



Simulations for Nuclear Reactions and Structure in Europe (SiNuRSE, JRA05)

GSI, RuG, CEA, ATOMKI, IFJ,
IFIN-HH, USC, CIEMAT, UCM

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KVI, University of Groningen

ENSAR meeting, Warsaw, June 18, 2013

Simulations for Nuclear Reactions and Structure in Europe (SiNuRSE)

- Develop event generators based on realistic physics models which are useful for the experimental activities pursued at the European facilities concerned by ENSAR.
- Benchmark these models against a wide set of available experimental data and against each other.
- Create a platform for simulations in which the user can easily switch between various modules.

The ultimate goal is to be able to combine an event generator from a specific application with the definition of the geometry from another code and the tracking of a yet another program.

- Verify the results against several detector types which are currently being developed for the ENSAR facilities.

Tasks

- **Task 1:** Deals with the event generators and their benchmarking.
- **Task 2:** Deals with the development of virtual Monte-Carlo platform and databases.
- **Task 3:** Involves a few well-chosen test cases relevant for several activities of the community.
- Total budget of 402 k€.

Milestones

Milestone number	Milestone name	Work package(s) involved	Expected date	Means of validation
<i>M-JRA05-1.1</i>	<i>Event generator for light ion induced reaction ready for benchmarking and for implementation into simulation codes</i>	<i>JRA05</i>	<i>24</i>	<i>Event generator vs. experimental data</i>
<i>M-JRA05-1.2</i>	<i>Event generator for heavy ion induced reaction ready for benchmarking and for implementation into simulation codes</i>	<i>JRA05</i>	<i>36</i>	<i>Event generator vs. experimental data</i>
<i>M-JRA05-1.3</i>	<i>Event generator for specific reactions ready for benchmarking and implementation into simulation codes</i>	<i>JRA05</i>	<i>24</i>	<i>Event generator vs. experimental data</i>
<i>M-JRA05-2</i>	<i>Choice for codes to be implemented in the virtual Monte-Carlo simulations</i>	<i>JRA05</i>	<i>24</i>	<i>Software prototype for evaluation</i>
<i>M-JRA05-3.1</i>	<i>Implementation of neutron detector geometry and event generator</i>	<i>JRA05</i>	<i>24</i>	<i>Characteristic histograms of the detector</i>
<i>M-JRA05-3.2</i>	<i>Implementation of fast ejectile and heavy-ion detectors and event generator</i>	<i>JRA05</i>	<i>24</i>	<i>Characteristic histograms of the detector</i>

Deliverables

Task 1

- *D-JRA05-1.1: Report on the benchmarking of the event generator for light ion induced reaction (Month 36) (CEA)*
- *D-JRA05-1.2: Report on the benchmarking of the event generator for heavy ion induced reaction (Month 48) (GSI)*
- *D-JRA05-1.3: Report on the benchmarking of the event generator for specific reactions (Month 48) (CIEMAT)*
- *D-JRA05-1.4: Report on the benchmarking of the event generator for fusion-evaporation reactions (Month 48) (IFJ)*

Task 2

- *D-JRA05-2: The platform for Monte-Carlo simulations (Month 48) (USC)*

Task 3

- *D-JRA05-3.1: Simulation results for various neutron detectors (Month 48) (ATOMKI)*
- *D-JRA05-3.2: Simulation results for fast ejectile and heavy-ion detectors (Month 48) (RUG)*
- *D-JRA05-3.3: Simulation results for a calorimeter (Month 48) (USC)*

Status

- First kick-off meeting on Jan. 24, 2011 in Amsterdam.
 - Every year a coordination meeting in Amsterdam.
 - Three coordinators for three tasks.
 - All the positions have been occupied to a large extent.
 - SiNuRSE colleagues from Spain have joined the GEANT4 collaboration and maintain their respective developments: the neutron cross section libraries and the gamma-ray event generators, respectively.
 - All milestones reached on time (within a couple of months).
 - Working towards the deliverables.
-

Subtasks for task 1

- **Subtask 1:** Development of an event generator for light-ion induced reactions (CEA, U-Liege).
- **Subtask 2:** Development of an event generator for heavy-ion induced reactions (GSI).
- **Subtask 3:** Development of an event generator for elastic proton-nucleus cross-sections and p-n reactions with focus on exotic nuclei (UCM).
- **Subtask 4:** Development of an event generator for beta-decay including delayed particle emission (n, p, alpha) (CSIC).
- **Subtask 5:** Development of a gamma ray event generator for neutron capture electromagnetic cascades (CIEMAT).
- **Subtask 6:** Development of a software tool which allows the use in GEANT4 of cross sections from correct (neutron and ions) reaction data bases for low-energy reactions (CIEMAT).
- **Subtask 7:** Development of an event generator for fusion-evaporation reactions (IFJ).
- **Subtask 8:** Improvement of Intra-Nuclear Cascade models for a better prediction of one-nucleon-removal channel (CEA).

Sub-tasks 1.1 and 1.8: light-ion induced reactions (CEA, Saclay, U-Liege)

■ Objectives:

- To improve/extend the INCL4 intra-nuclear cascade model proven successful on nucleon-induced reactions
- To implement it (C++ version) into GEANT4 for simulations of both nuclear structure experiments and hadrontherapy applications

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David¹⁾, S. Leray¹⁾, A. Obertelli¹⁾

¹⁾ CEA/Saclay, ²⁾ Liège University

➡ **Sub-Task 1: light ion-induced reactions**

➡ **Sub-Task 8: better prediction of one-nucleon-removal**

Sub task 1.1: Development of an event generator for light-ion induced reactions (CEA, Saclay, U-Liege)

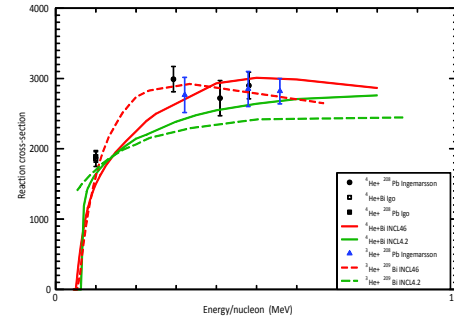
Model development:

- New version of the model for nucleon and LCP - induced reactions: INCL4.6 (A. Boudard et al., PRC 87, 014606 (2013)) improved in particular at low energies and for LCP-induced reactions (coupled to ABLA07)
- Implementation of the INCL4.6 modifications into the INCL++ version
- Improvement of the light-ion induced part of INCL++

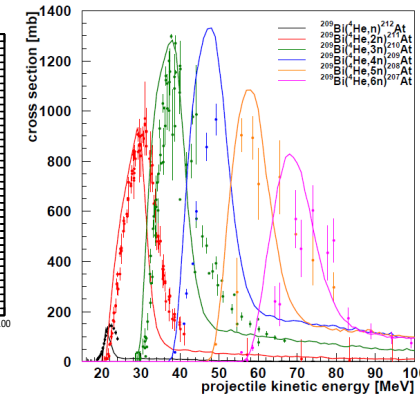
Implementation into GEANT4:

- Release 9.6: INCL++ with LI extension up to ^{18}O coupled to G4-deexcitation
- New physics lists: QGSP_INCLXX (+ QGSP_INCLXX_HP, FTFP_INCLXX, FTFP_INCLXX_HP to appear with next β -release)

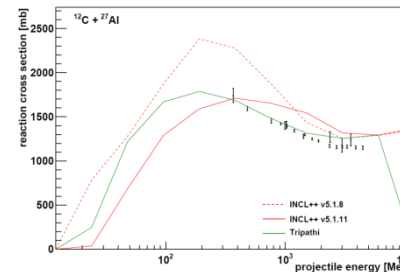
He-Bi/Pb total reaction cross-section



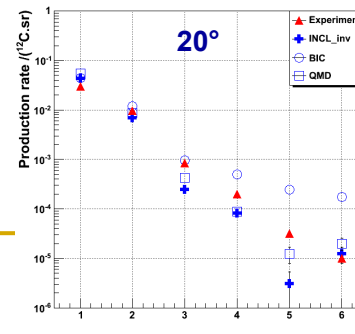
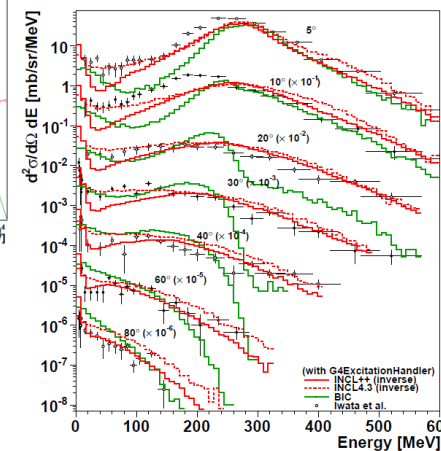
Excitation functions



$^{12}\text{C}+\text{Al}$ total reaction cross-section



$^{12}\text{C} + ^{12}\text{C}$ 290 MeV/u



^{12}C (95 A MeV) on 5 mm PMMA Charge distributions

Sub task 1.8: Improvement of Intra-Nuclear Cascade models for a better prediction of one-nucleon-removal channel (CEA)

Analysis as a function of the cost for one nucleon removal :

$\Delta C = S_n - S_p$ if a neutron is removed

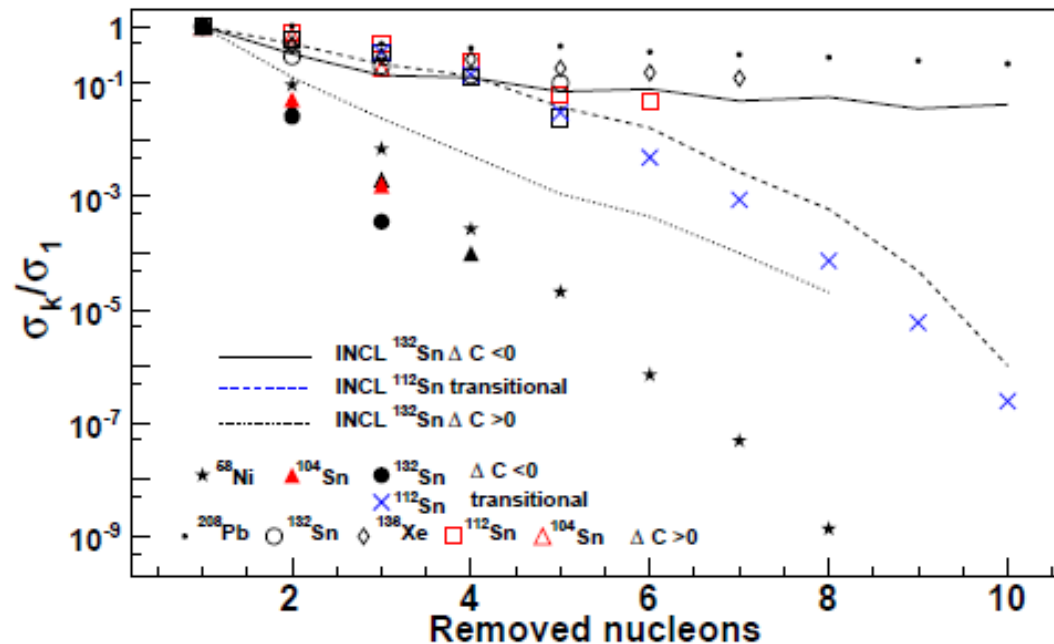
$\Delta C = S_p - S_n$ if a proton is removed

(Coulomb barrier corrected)

→ universal behaviour depending only on $\Delta C < 0$ or > 0

→ Evaporation always lead to the removal of the cheapest species

Experiment RIKEN-RIBF ^{104}Sn and ^{112}Sn on C and H targets at 174 and 191 MeV/nucleon



From Audirac et al., submitted to publication

INCL4 (and other INC models) fails to reproduce the removal of the most bound nuclear species due to a too low excitation energy associated with the removal of one nucleon in the cascade stage: work in progress to find a remedy

Sub-task 1.2: Development of an event generator for heavy-ion induced reactions (GSI)

Latest improvements in the de-excitation code ABLA:

1. Implementation of a new analytical parameterization of the barrier for the emission of LCPs and IMFs and its position, according to W.W. Qu et al., NPA 868 (2011) 1.
 2. Inclusion of ${}^6\text{He}$ as evaporative LCP in addition to ${}^{1,2,3}\text{H}$ and ${}^{3,4}\text{He}$.
 3. Possibility to use experimental ground-state masses.
 4. Work has also been done in the modeling of low-energy fission. The tunneling through the fission barrier is included in an analytical way, which is an important technical achievement because it reduces the computing time.
-

Multiplicities of evaporated n and LCPs

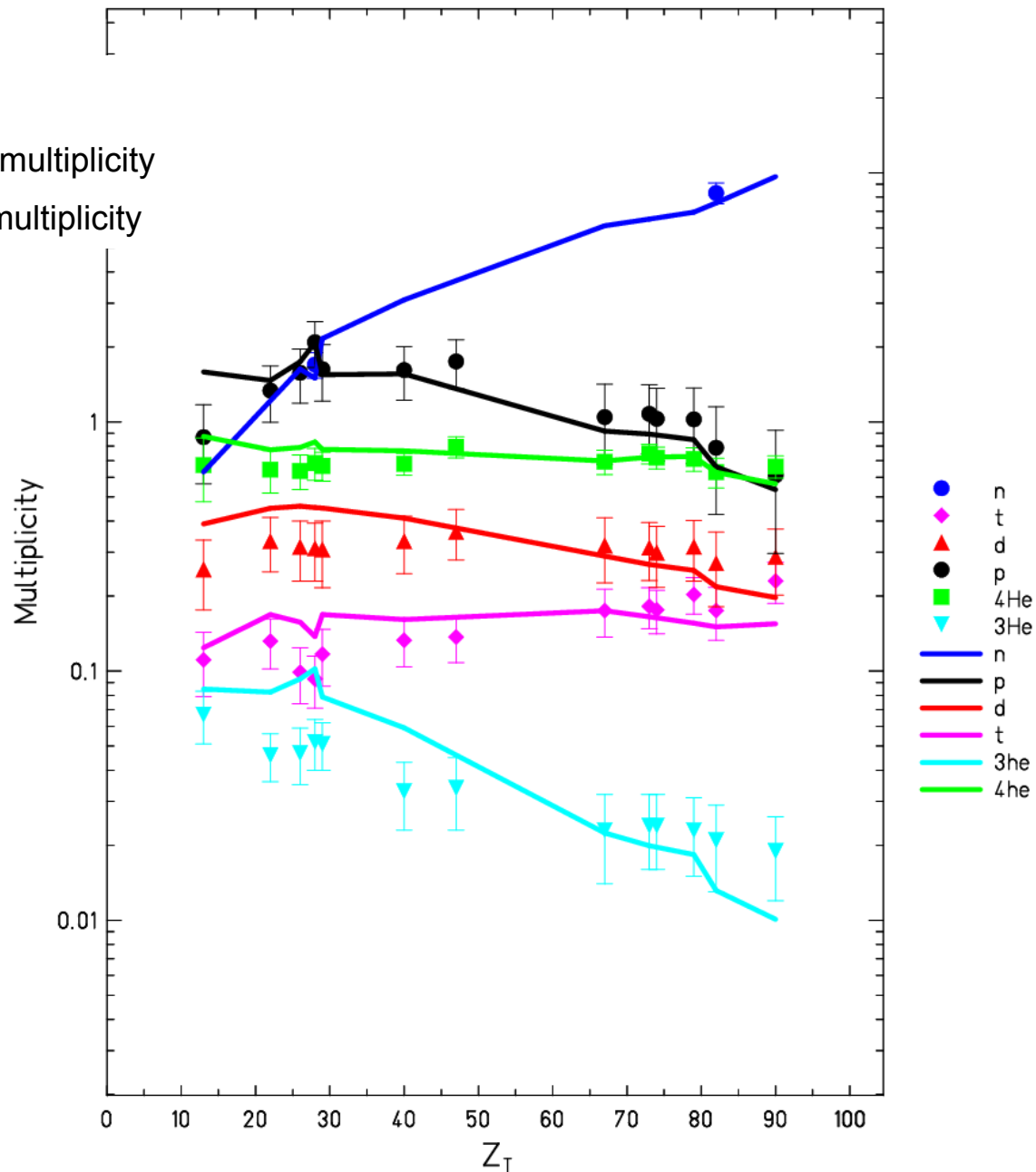
1200 MeV p + target

Average evaporated neutron (2-20 MeV) multiplicity

Average evaporated LCPs (0-100 MeV) multiplicity

Points – experimental data taken from the Spallation benchmark database

Lines – ABLA's predictions



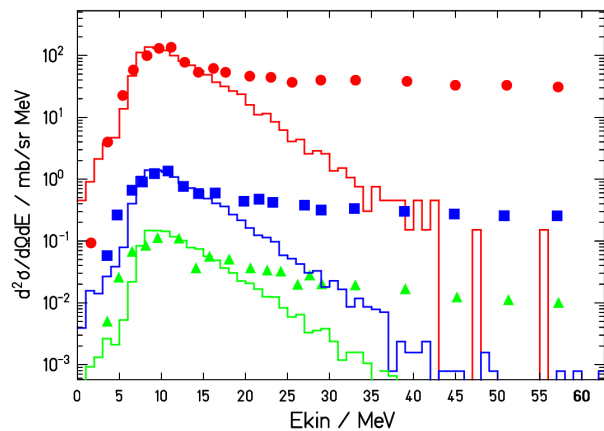
Double differential cross sections for LCPs

Only evaporative part of calculated spectra (ABLA) is shown

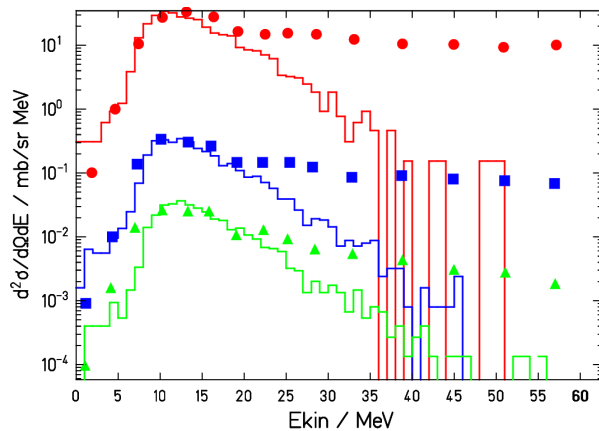
1200 MeV p + ^{181}Ta

Data from COSY, C.-M. Herbach et al., Nucl. Phys. A 765 (2006) 426

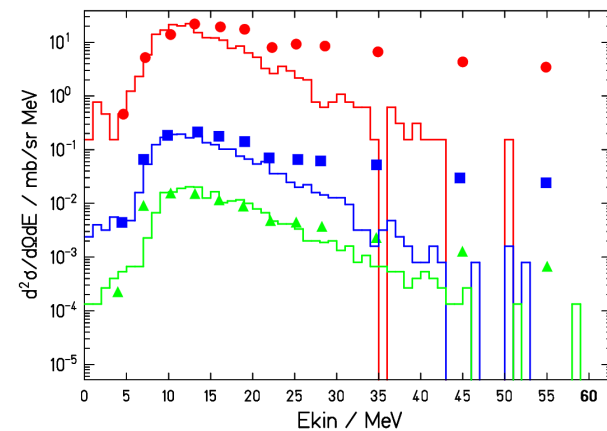
Proton



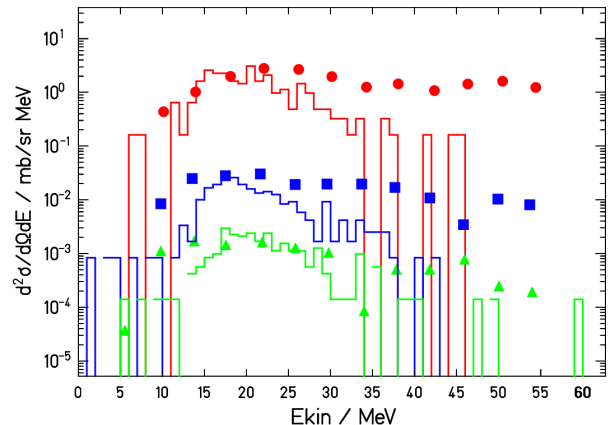
Deuteron



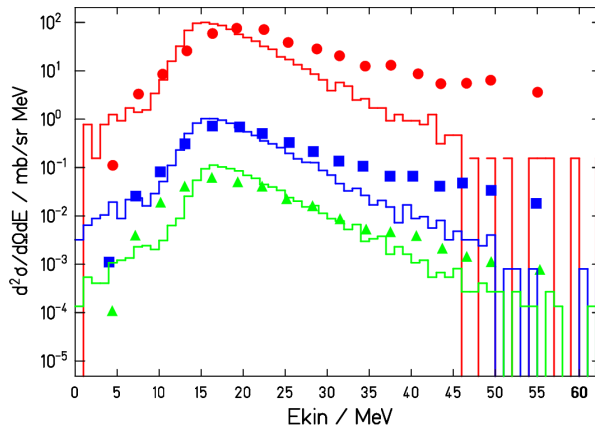
Triton



^3He



Alpha



Scaling factors for displaying:

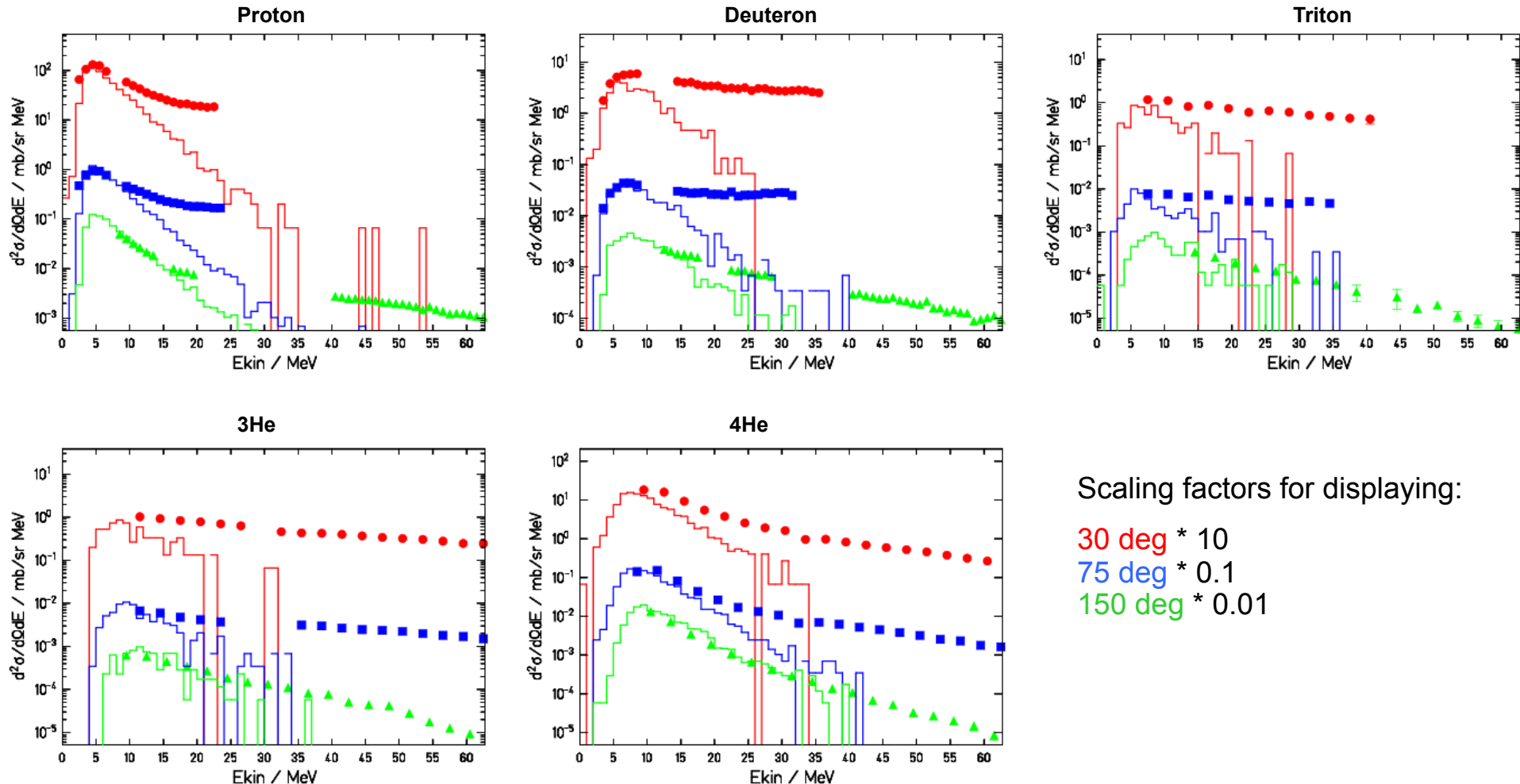
30 deg * 10
75 deg * 0.1
150 deg * 0.01

Double differential cross sections for LCPs

Only evaporative part of calculated spectra (ABLA) is shown

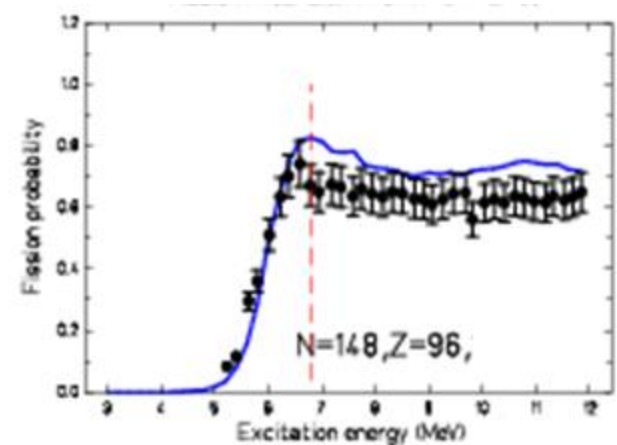
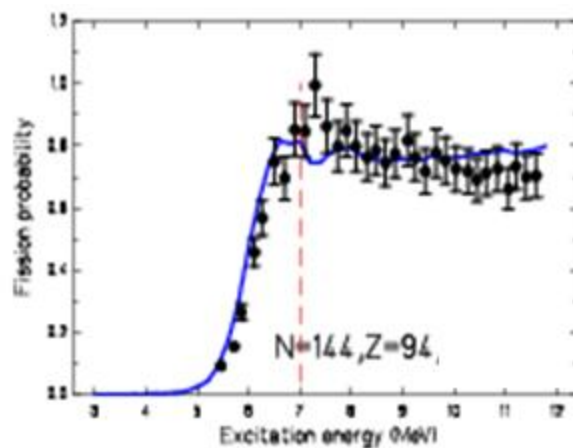
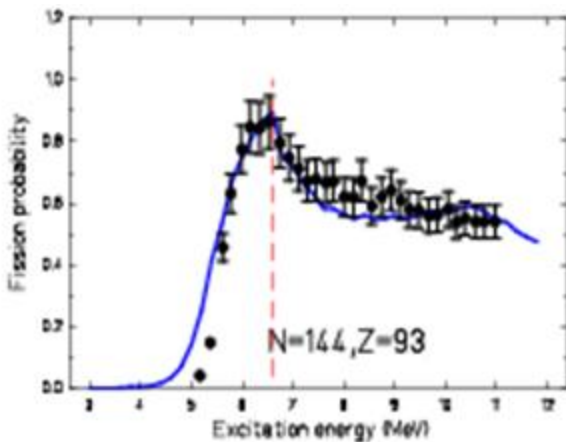
175 MeV p + ^{58}Ni

Data from COSY, A.Budzanowski et al., Phys. Rev. C80 (2009) 054604.

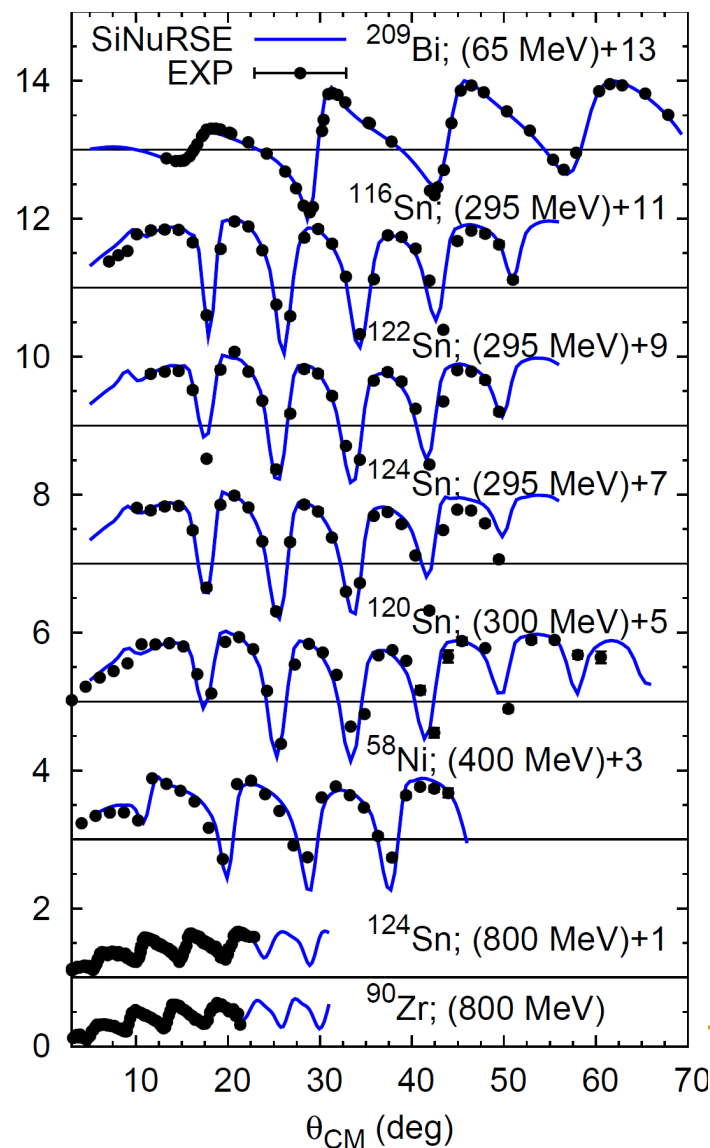
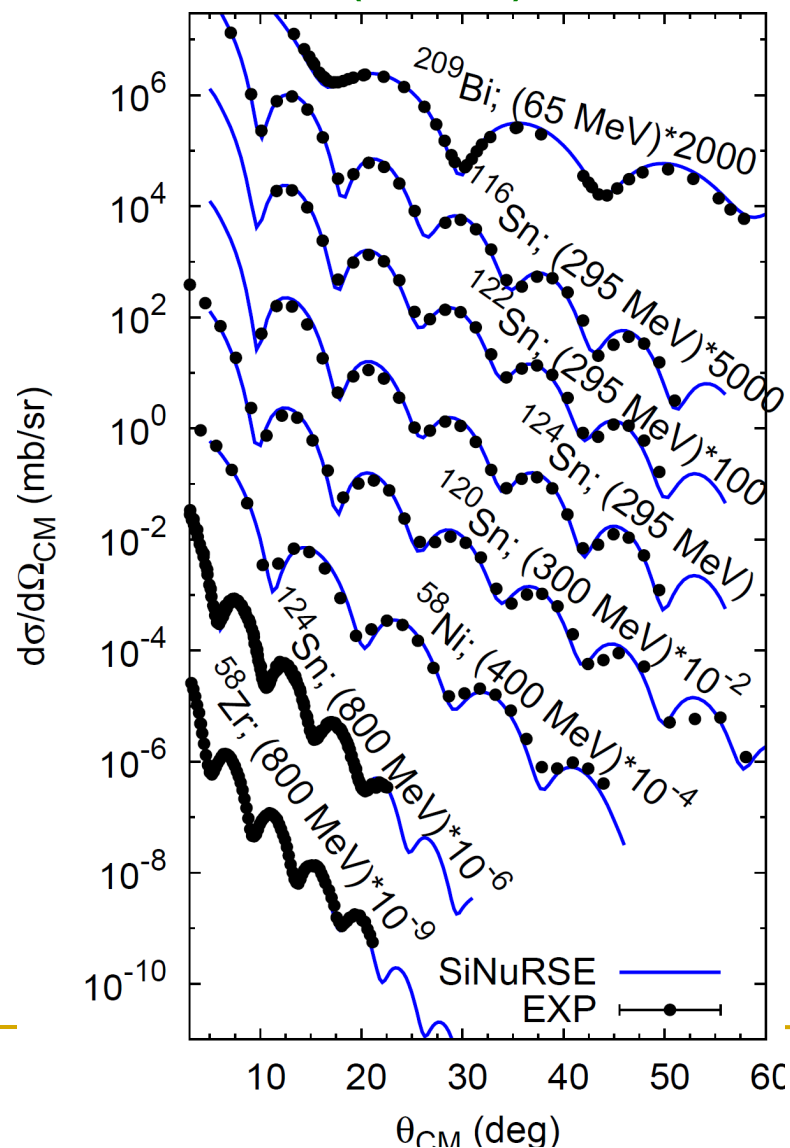


Fission excitation functions

- Black points – experimental data (A. Gavron et al, Phys. Rev. C13 (1976) 2374)
- Blue lines – ABLA07 predictions



Sub-task 1.3: Development of an event generator for elastic proton-nucleus cross-sections and p-n reactions with focus on exotic nuclei (UCM)



Sub-tasks 1.5 and 1.6: Development of a gamma ray event Generator for neutron capture electromagnetic cascades & Development of a Software tool which allows the use in GEANT4 of cross sections from correct (neutron and ions) reaction data bases for low-energy reactions (CIEMAT).

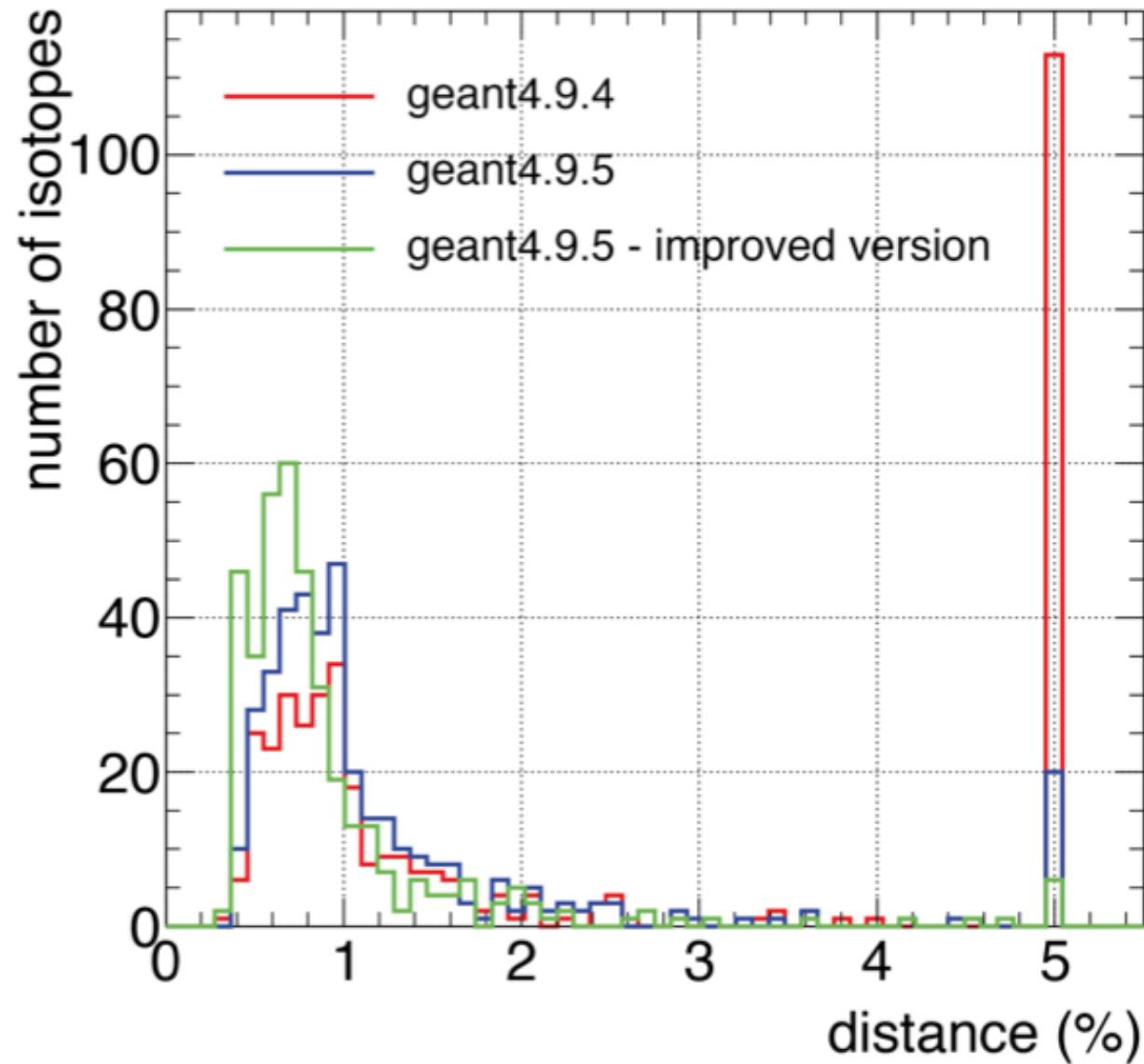
- Eight different ENDF libraries have been translated into the GEANT4 format.
 - The libraries have been reprocessed with the PREPRO libraries.
 - A computer code has been developed to perform the translation into G4NDL.
- Several (important) GEANT4 bugs have been found and corrected (inelastic reactions, distribution probability classes, ...).
- New GEANT4 code has been developed for generating capture photons in MF=6 format.
- In the translation process:
 - Some bugs in the processed ENDF files have been found as well.
 - The number of Legendre polynomials has been restricted up to 30 (instead of 64).
 - Some angular distributions have been assumed to be isotropic in the CMS, when that information is required by GEANT4 and it is missing in the ENDF files.
 - Information concerning recoil nuclei hasn't been translated.
 - Some fission neutrons described in MF=6 format have been translated into MF=4,5 format.
- A validation procedure has been established and carried out for the ENDFB-VII library, by comparing GEANT4 with MCNPX. The validation requires ~1200 simulations for each library (4 per isotope) = 2 weeks of CPU at CIEMAT's supercomputer EULER.

Sub-tasks 1.5 and 1.6: Development of a gamma ray event Generator for neutron capture electromagnetic cascades & Development of a Software tool which allows the use in GEANT4 of cross sections from correct (neutron and ions) reaction data bases for low-energy reactions (CIEMAT).

The following ENDF-6 format libraries have been translated into the GEANT4 format:

- ENDF-VII.0 (USA) – 385 isotopes – ENDF-VI.8 (USA) – 317 isotopes – JEFF-3.0 (EU) – 373 isotopes
 - JEFF-3.1 (EU) – 334 isotopes
 - JENDL-4.0 (Japan) – 400 isotopes
 - JENDL-3.3 (Japan) – 332 isotopes
 - BROND-2.2 (Russia) – 120 isotopes
 - CENDL-3.1 (China) – 239 isotopes
 - G4NDL-3.14 (GEANT4) – 181 isotopes (only ^{235}U and ^{238}U) – TENDL 2009, 2010, 2011, 2012
-

Sub-tasks 1.5 and 1.6



All the new libraries are publicly available at the
IAEA Nuclear Data website (<http://www-nds.iaea.org/geant4/>)

International Atomic Energy Agency
Nuclear Data Services
Provided by the Nuclear Data Section

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Hot Topics » ENDF/B-VII.1 • JENDL-4 • TENDL-2010 • IBANDL News » 2012/01/16 ENDF/B-VII.1 - U.S. Evaluated Nuclear Data Library, issued in December 2011

Quick Links
ADS-Lib
Atomic Mass Data Centre
CINDA
Charged particle reference cross section
DROSG-2000
EMPIRE-II
ENDF Archive
ENDF Retrieval
ENDF-6 Codes
ENDF-6 Format
ENDVER
ENSDF
ENSDF ASCII Files
ENSDF programs
EXFOR
FENDL-2.1
Fission Yields
GANDR
IBANDL
INDL/TSL
IRDF-2002

New evaluated neutron cross section libraries for the GEANT4 code

Emilio Mendoza and Daniel Cano-Ott, Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Spain

Geant4 is a general purpose toolkit for the simulation of the passage of particles through matter. Primary focus of Geant4 was on preparation of experiments for CERN Large Hadron Collider. Other areas of application are growing and include high energy, nuclear and accelerator physics, studies in hadronic therapy, tomography, space dosimetry, and others. Geant4 physics includes different models for simulation of interactions of hadrons with nuclei.

The present web page contains selected nuclear data from evaluated data libraries for high precision transport of low energy neutrons.

- Documentation**
Please [READ THE DETAILED INSTRUCTIONS](#) carefully before starting the installation of the new source code and the neutron data libraries. You will be modifying a standard release of the GEANT4 source code and its performance can be affected severely in case of an incorrect installation.
- Source code**

Content
[GEANT4 Home](#)
[Documentation](#)
[Source code](#)
[Libraries](#)

Links
[GEANT4 \(CERN\)](#)

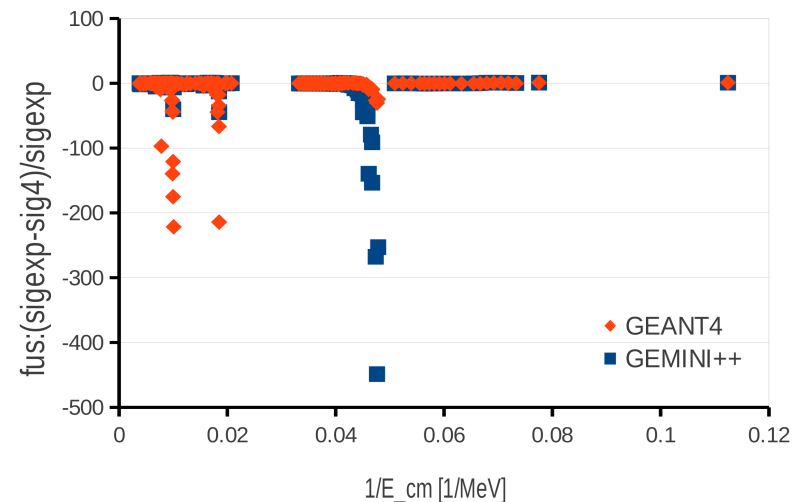
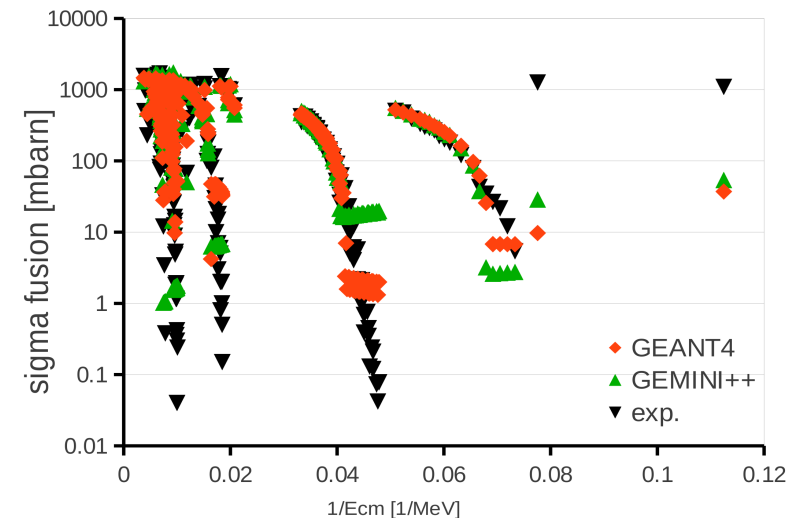
Contacts
[Emilio Mendoza](#)
[Cembranos](#)
[Daniel Cano-Ott](#)
[Roberto Capote](#)

Sub-task 1.7: Development of an event generator for fusion-evaporation reactions (IFJ)

Test of the fusion part

<http://nrv.jinr.ru/nrv/webnrv/fusion/reactions.ph>

reaction	E_{lab} [MeV]	$\sigma_{\text{Exp.}}$ [mb]	σ_{Bass} [mb]	σ_{Geant4} [mb]
6Li+181Ta	74.8	1322	1678	1198
	94.4	1647	1721	847
6Li+208Pb	74.8	1356	1737	1260
	94.4		1801	923
35Cl+27Al	120	1140	1012	1023
	90	637	549	564
35Cl+62Ni	140	980	946	960



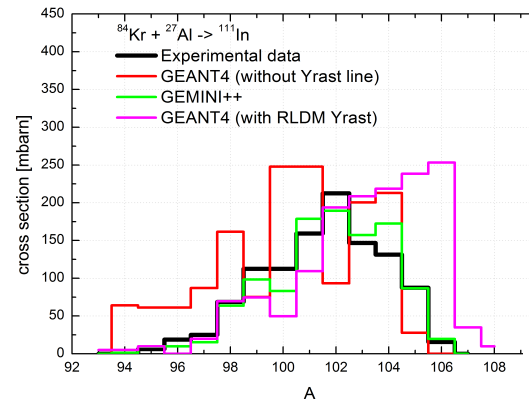
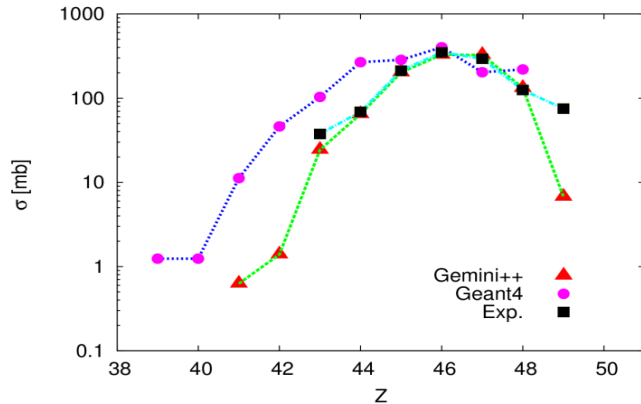
The fusion cross-sections obtained with the new GEANT4 class and with GEMINI++ are compared to existing 250 reactions with different symmetric and asymmetric entrance channels and wide range of excitation energy.

Sub-task 1.7

Test of the evaporation part

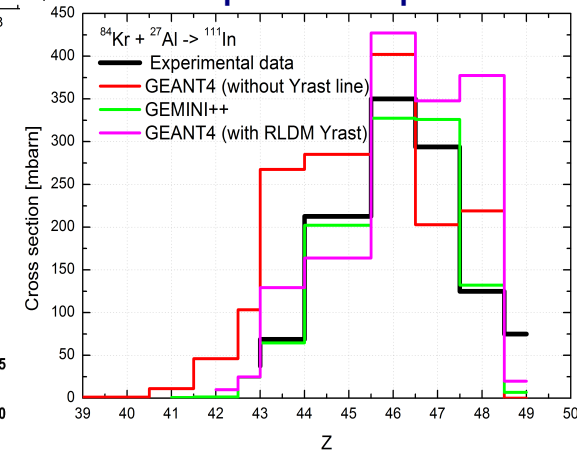
Hauser-Feschbach

Weisskopf



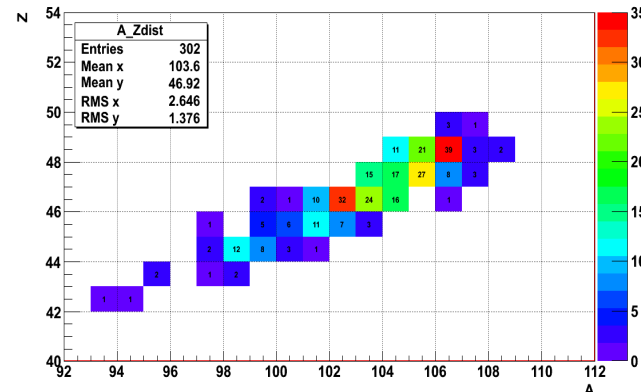
No yrast – too many evaporated particles

Yrast for spherical shape – too little evaporated particles



F. W. Schneider et al. NPA371.493

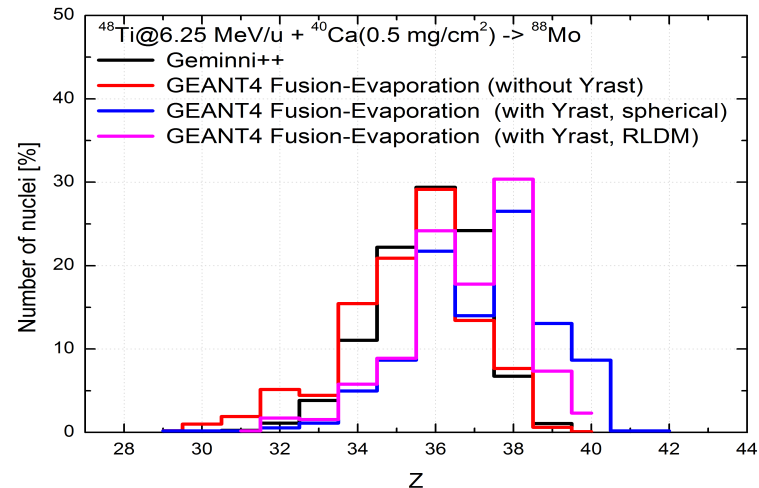
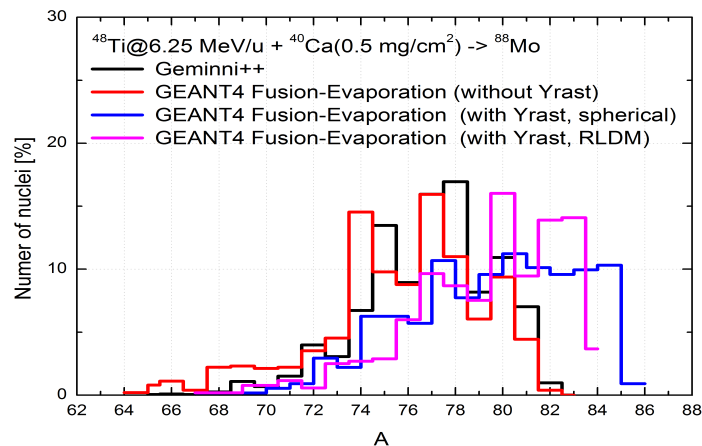
With Weisskopf model,
It was not possible to
reproduce the
experimental charge
distribution



The isotopic distribution
for the results obtained
with the fusion-evaporation
class of GEANT4 with
RLDM yrast line.

Sub-task 1.7

The prediction of the fusion-evaporation GEANT4 class for ^{88}Mo



Summary:

1. The energy loss in the target is taken into account.
2. Reproduction of the fusion cross-section is very good.
3. The Weiskopf model of the evaporation has been tested.
4. The Hauser-Feschbach model was tested without any yrast line and with yrast line for spherical shapes and for the yrast line coming from the RLDM approach.
5. The results have been compared with existing data and the prediction for ^{88}Mo has been compared with state-of-art statistical code GEMINI++.

Subtasks for task 2

- **Subtask 1:** Basic framework structure, code management (USC);
- **Subtask 2:** Parameters database management (RUG);
- **Subtask 3:** Detector integration, quality assessment (IFIN-HH, ISS).

Subtask 2.1: Basic framework structure, code management (USC)

■ **ENSARRoot basic code:** <http://fpsalmon.usc.es/svn/ensarroot/trunk>

- Derived from FAIRRoot, based on ROOT VMC and running G3 and G4.
- Including event display classes for common detectors, explicit ion support (generators, display info, ...), analysis macros, examples, ...

■ **Code Maintenance and management:**

- A set of code conventions, included in the framework documentation.
- A set of macros and routines for the CDash/CTest/CMake automatic code checking and for the Quality Assessment, also in the documentation.
- A Howto about using Cdash/CTest checking and the included examples.

■ **Code repository and www maintenance:**

- A www page: <http://igfae.usc.es/~sinurse/> or, directly linked in the ENSAR JRA: <http://www.ensarfp7.eu/what-is-ensar/activities/jra>

STATUS: preliminary macros, code repository and www pages working.

STILL TO DO: complete the documentation, in particular how-to's for automatic maintenance and QA.

~~DELIVERABLES: The ENSARRoot code. Complete documentation including tutorials. The www pages themselves and documents repository.~~

Subtask 2.1: Basic framework structure, code management (USC)

The image displays the SiNuRSE website and a Subversion repository browser. The website, titled "Simulations for Nuclear Reactions and Structure in Europe", provides information about the project and its collaboration partners. The repository browser shows the structure of the "ensarroot/trunk" repository, listing various subdirectories and files.

SiNuRSE Website Content:

- Navigation:** Home, The Project, The Collaboration, Documents, Downloads, How-To's, Links.
- Left Sidebar:** News, Meetings, Milestones, Deliverables, Time Schedule.
- Main Content:**
 - List of the involved universities and research centers in SiNuRSE:**
 - GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, Germany ([GSI](#)): M.V. Ricciardi
 - Kernfysisch Versnellend Instituut, University of Groningen, The Netherlands ([RUG-KVI](#)): N. Kalantar, M. Babai, J. Messchendorp
 - French Atomic Energy Commission at Saclay, France ([CEA-Saclay](#)): S. Leray, D. Mancusi

Subversion Repository Browser Content:

Repository: repos: ensarroot/trunk

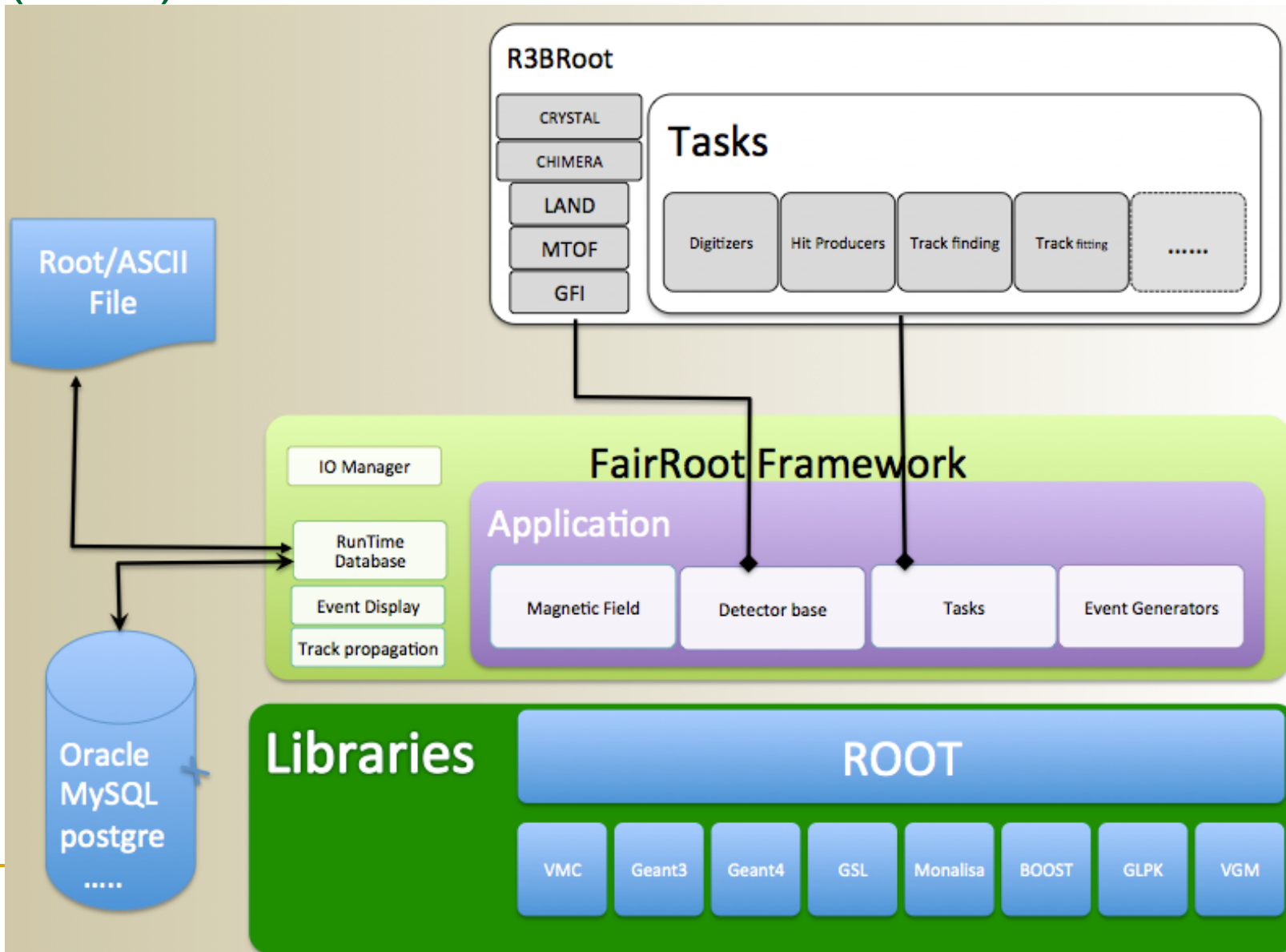
URL: fpsalmon.usc.es/svn/ensarroot/trunk/

Navigation: home, up, folder history, refresh

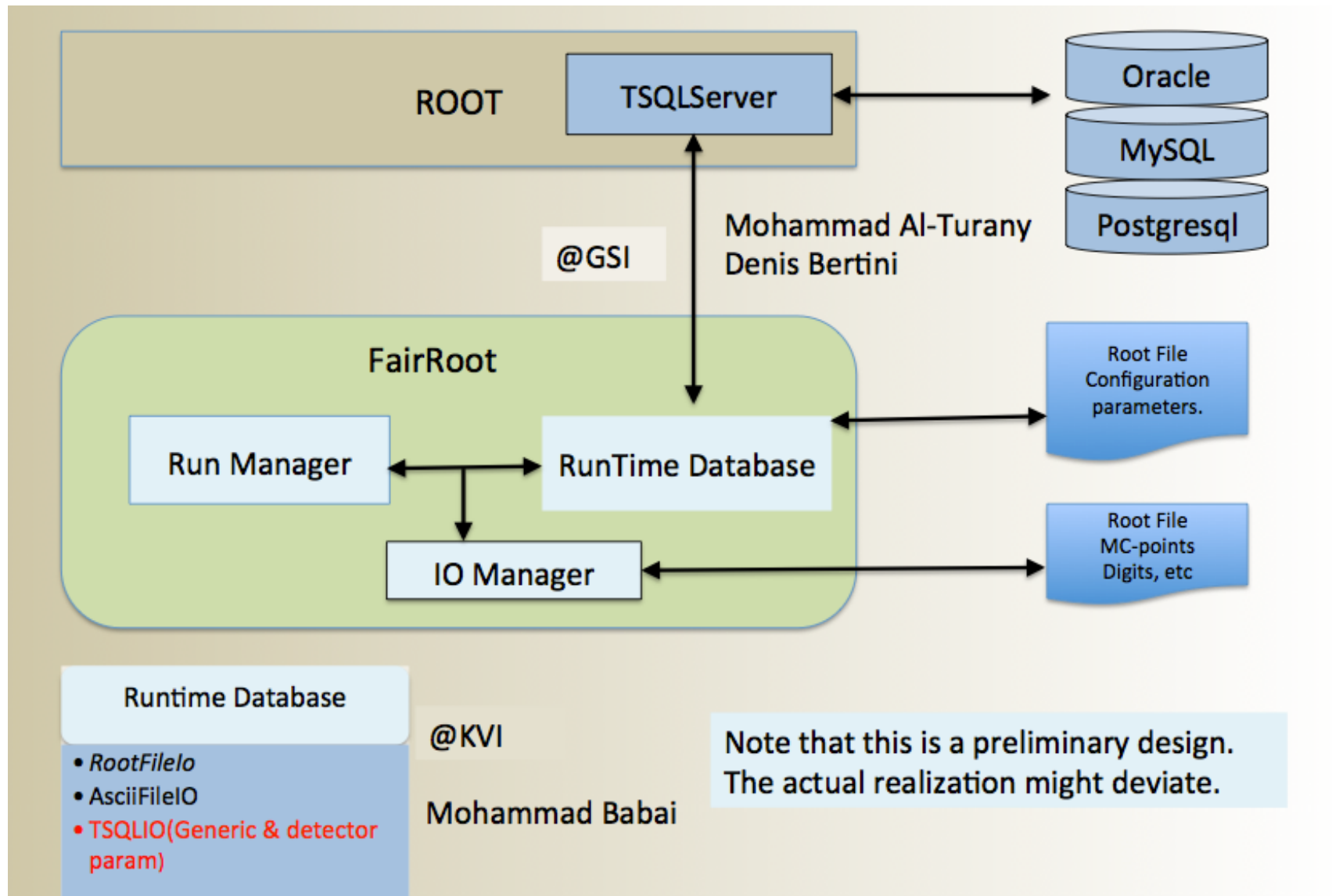
Current View: trunk

Item	open	view history
ensarbase	open	view history
ensardata	open	view history
ensarevtdisplay	open	view history
ensargen	open	view history
gconfig	open	view history
macros	open	view history
mcstack	open	view history
mydet	open	view history
plists	open	view history
CMakeLists.txt	open	view history
CTestConfig.cmake	open	view history
CTestCustom.cmake	open	view history
EnsarRoot_test.cmake	open	view history

Subtask 2.2: Parameters database management (RUG)



Subtask 2.2: Parameters database management (RUG)



Subtask 2.3: Detector integration, quality assessment (IFIN-HH, ISS)

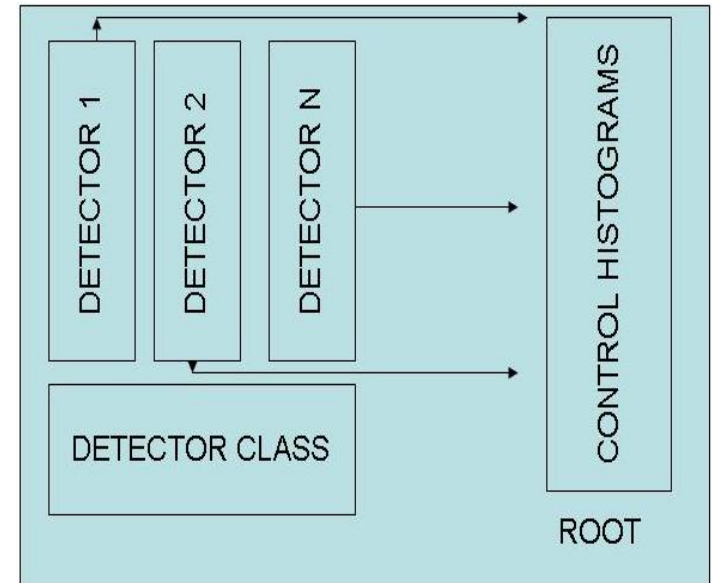
1. The geometry of the detector is implemented directly in the framework based on the TGeo geometry definitions using `EnsarDetector::ConstructGeometry()`;
2. Already implemented two type of template detectors:
 - Template scintillator detector: 200 x 20 x 5 cm of polyvinyltoluene scintillator material;
 - Template silicon detector: 1 x 1 x 0.01 cm of silicon material
3. Documenting of the corresponding classes (*EnsarScintillatorDetector1.cxx*, *EnsarScintillatorDetector1_ContFact.cxx*, *EnsarScintillatorDetector1_Geo.cxx*, *EnsarScintillatorDetector1_GeoPar.cxx*, *EnsarScintillatorDetector1_Point.cxx*, same for silicon detector etc.);

Subtask 2.3: Detector integration, quality assessment (IFIN-HH, ISS)

The Quality Monitoring (QM) structure

The QM is performed in three steps:

1. For each detector class build quality control histograms classes (a template for a scintillator detector in this case). At this step QM data objects characterizing detector data-taking are built.
2. At the second step QM data objects for a given level and a given detector are stored controlling a *TList* type class.
3. The last step is building a checking class for the different QM parameters with user defined data.

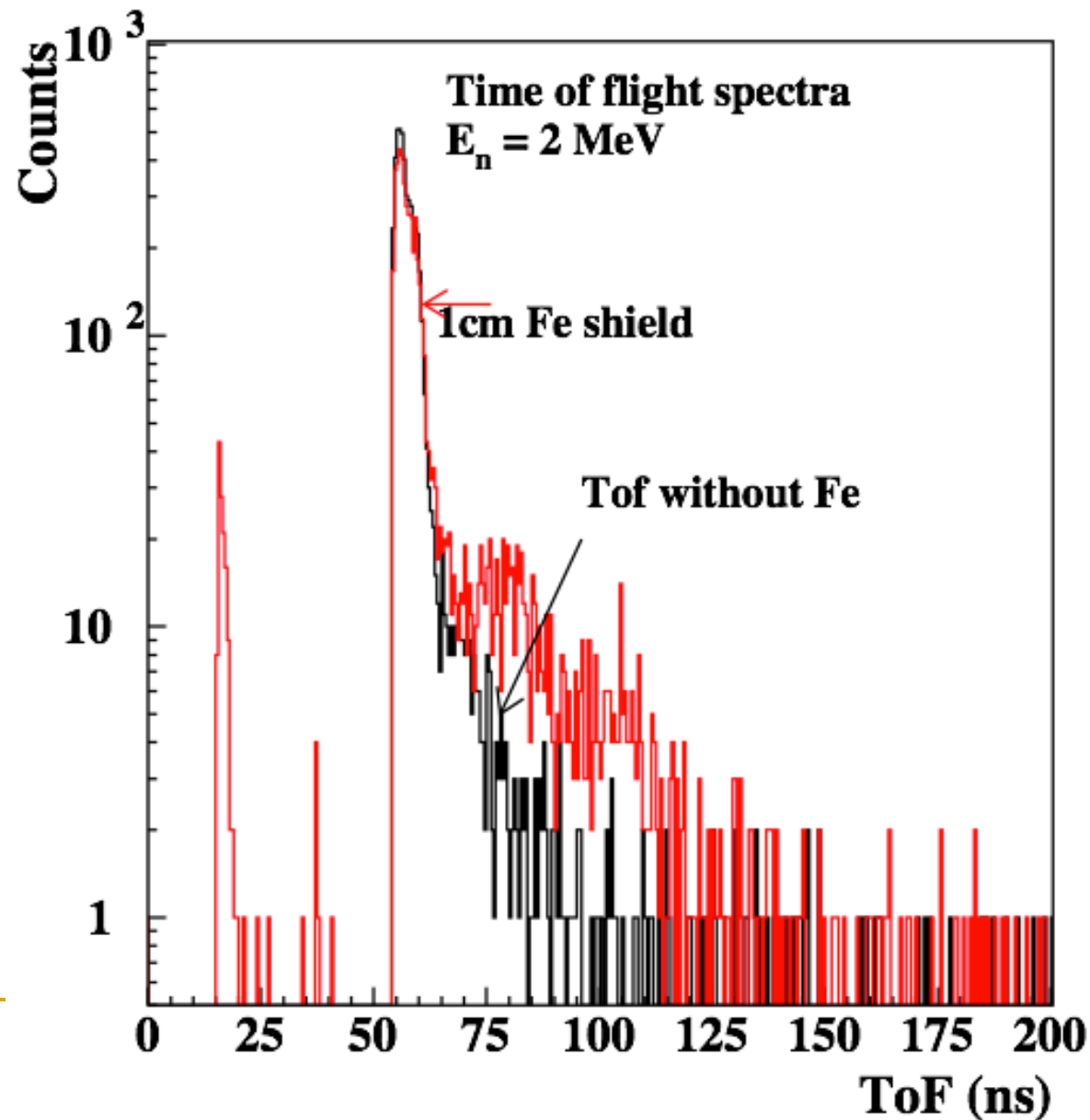


Class structure for detector and monitoring histogram

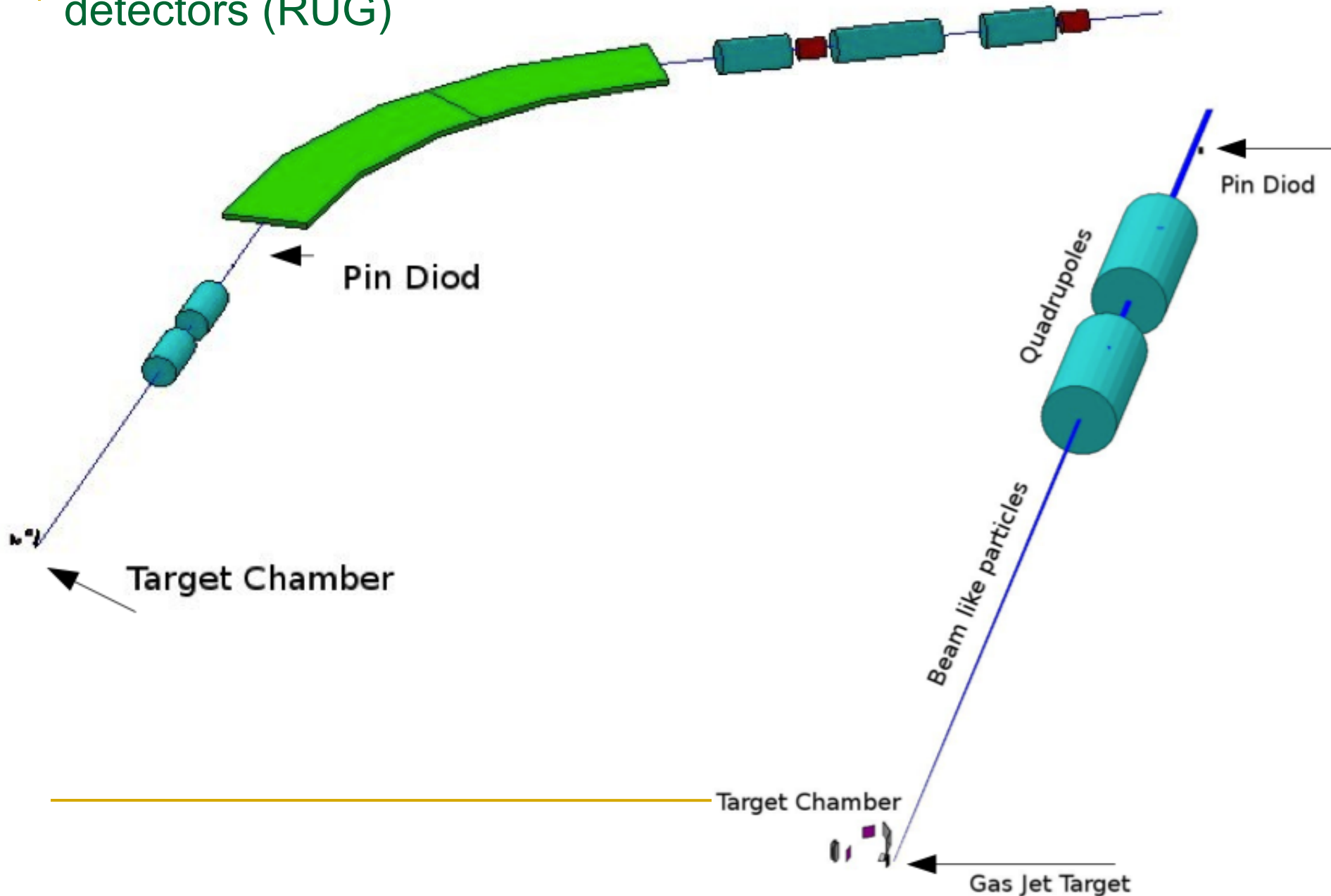
Subtasks for task 3

- **Subtask 1:** The response of neutron detection systems (ATOMKI);
- **Subtask 2:** The response of fast ejectile and heavy-ion detectors (RUG);
- **Subtask 3:** The response of a calorimeter (USC).

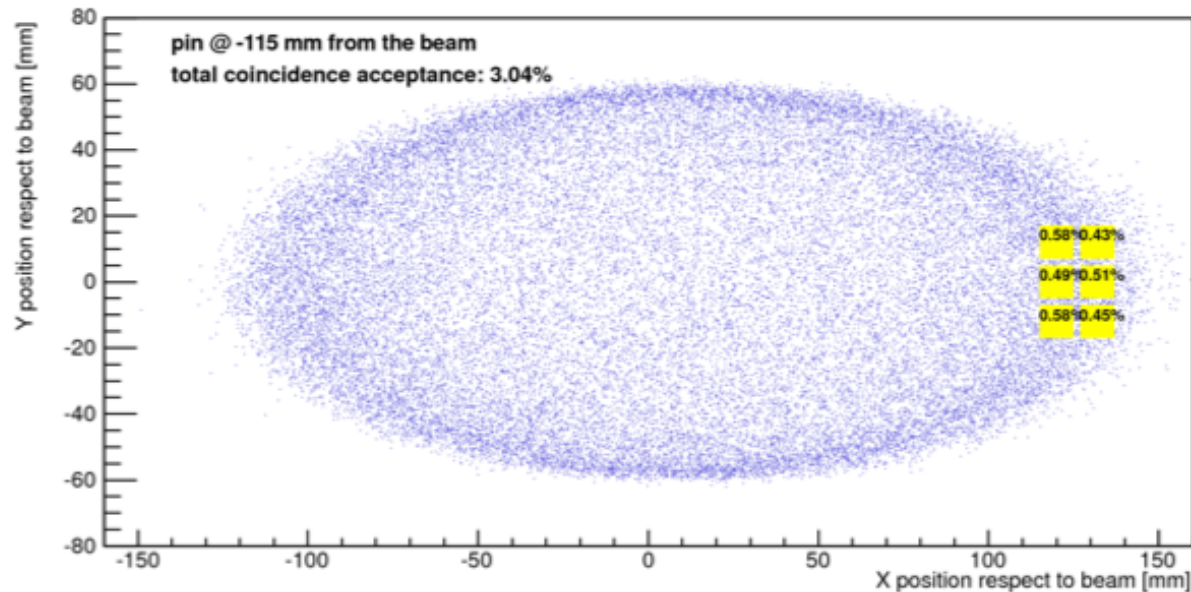
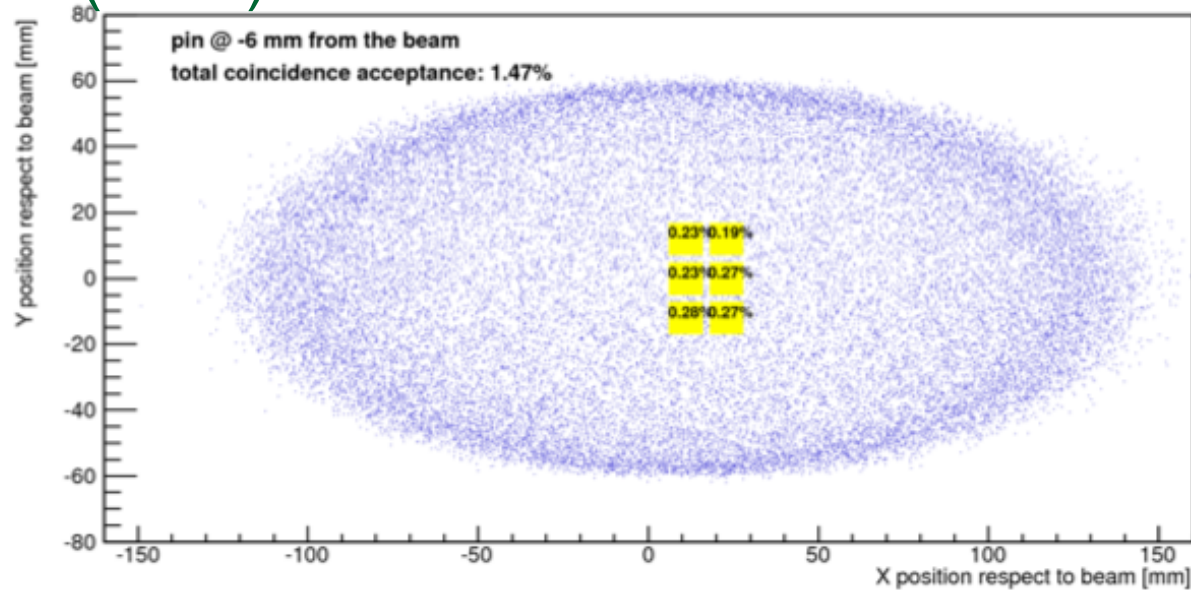
Sub-task 3.1: Response of neutron detection syst. (ATOMKI)



Sub-task 3.2: Response of fast ejectile and heavy-ion detectors (RUG)

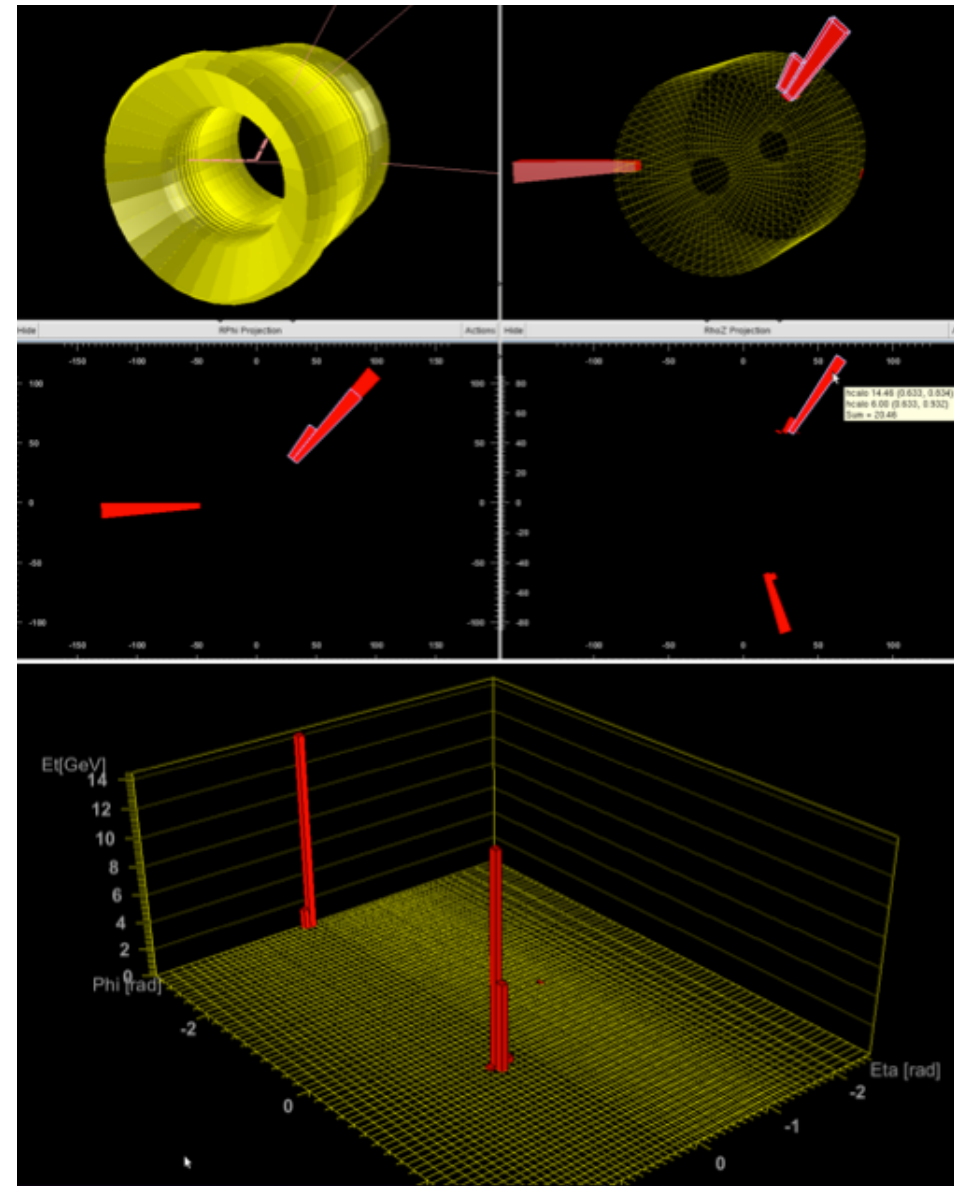


Sub-task 3.2: Response of fast ejectile and heavy-ion detectors (RUG)



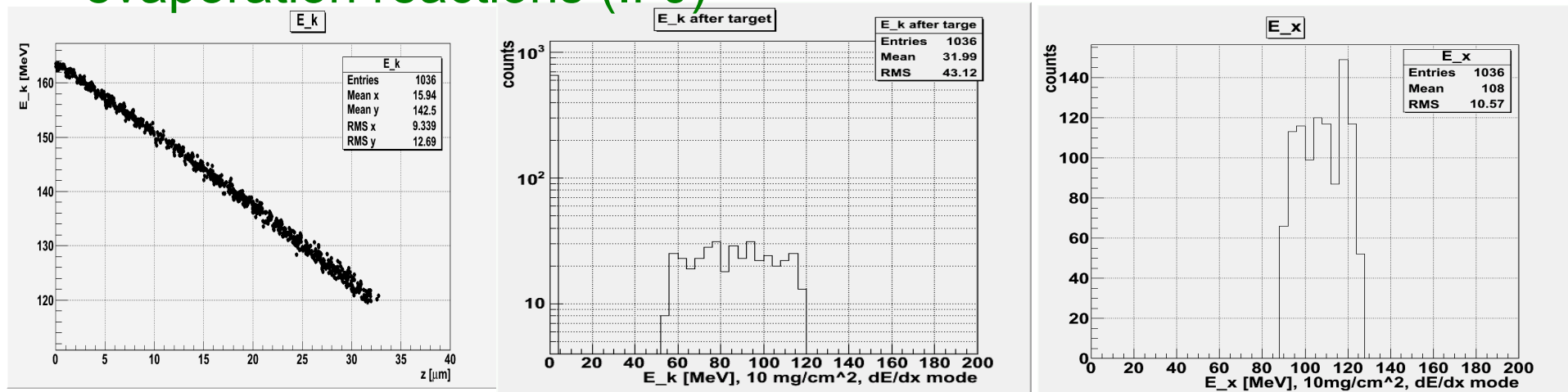
Sub-task 3.3: response of a calorimeter (USC) CALIFA @ R3B

- Development of digitization techniques.
- Geometry. Basics and methods for assemblies exemplifies in a big array construction (CALIFA).
- Basic energy digitization.
- Non-proportionality in light collection: curves for relative light-yield.
- Non-uniformity considered as a global mean effect or from non-uniformity experimental curves.
- Other effects (energy deposition depth, electronics, crystal-shape effect, ...).
- Algorithms for calibration, signal reconstruction and analysis, Addback mechanism.
- Data visualization.

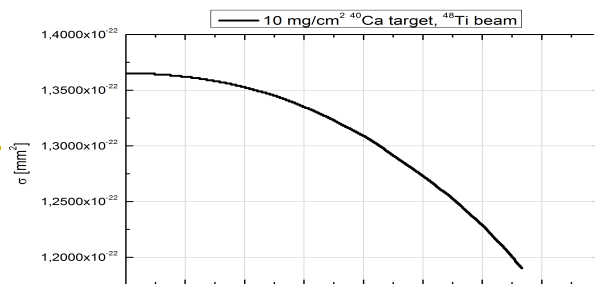
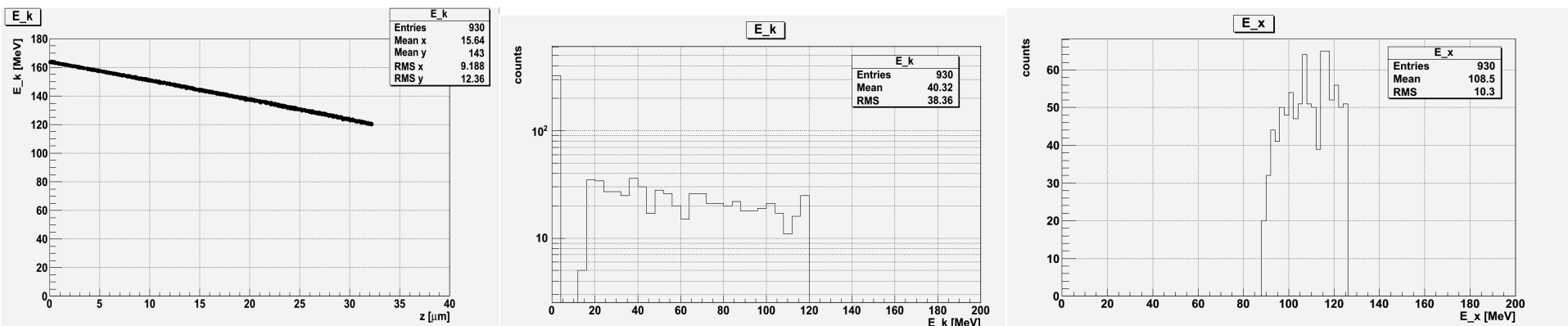


Thank you!

Sub-task 1.7: Development of an event generator for fusion-evaporation reactions (IFJ)



The option with the changing the fusion cross-section by the energy lost in target.



Data containers for unified access and analysis

At this moment we are constructing a complex hierarchy (templates) of classes that would allow the storage of events and their information.

□ There are 3 distinct type of information that one experiment would want to store:

1. *RAW data* – digitized data from detectors with the associated metadata stored in an database;

- custom format of writing data - must provide custom readers for general data retrieval

2. *Event Summary Data (ESD)* – processed raw data that contains all fundamental data, triggers, clusters, individual specific detector data, run and detectors parameters, etc.

- template structure for detector data and signals (tracks, hits, digits collections) ; built by reconstruction - processed for physics data

3. *Analysis Output Data (AOD)* - identified and reconstructed data such as tracks, jets, calorimeter clusters and individual physical information from detectors

- template for tracks, V0s, vertices, jets, clusters, cells, etc...

□ At this moment we are evaluating 2 hierarchies of fundamental types for particle, track, hit, digit, event paradigms:

1. constructed from scratch with inheritance from *TObject*;
2. inheritance from similar structure from ROOT *TParticle* and constructing logically: tracks, hits and the event.

An unified hierarchy of this objects would allow the possibility of parallel processing and analysis, complex schema evolution and future developments of stored data.

We are looking for the most simple structure in order to obtain an product with the simple maintenance required and best performance in analysis.

Event display and detector display examples for different detectors

1. Identification of common elements of event display with monitoring and analysis systems in order to avoid duplication of effort:

- an event display based on ROOT could be easily integrated into EnsarRoot software infrastructure;
- *TEveGeoNode* class provides a simple and natural means of building detector geometry and placing hits within that geometry
- graphical displays already contain much of the basic functionality that we need without much additional coding: *rotate and zoom; click and inspect objects on canvas, display using OpenGL, etc.*
- very poor documentation. ROOT User's Guide useful only for getting started which result in a disproportionate amount of time to implement.

2. Identification of generic graphics classes for detector and event objects; *R3BRoot* was used as testing ground for this task, therefore the classes that we develop includes this terminology:

- ❖ Updating Monte Carlo Root classes such as *R3BEventManager*, *R3BEventManagerEditor*
- ❖ Creating classes *R3BLandEventDisplay* and *R3BLandHitEventDisplay* and testing.

3. Development of components for the construction of stand-alone graphical user interfaces:

- ❖ construct stand-alone Event Viewer for LAND-like detector starting from CALIFA Event Viewer
- ❖ construct stand-alone Detector Display for LAND-like detector starting from EVE Detector Display
- ❖ implement in EnsarROOT the Event Viewer Classes for LAND type detectors
- ❖ working in constructing different examples for different archetypal detectors (scintillators in particular) which should demonstrate the usage of Event Display classes