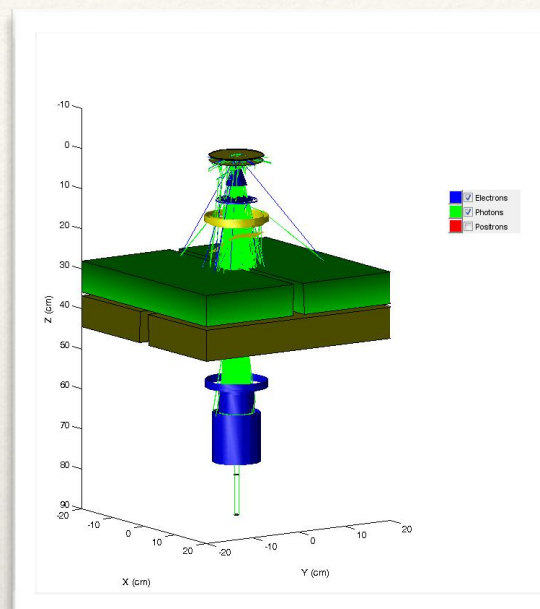


From the computational point of view the photo-nuclear (photo-neutron, in the specific case) process simulations are heavy since the cross section are small wrt other EM/hadronic processes. In order to have statistically accurate results for the neutron yield, very high statistics is needed. The possibility to use parallel calculations on CRESCO Cluster was a fundamental option to achieve statistically significant results

Simulation of Radiation Beams Used for Advanced Radiotherapy Modalities by Modelling Clinical Radiation Facilities

(M.Pimpinella, L.Silvi and C.Caporali)

- ❖ The most time consuming calculations are related to tuning the simulation parameters with experimental data (dose released).
- ❖ Availability of high performance calculation systems allows a more accurate beam characterization and therefore helps to improve reliability of clinical dosimetry.
- ❖ Recently small photon beams used for stereotactic radiotherapy have been successfully simulated in the framework of a European metrology project aiming at developing measurement procedures appropriate in beam sizes below 2 cm.

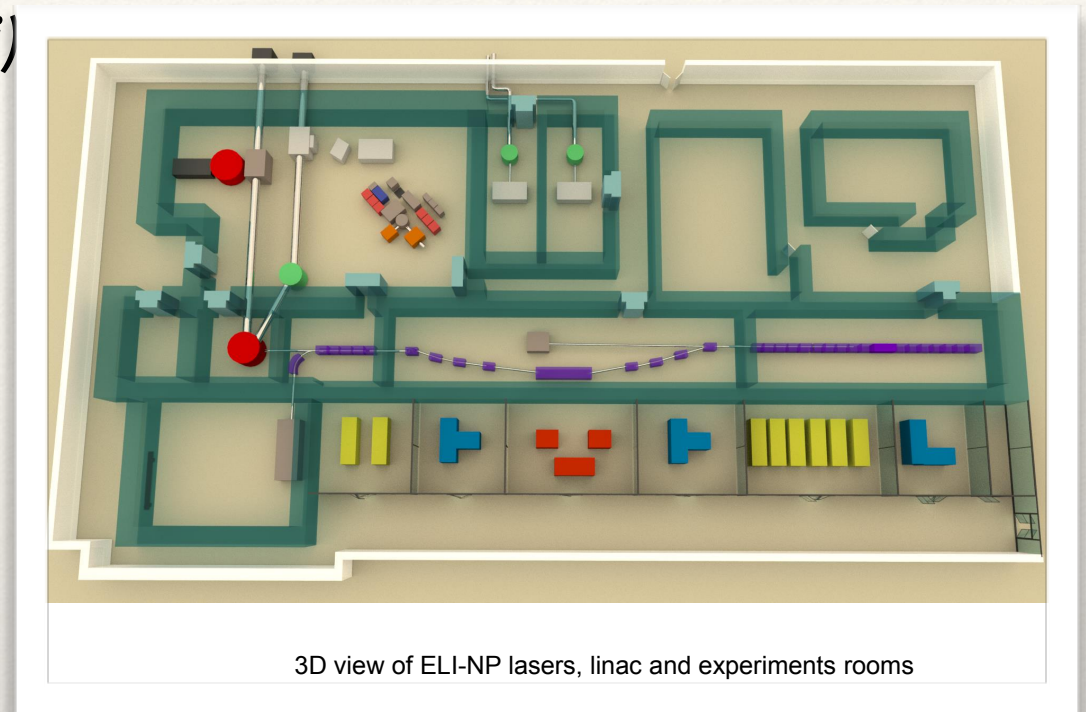
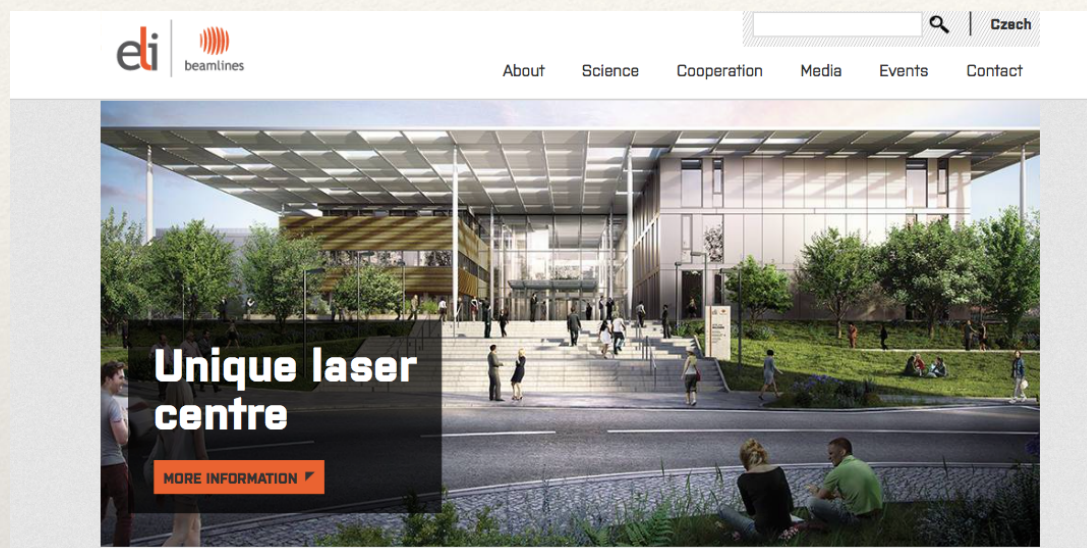


Overview of Some Representative Application Cases of FEA Codes

Thermal design of Dump of ELI

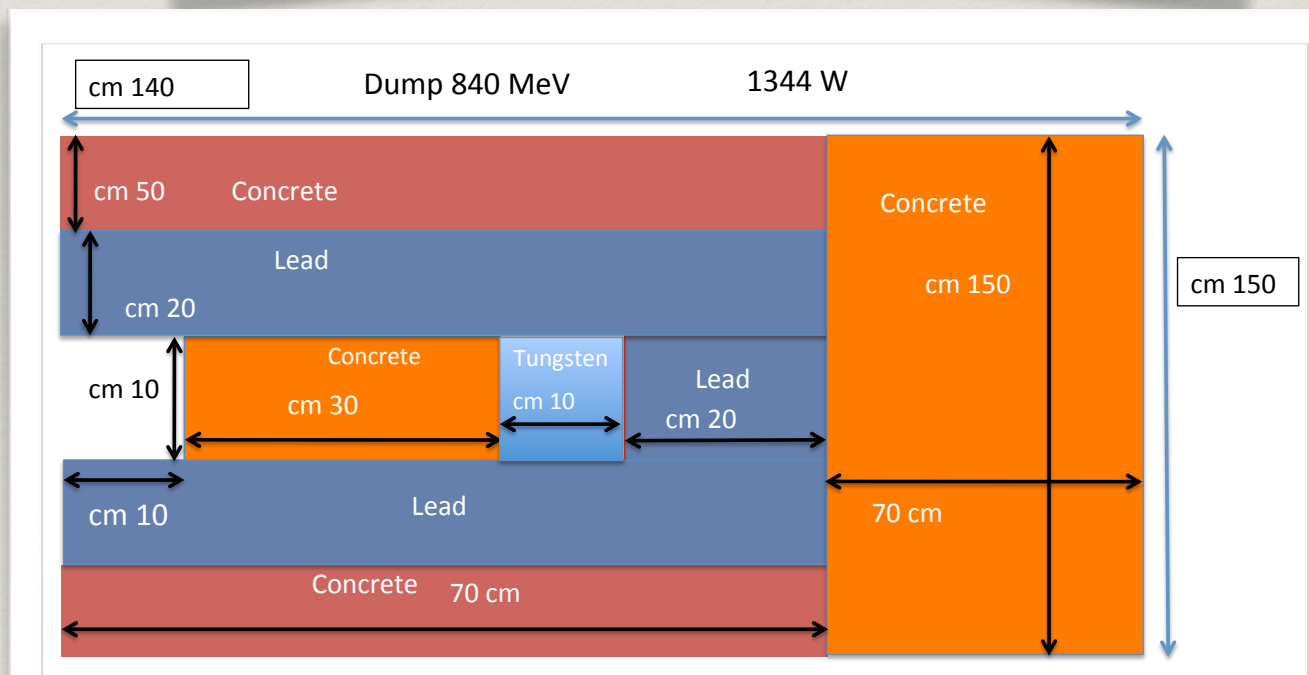
“Extreme Light Infrastructure - Nuclear Physics ELI - NP”

In collaboration with INFN (Laboratori Nazionali di Frascati)



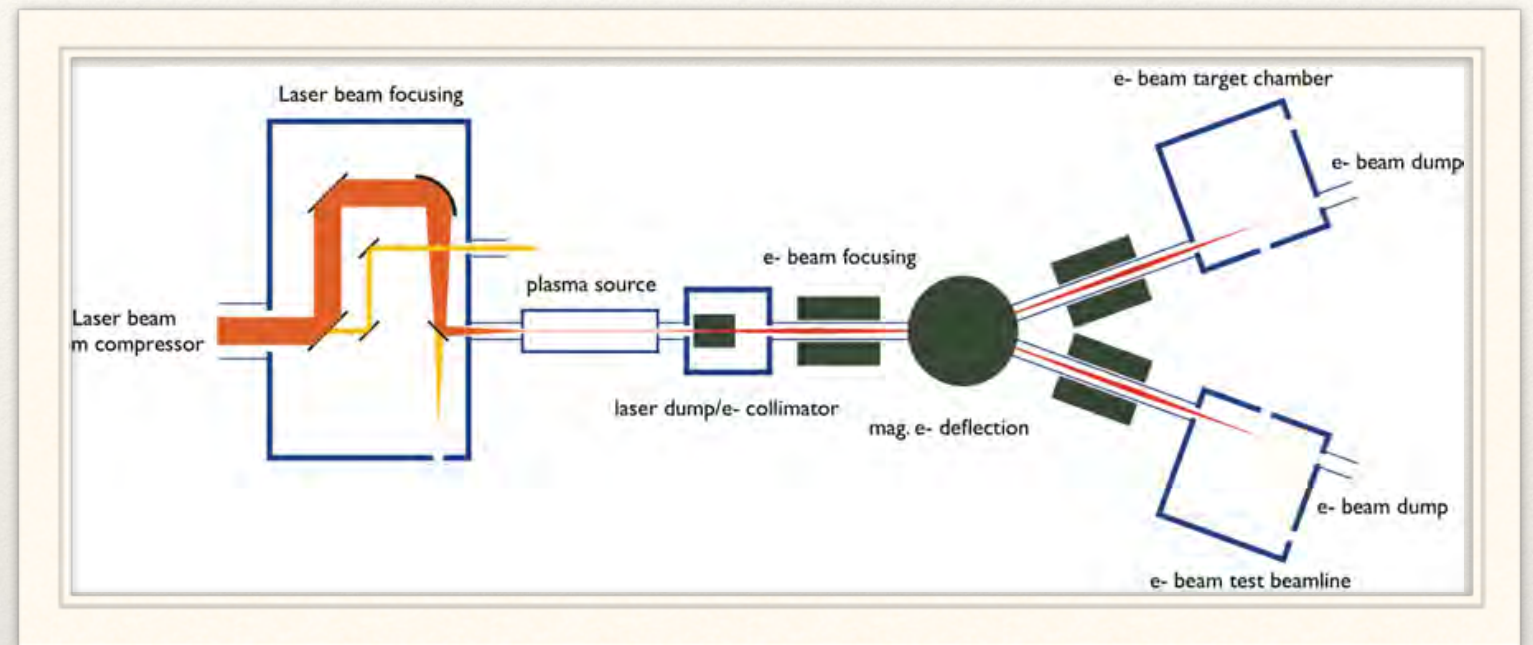
<http://www.eli-beams.eu>

- ❖ Temperature distribution simulations inside the dump for the higher energy electron beam (800 MeV).
- ❖ Both static and transient analysis



Eli Beam Dump and Thermal Load Scenario

- Particle type= electron
- Energy =840 MeV
- Average rate= $9.9\text{E}+12\text{ s}^{-1}$
- Divergence= 2 mrad
- Spot size (dump inlet)= 1 cm
- Overall power deposited: 1340 W
- Duty cycle: 172 h of continuously beam released at maximum power + 12 h

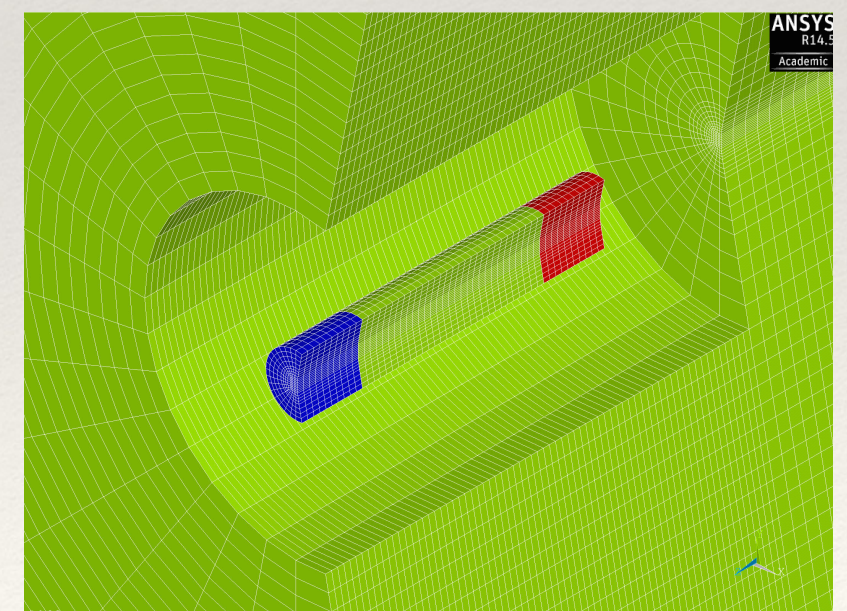
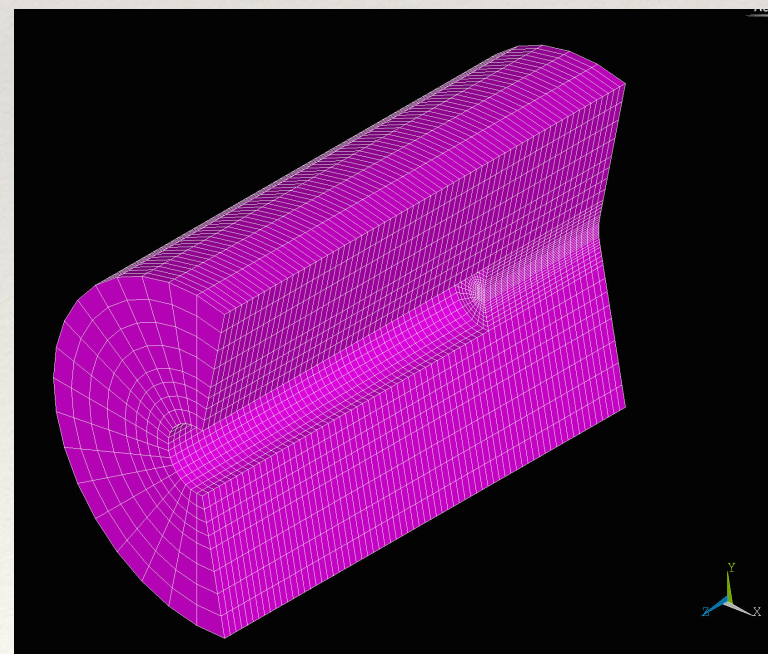
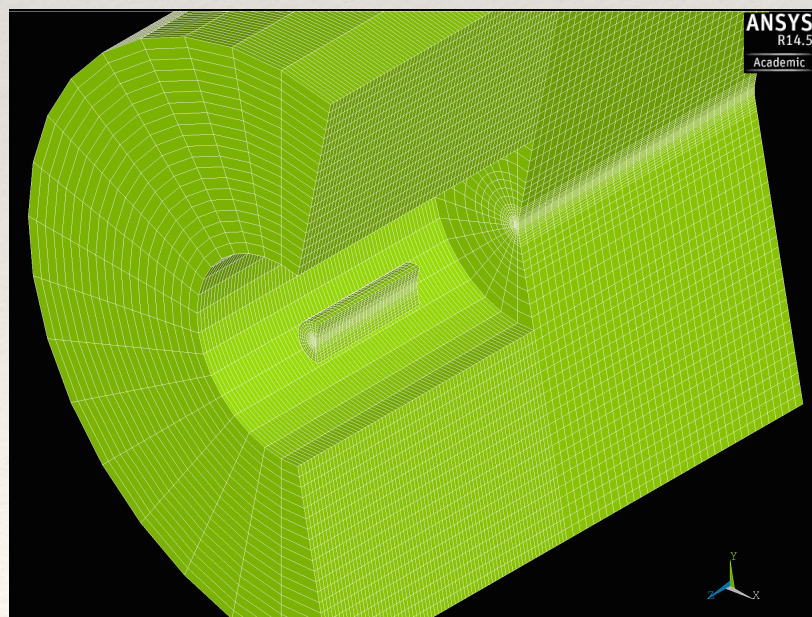
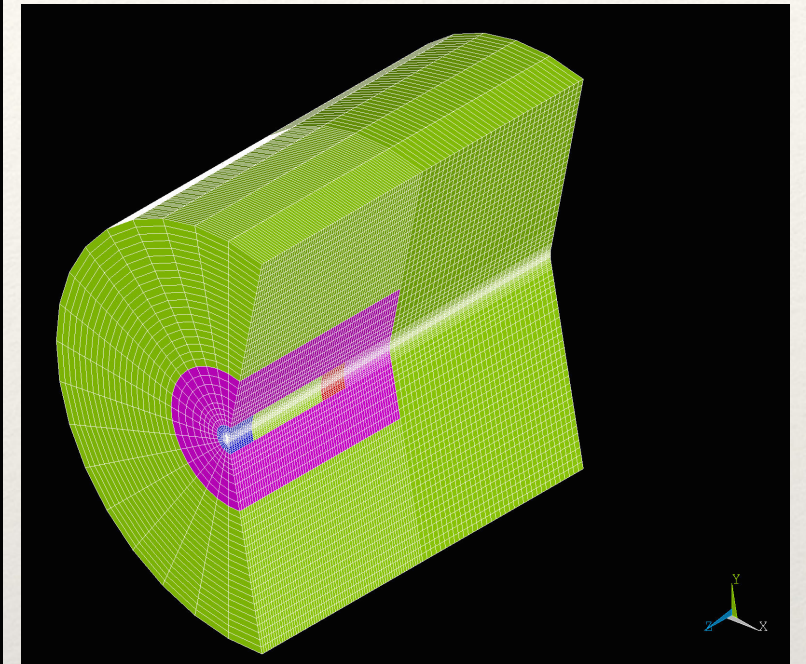
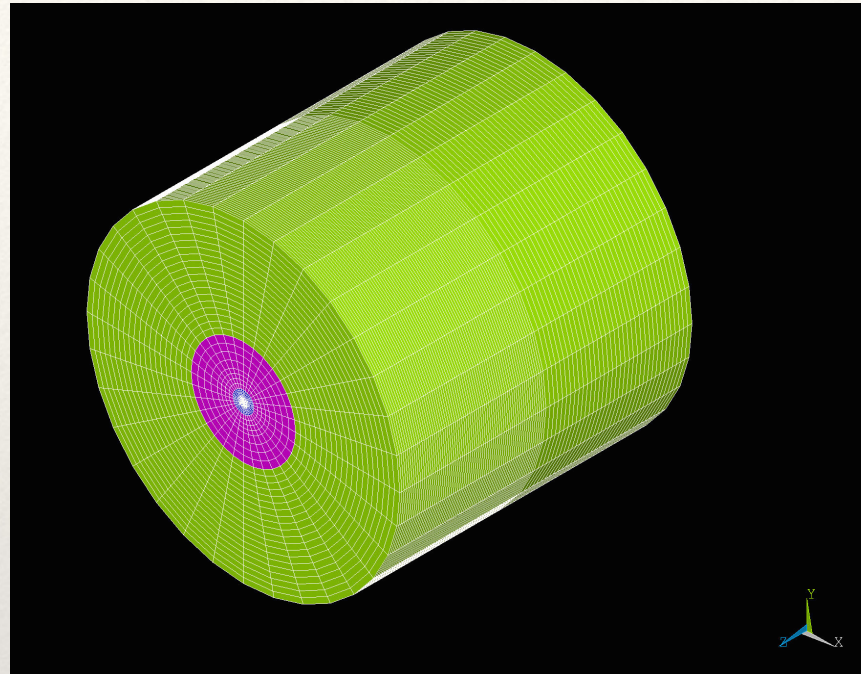
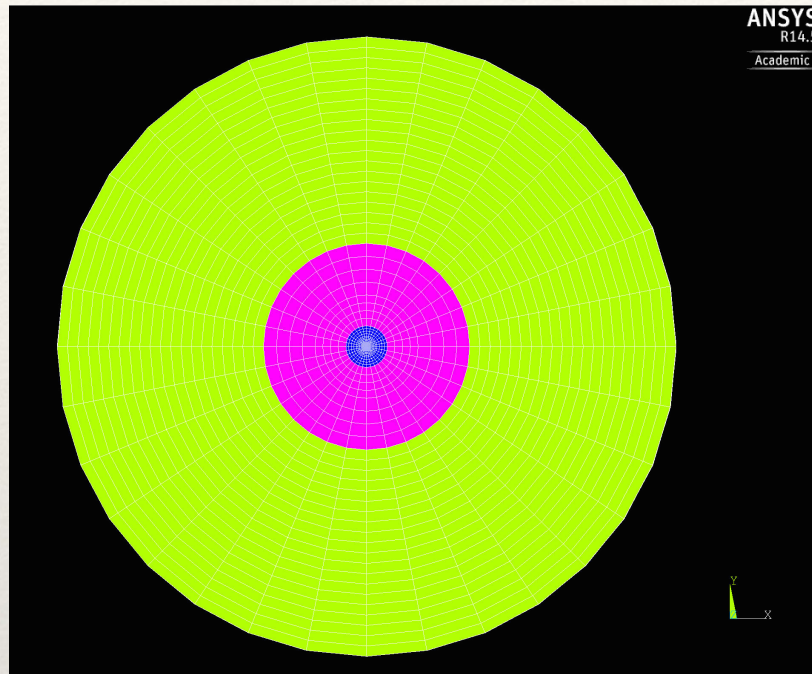


SCENARIO 1

- ❖ Thermal Transient Analysis
- ❖ Initial Condition: uniform temperature at 293.15 K
- ❖ Thermal load applied as power density generation (W/m^3)
- ❖ Max time of load application 168 h (7days continuously) +8 hours of cool-down phase
- ❖ Boundary conditions: all external surface are adiabatic
- ❖ Goal: check when the lead melting can start

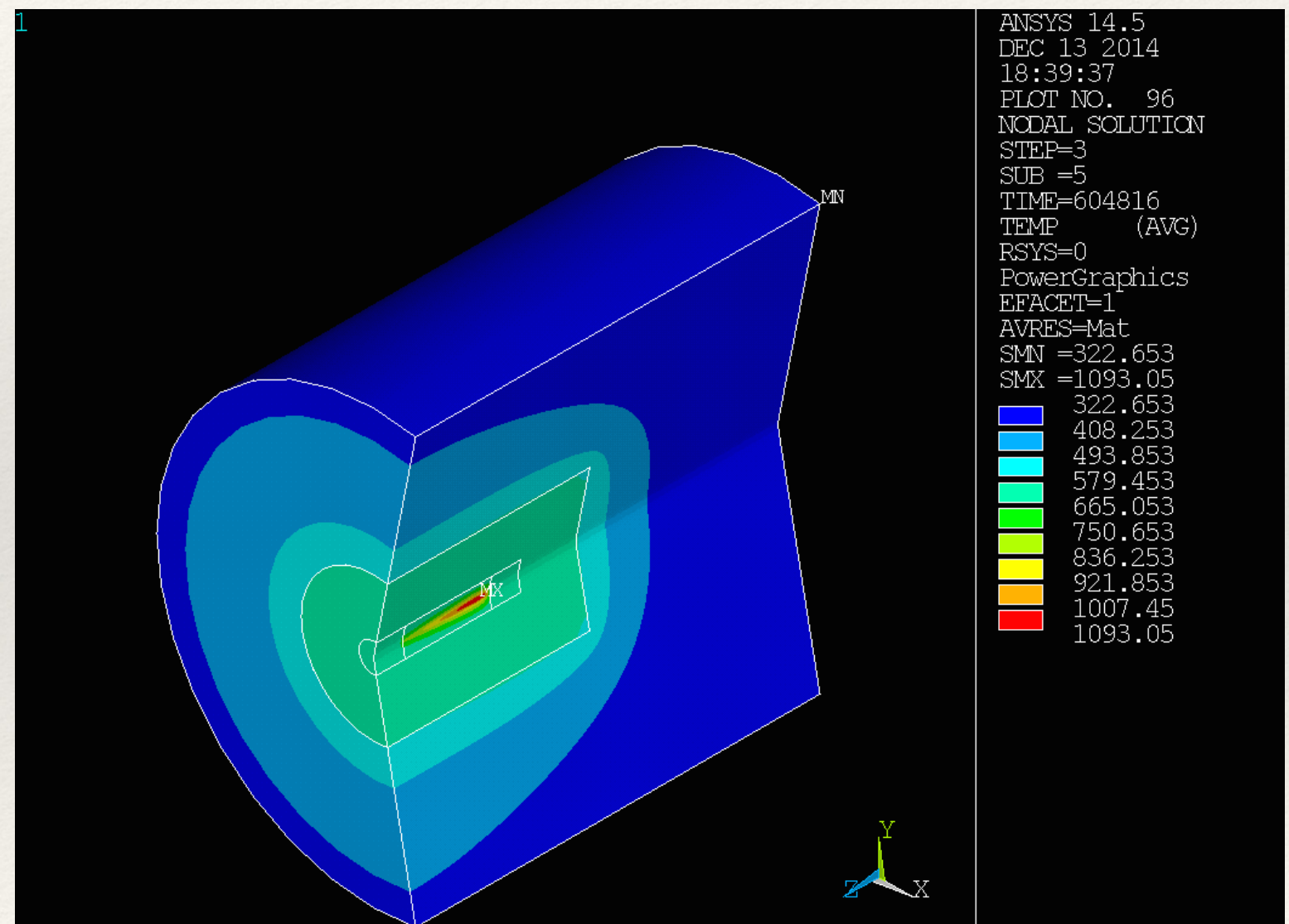
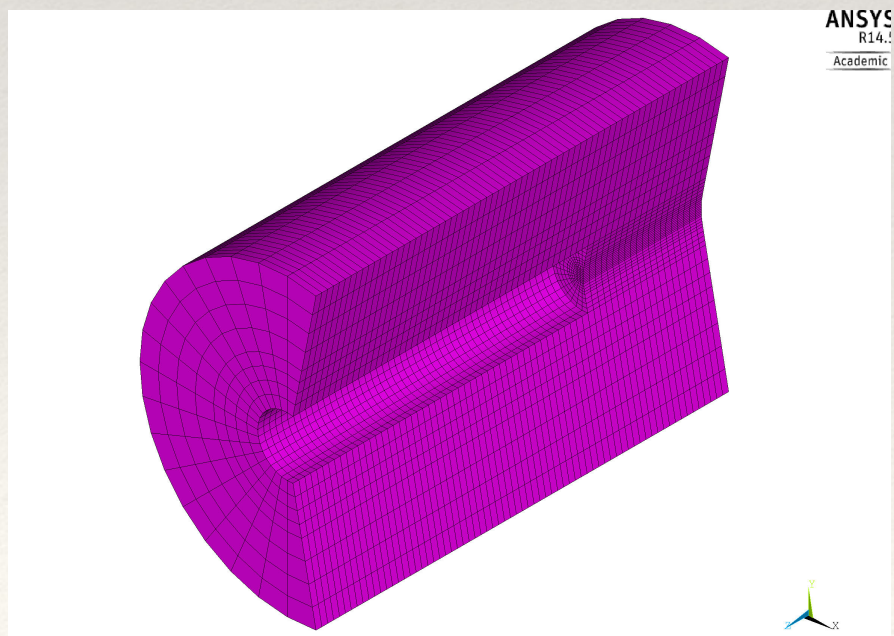
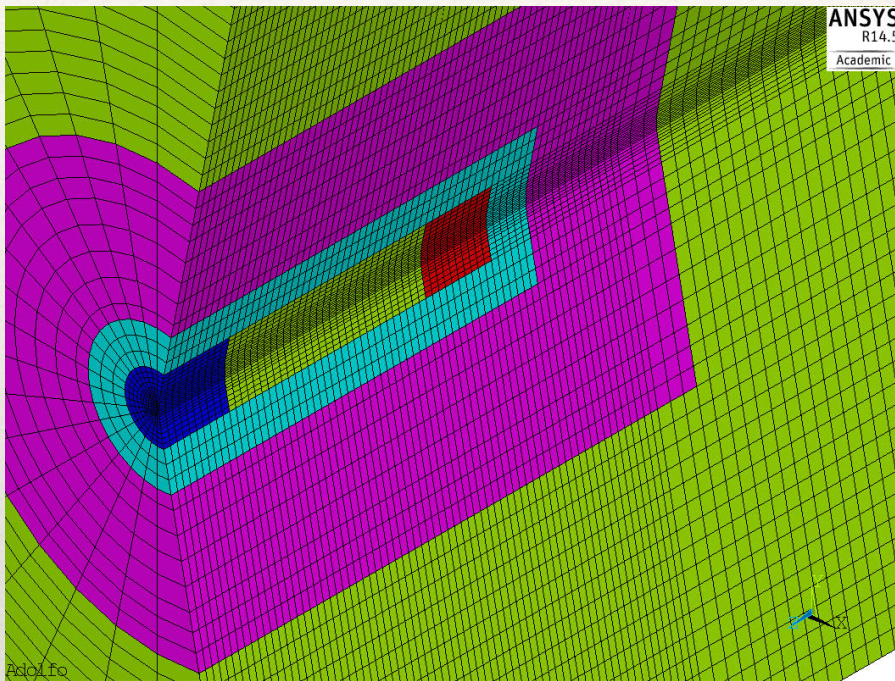
The Finite Elements Model

- 3D Mapped mesh. Element solid70.
- green elements =concrete; pink elements=lead; blu elements= air;red elements=tungsten



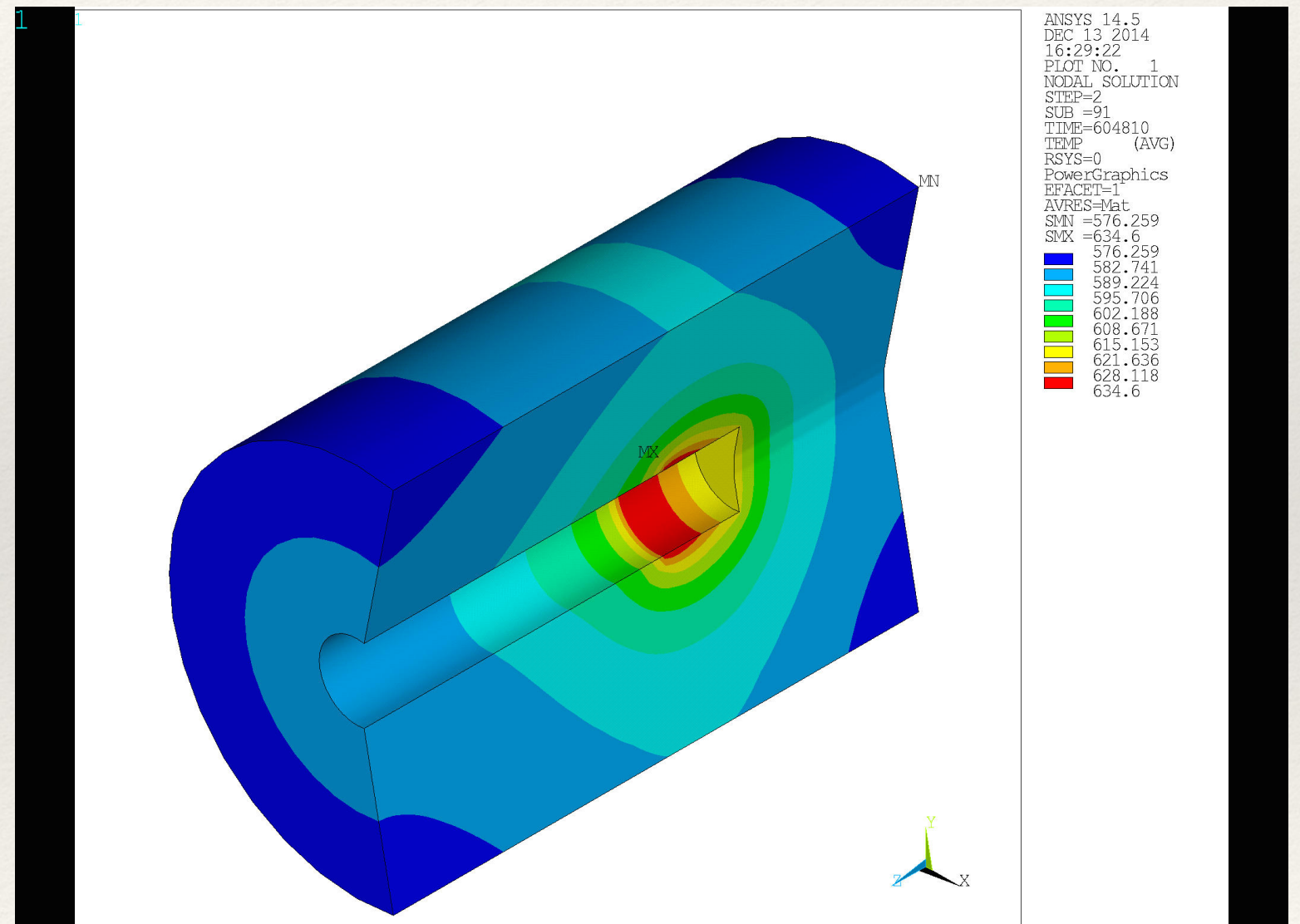
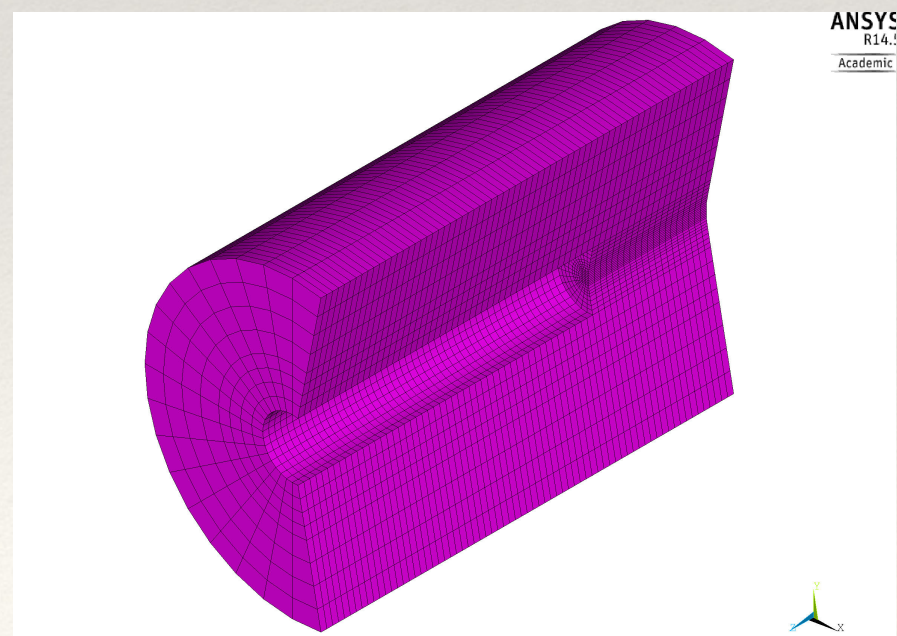
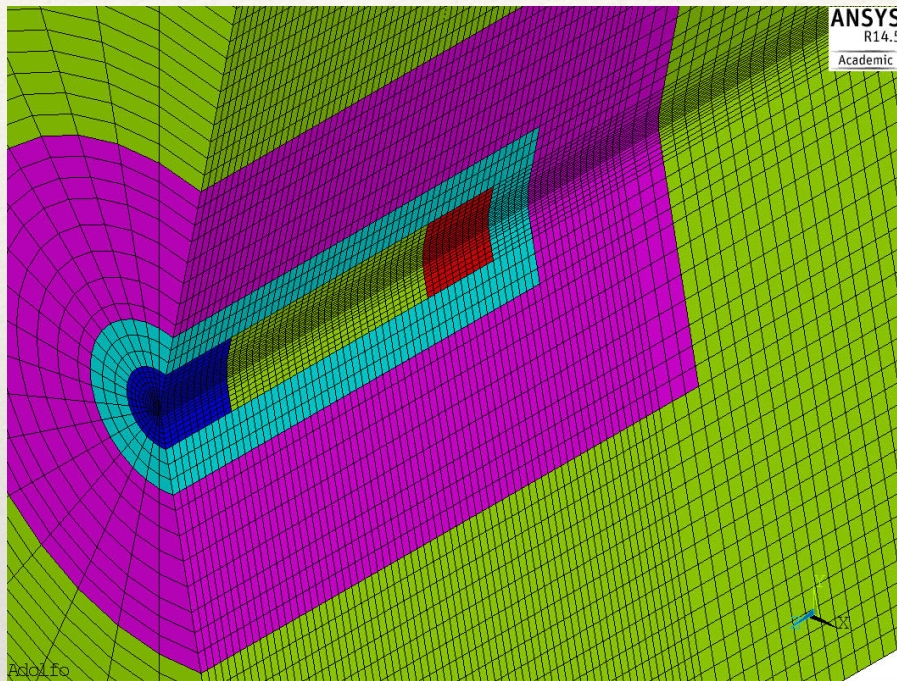
Preliminary Results

After 168 h of continuously deposited beam, the lead shell reaches its melting temperature (600 K)



Preliminary Results

After 168 h of continuously deposited beam, the lead shell reaches its melting temperature (600 K)



Conclusions and Acknowledgements

- ❖ Intensive simulation activities are routinely carried out in INMRI ENEA
- ❖ The quality and quantity of the scientific work have been increased substantially thanks to the high performance of CRESCO cluster
- ❖ Future plan foresees even more intense simulation activity. Participation to the EMPIR PRT: *metrology for accuracy of dose to patients in hadron therapy*. Task on neutron dose simulations with the major neutron transport Monte Carlo codes, for benchmarking purposes.
- ❖ **A fundamental support and high qualified assistance have been provided by the UTICT service with fruitful and synergic interactions.**

**Thank You for Your
Attention!**