The Abdus Salam International Centre for Theoretical Physics

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School on Physics, Technology and Applications of Accelerator Driven Systems (ADS)

19 - 30 November 2007

Nuclear Reactions and Related Data Libraries at High Energy.

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Nuclear reactions at high energy

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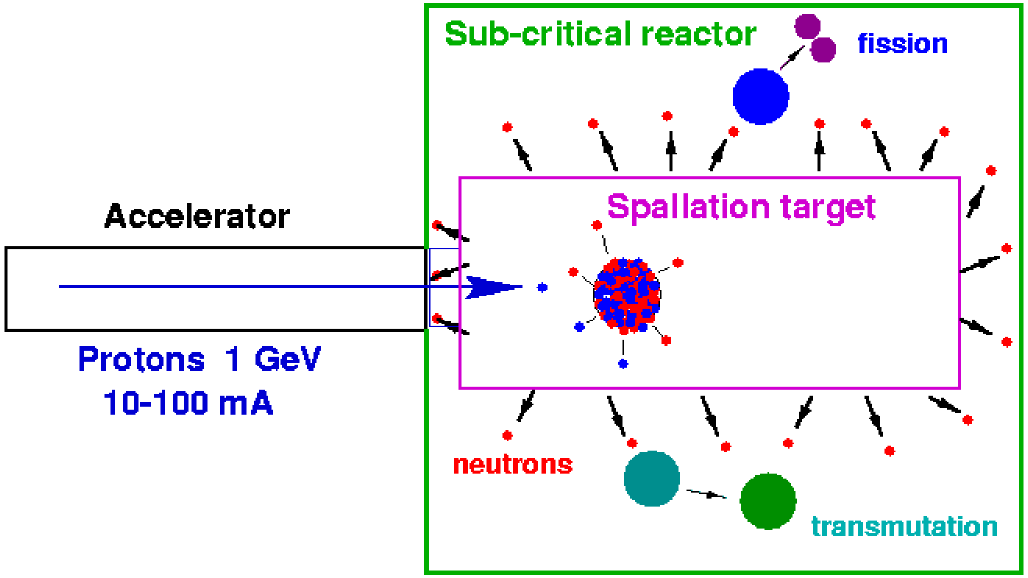
Accelerator-driven sub-critical reactors



A spallation target

- which produces an intense neutron flux though high-energy reactions of protons with a high-Z target

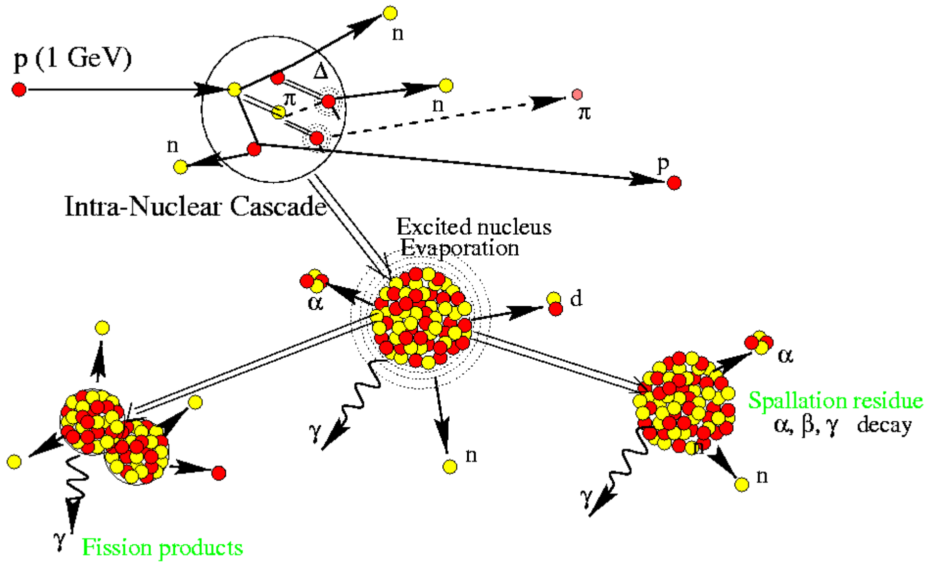
surrounded by a sub-critical reactor

- driven by the external source
- in which transmutation of minor actinides is achieved

Outline

- Introduction
  - ➥ Spallation reactions
- Specific features of high-energy reactions
  - ➥ Neutron production
  - ➥ Residue production
- Spallation reaction modelling
  - ➥ Basic assumptions
  - ➥ The different models (INC and de-excitation)
  - ➥ Comparisons to elementary experimental data: neutrons, light charged particles, residues
  - ➥ Predictions of the simulation codes for applications

Spallation reactions

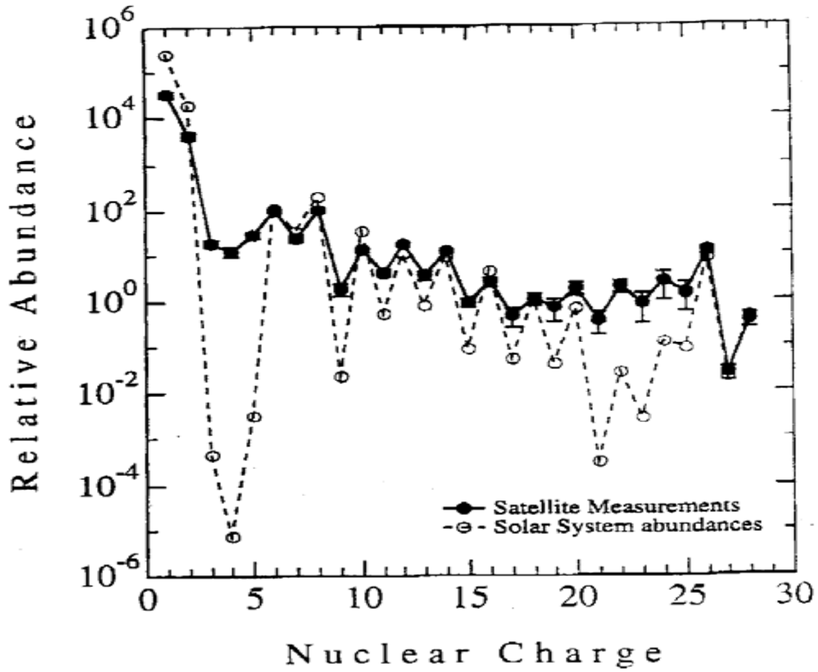


- **Definition:**

  interaction of a high energy (> 100 MeV) light particle with a nucleus leading to emission of light particles (mostly neutrons) and leaving a heavy residue

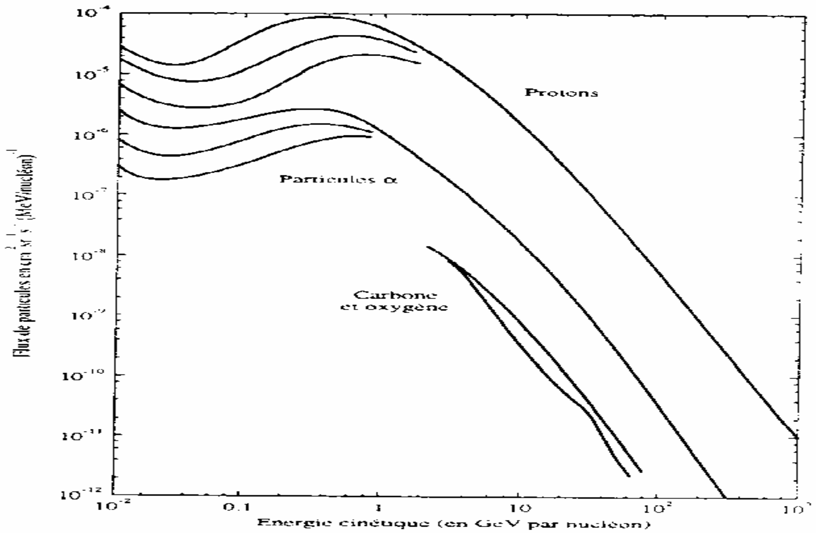
- **History:**
  - **observation of particle cascades in cosmic rays interactions** (G.Rossi, ZP82 (1933) 151)
  - **first accelerators: many nucleons emitted by the target nucleus** (Cunningham, PR72 (1947) 739)
  - **Two step mechanism** (Serber, PR72 (1947) 1114) **intranuclear cascade + de-excitation**

Astrophysics



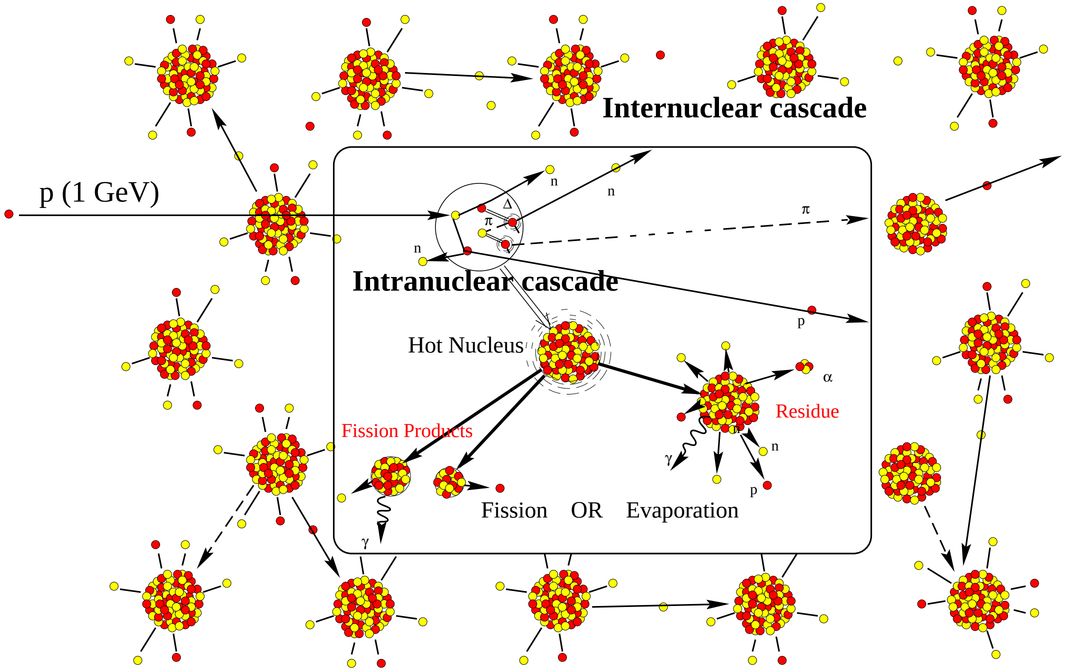
- **Secondary reactions of cosmic rays in interstellar medium (90% of hydrogen)**
  - **explanation of abundance of isotopes**
  - **decide among models for galactic nucleosynthesis**
  - **origin of cosmic rays**
- **Composition of meteorites**

Spallation reactions in space instruments



- **Cosmic ray bombardment of the spacecraft and instruments**
  - ➢ **Radiation damage on electronics**
  - ➢ **Radioprotection of space crew**
  - ➢ **Noise due to secondary neutrons, gammas from spallation residues → ex: INTEGRAL mission devoted to high resolution γ-ray astronomy**

Spallation neutron production

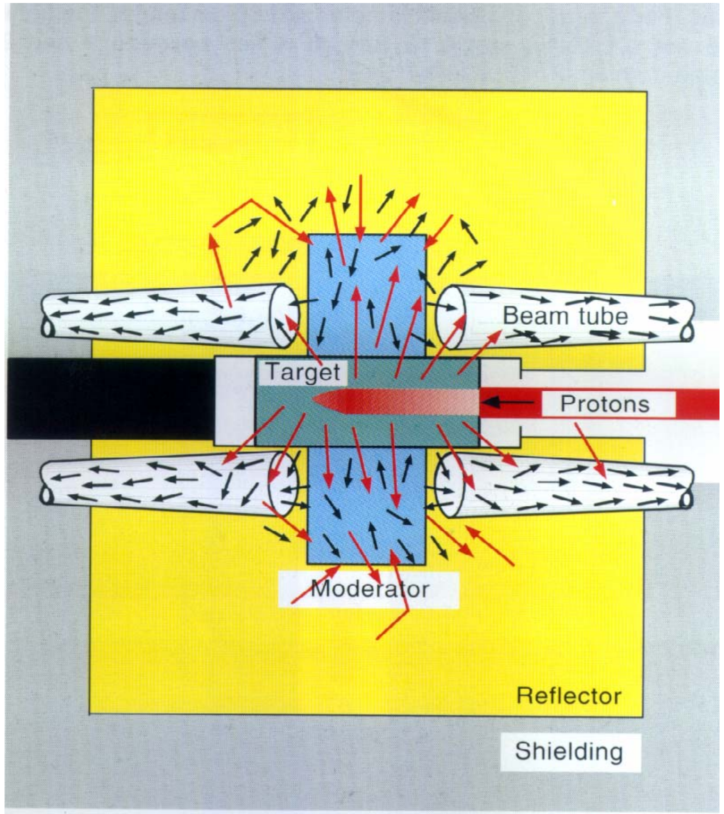


In a thick target:
internuclear cascade

➔ large number of produced neutrons

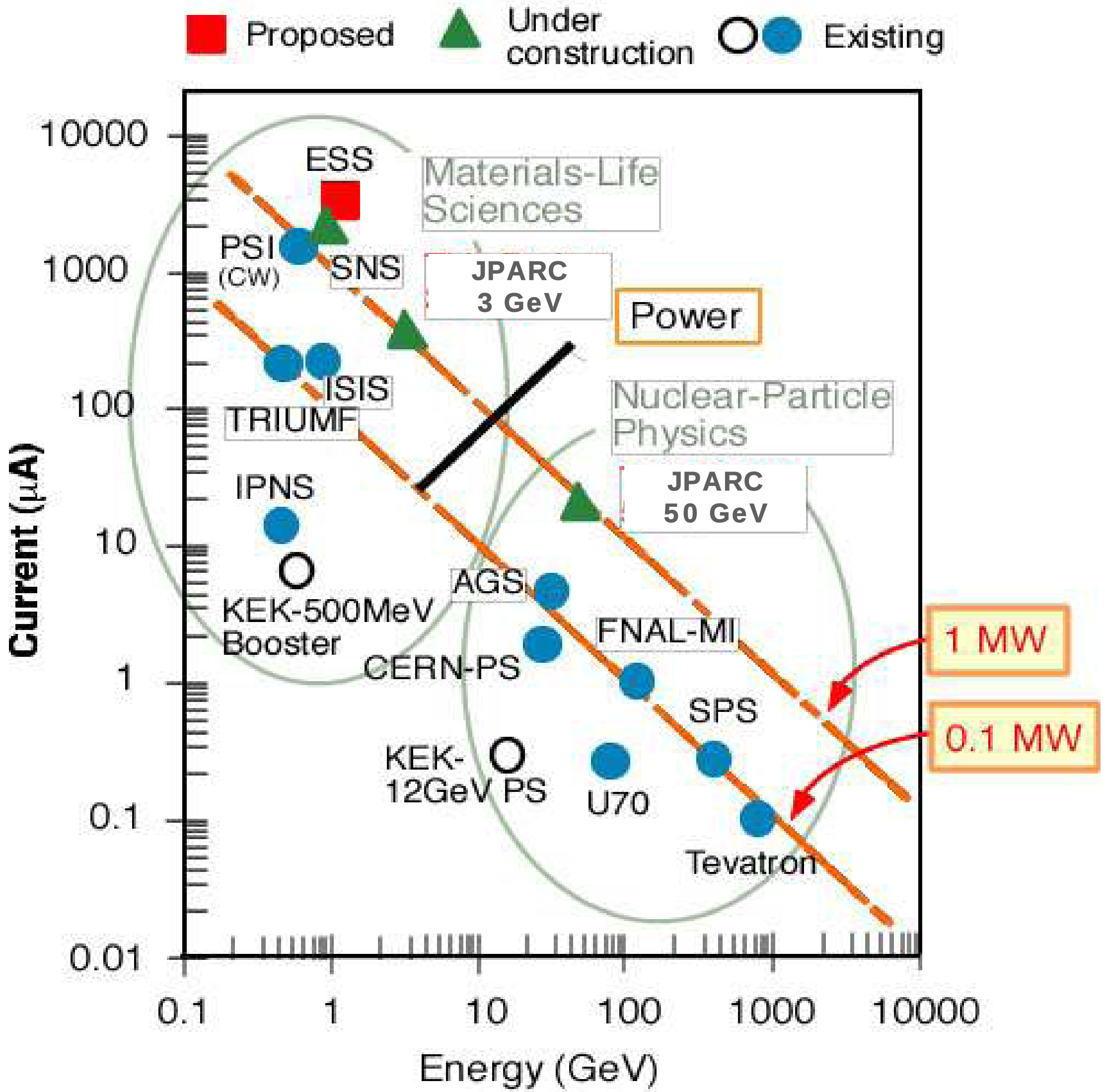
- **In a heavy metal target (Pb, W, Ta, Pb-Bi) around 20 neutrons per incident proton and GeV**
- **Applications:**
  - ↪ **ADS**
  - ↪ **Spallation neutron sources**
  - ↪ **Rare isotope beams (RIB)**

Spallation neutron sources



- **Moderation of spallation neutrons in (heavy) water**
- **Reflectors to direct escaping neutrons into beam tubes**
  - **pulsed sources (ISIS, SNS, JSNS): well-defined time structure, high peak flux**
    - ➔ **tof experiments**
  - **continuous sources (SINQ): high neutron flux in a large volume**
    - ➔ **irradiation experiments, imaging**

Spallation sources



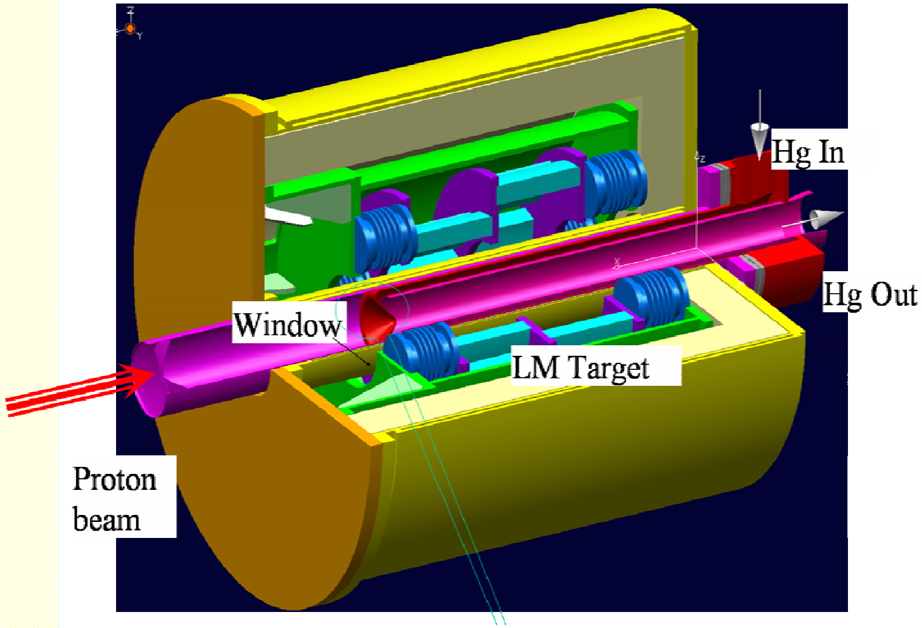
Rare isotope production

- **Direct methods**
  - ISOL p (1 GeV) + A
    - ➔ low energy RIB
  - fragmentation of GeV/A heavy ions
    - ➔ high energy RIB
- **Converter methods**
  - use of produced neutrons to induce fission
    - ➔ low energy RIB
  - use of neutrons to produce
    - ➔isotopes for medicine

Reference Multi MW Target Station

EURISOL Design Study

Hg converter and secondary fission targets



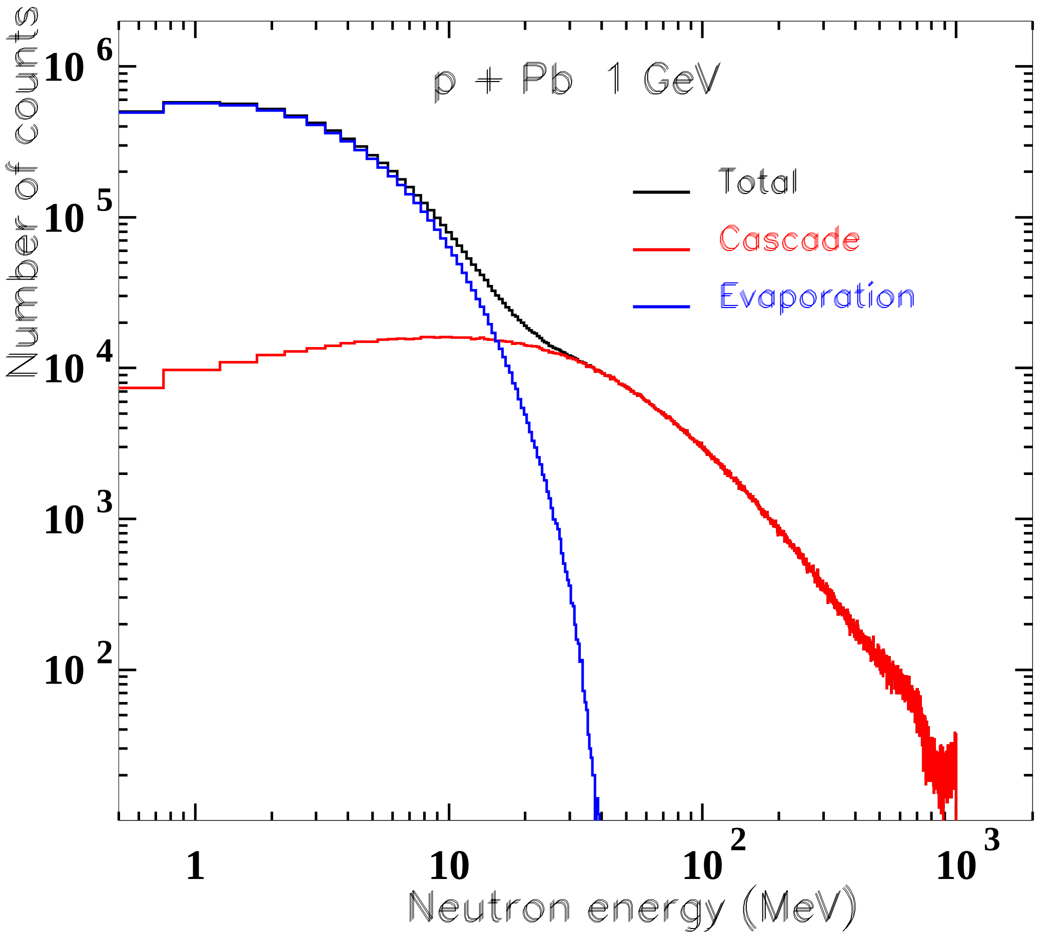
From Y. Kadi, EURISOL week
27-30 November 2006

Interactions in a thin target

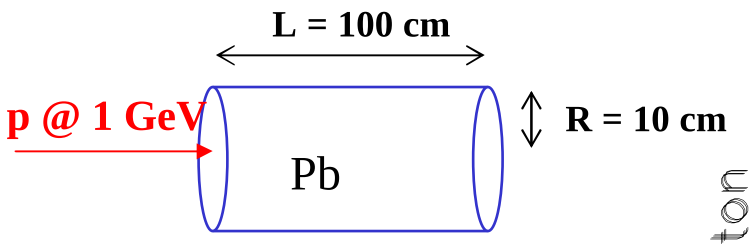
➢~2 neutrons with E>20 MeV (intra-nuclear cascade)

➢~15 neutrons with E<20MeV (evaporation)

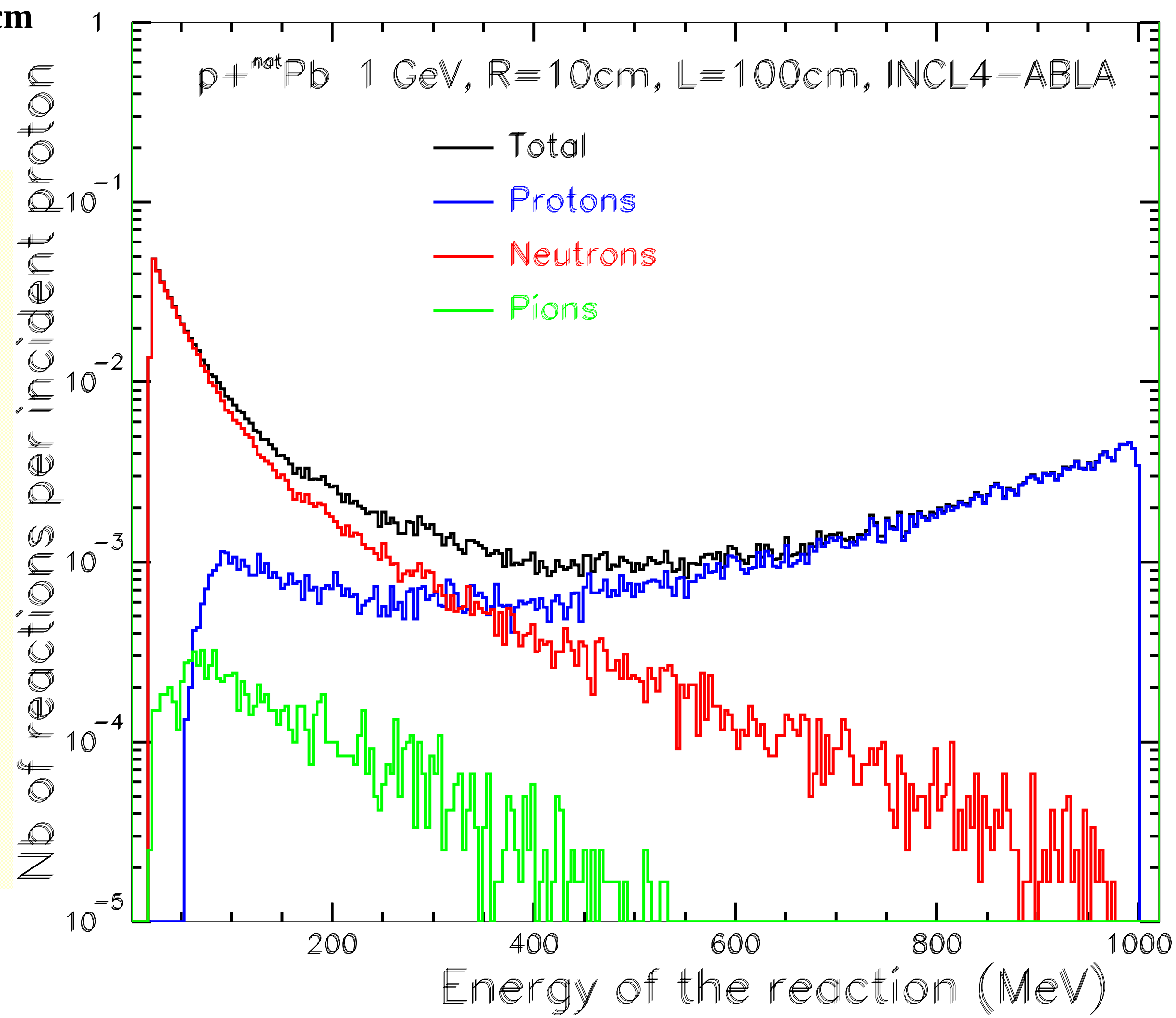
➢ But energy carried out by cascade neutrons = 85% (95% for protons)



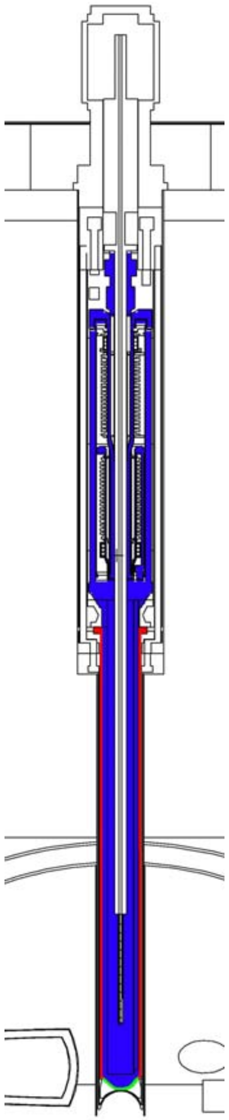
Interactions in a thick target



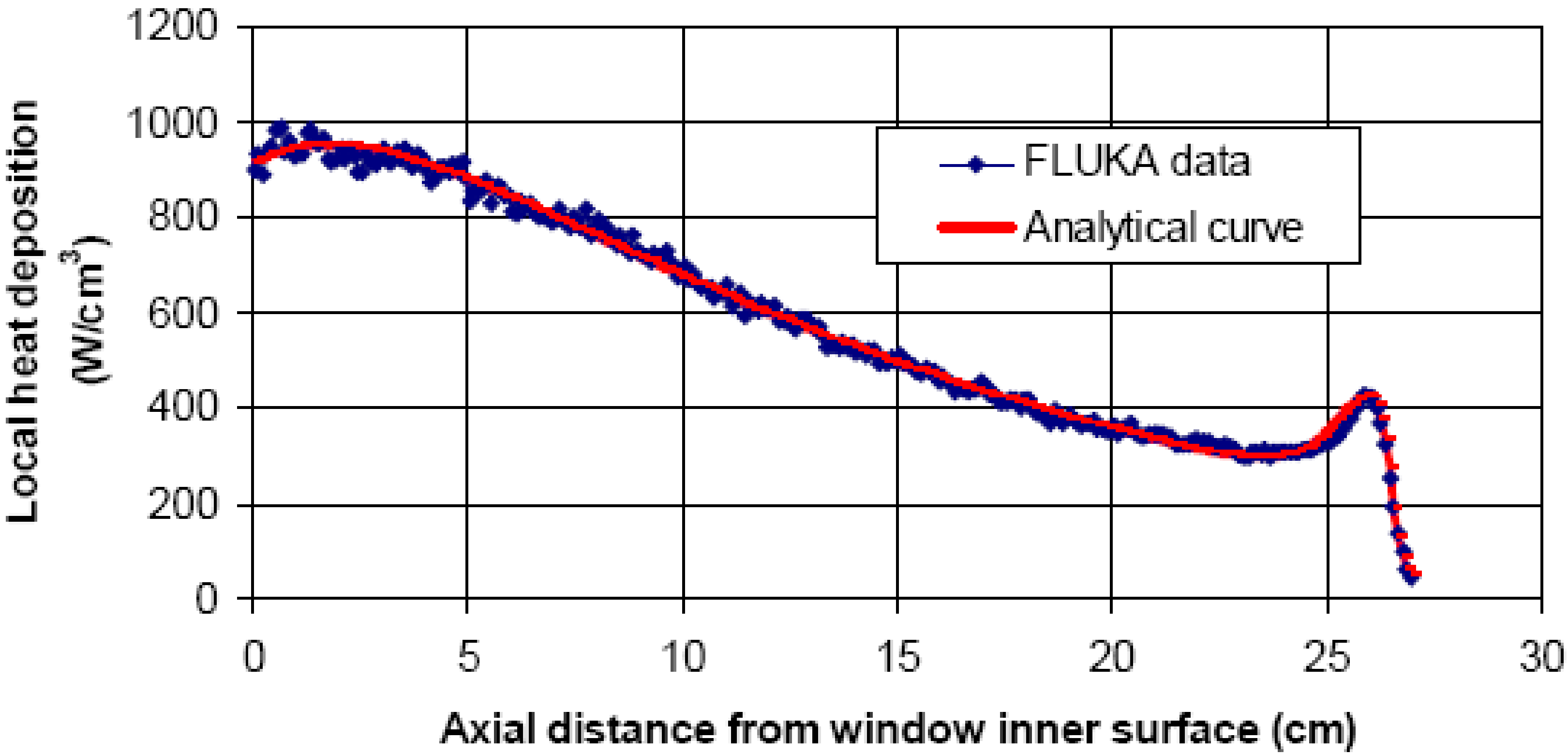
- Protons interact before slowing down
- 3.5 reactions per incident proton in average
- Large number of secondary neutron interactions



Heat deposition in a thick target



MEGAPIE target: 600 MeV protons on Pb-Bi



From T. Kirchner, Workshop MEGAPIE, 2002

DPA in JNSN

Component	Position of maximum value	Maximum DPA (DPA/5000 MW h)			
		Total	Proton	Neutron	Rutherford scattering
Target					
Target container vessel	Center of front window	3.9	0.81	3.09	0.18
Inner water-cooled containment shroud	Center of front window	2.2	0.84	1.36	0.13
Outer water-cooled containment shroud	Center of front window	2.2	0.84	1.36	0.11
Reflector					
Reflector vessel	Center of vessel nearest target	2.8	0.02	2.78	0.03
Moderator					
Coupled moderator vessel	Center of vessel nearest target	2.8	0.02	2.78	0.02
Proton-beam window					
Upstream window	Center of window	0.40	0.33	0.07	0.07
Downstream window	Center of window	0.44	0.34	0.1	0.06
Water-cooled shield					
Vessel	Around proton-beam entrance hole	0.16	0.00	0.16	0.00
Middle-section					
Vessel	Around proton-beam entrance hole	0.04	0.01	0.03	0.00

Power: 1MW (3 GeV, 0.33 mA)

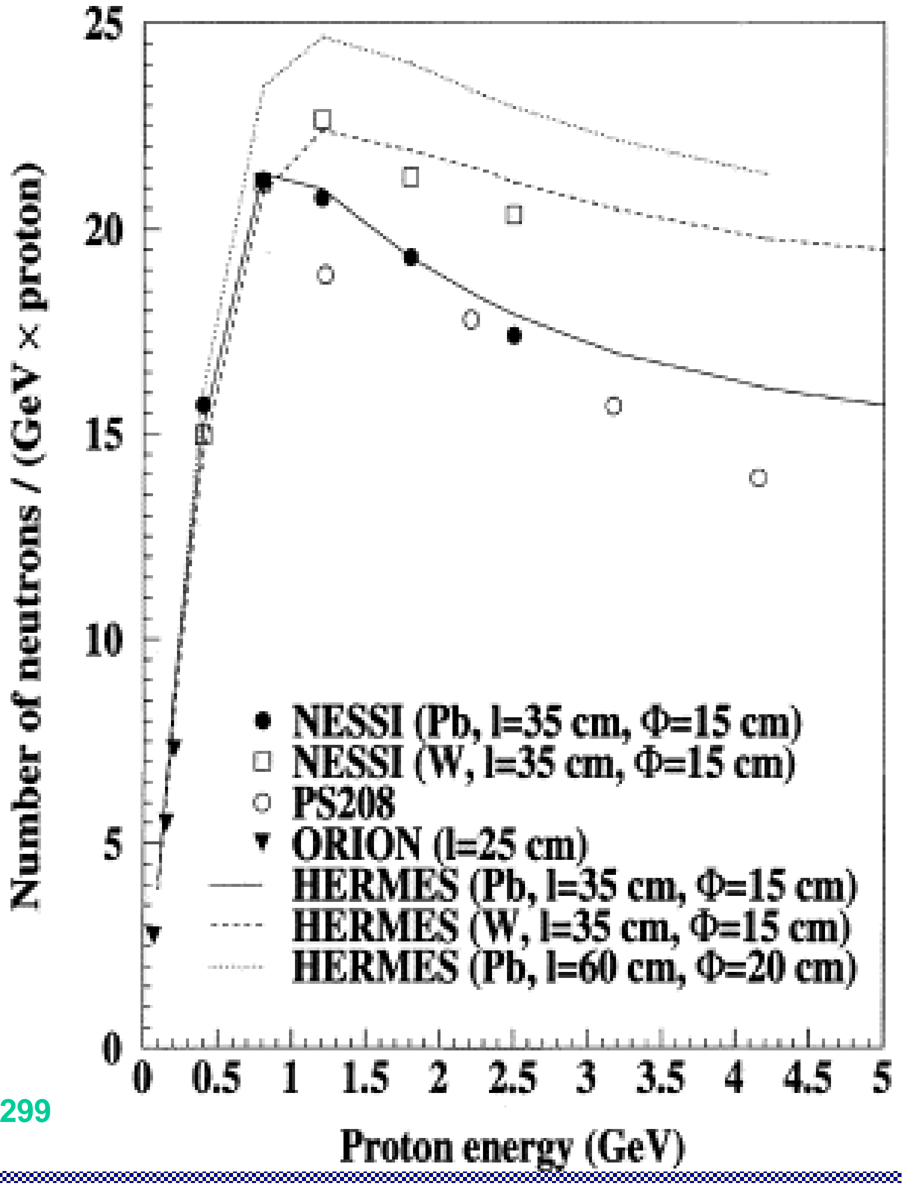
Proton beam window : A5083, 2.5 mm x 2 plates
Target vessel : 316L stainless steel
Reflector vessel : iron

From Harada et al., J. of Nucl. Mater. 343 (2005) 197

Spallation neutron production

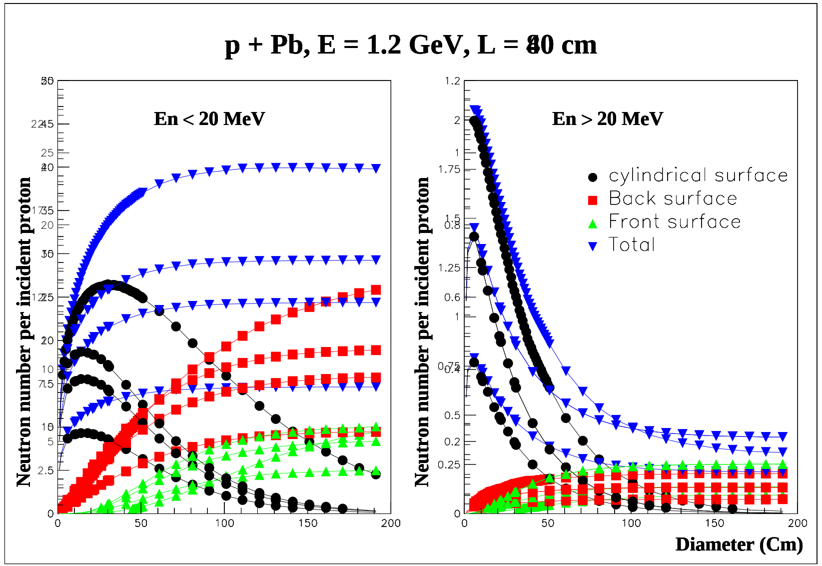
- In a heavy metal target (Pb, W, Ta, Pb-Bi) around **20 neutrons per incident proton and GeV**

- Maximum efficiency around 1 GeV



From Letourneau et al., NIM B170 (2000) 299

Choice of incident energy

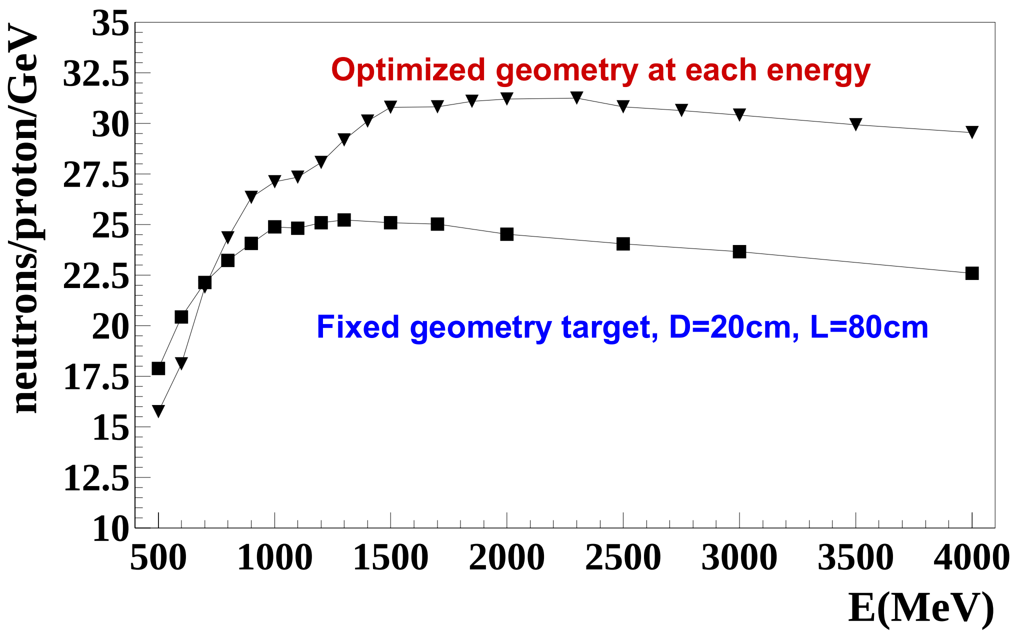


Target length and diameter optimization

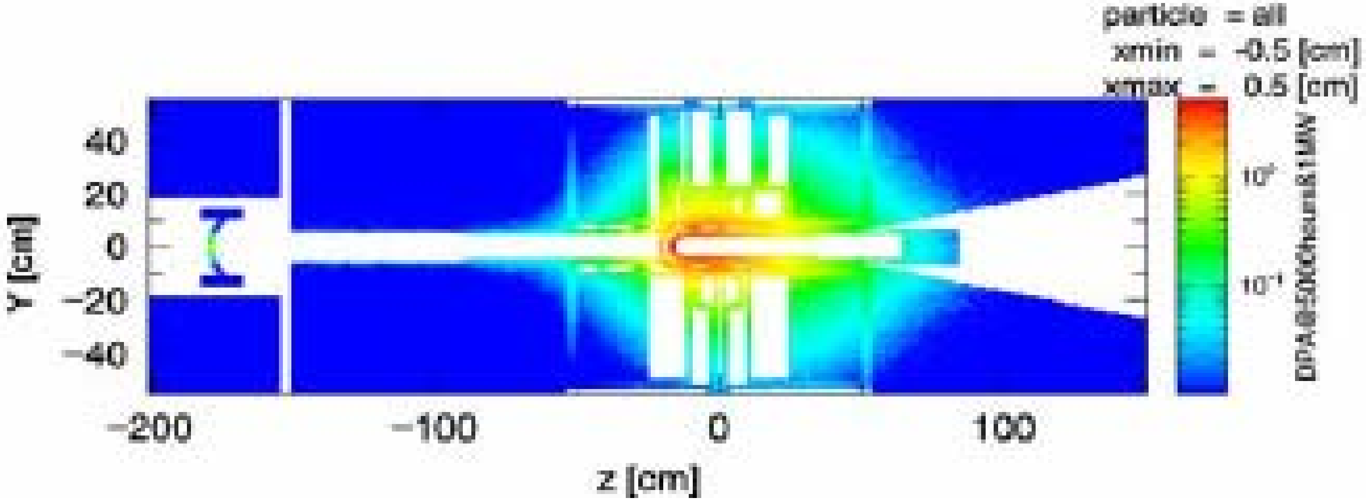
➔ **maximize lateral low energy n**

➔ **minimize high-energy leaks**

From F. Lavaud, SPhN report 1998 and SL, J. Phys. IV 9 (1999) 57



DPA



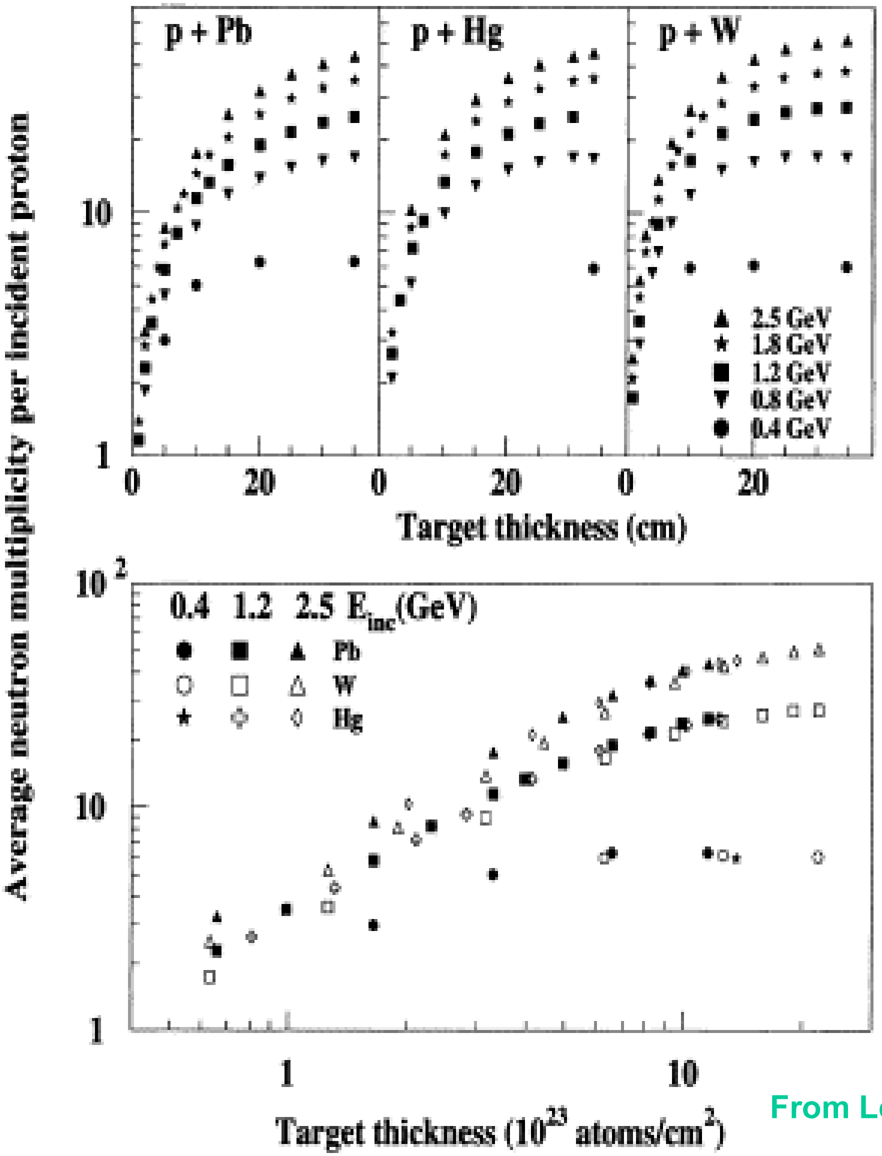
Effect of proton beam energy at same power (1 MW)
3 GeV – 0.33 mA compared to 1 GeV – 1 mA

Case[a]	Peak current density (μA/cm²)	Maximum DPA (DPA/5000 MW h)			
		Proton-beam window	Target container vessel	Reflector vessel	Moderator vessel
3	4.3	0.4	3.9	2.8	2.8
4	13.0	1.3	6.7	3.4	3.4

[a] Proton-beam condition per MW: Case 3: 3 GeV and 0.333 mA in total, Case 4: 1 GeV, 1 mA in total.

From Harada et al., J. of Nucl. Mater. 343 (2005) 197

Choice of material



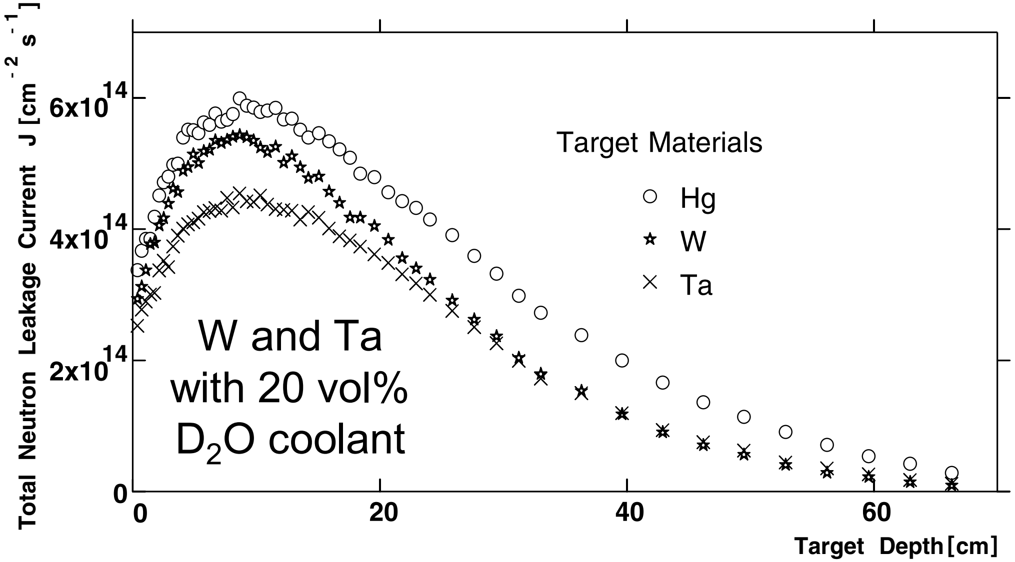
Neutron production

- ➢ increases with target thickness and saturates above 30 cm
- ➢ is similar for W to Pb for the same atom density

➔ choice of material from technological criteria

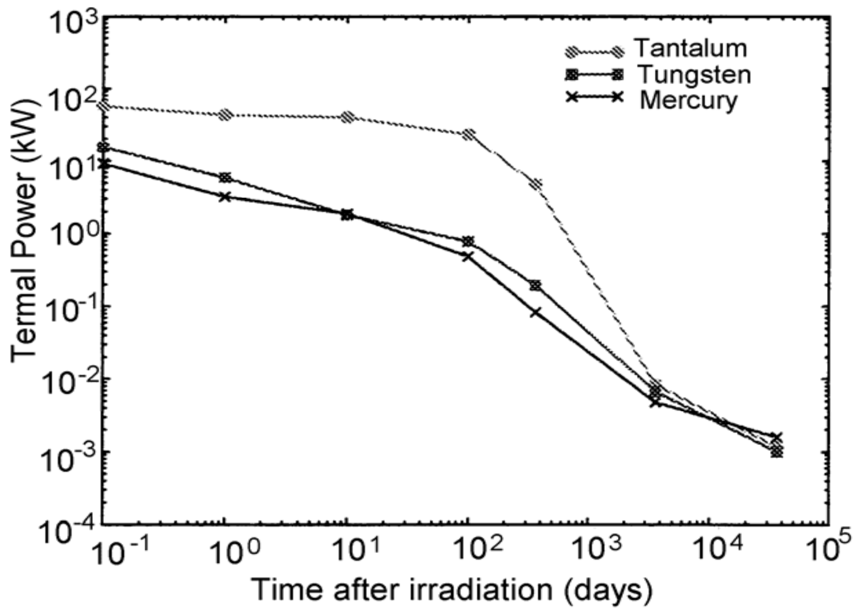
From Letourneau et al., NIM B170 (2000) 299

The choice of Hg as a Target



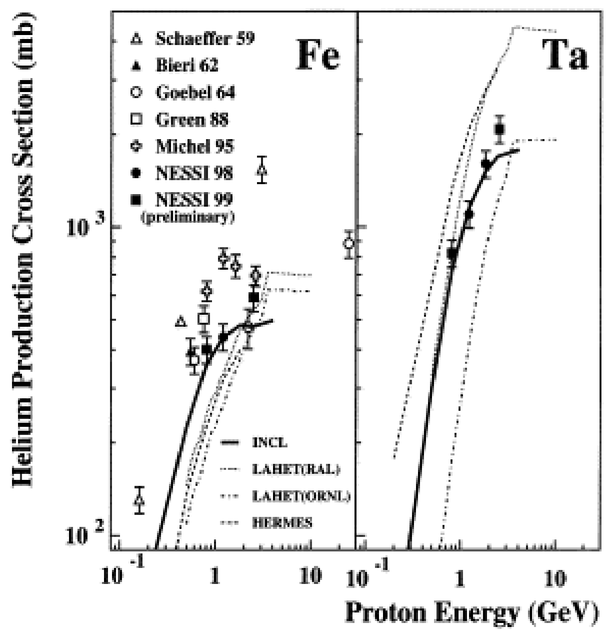
Calculated neutron leakage from a target of ESS geometry for different target materials

Calculated decay power for 200 days of operation in a 5 MW beam



From Y. Kadi, EURISOL week
27-30 November 2006

Helium and hydrogen production



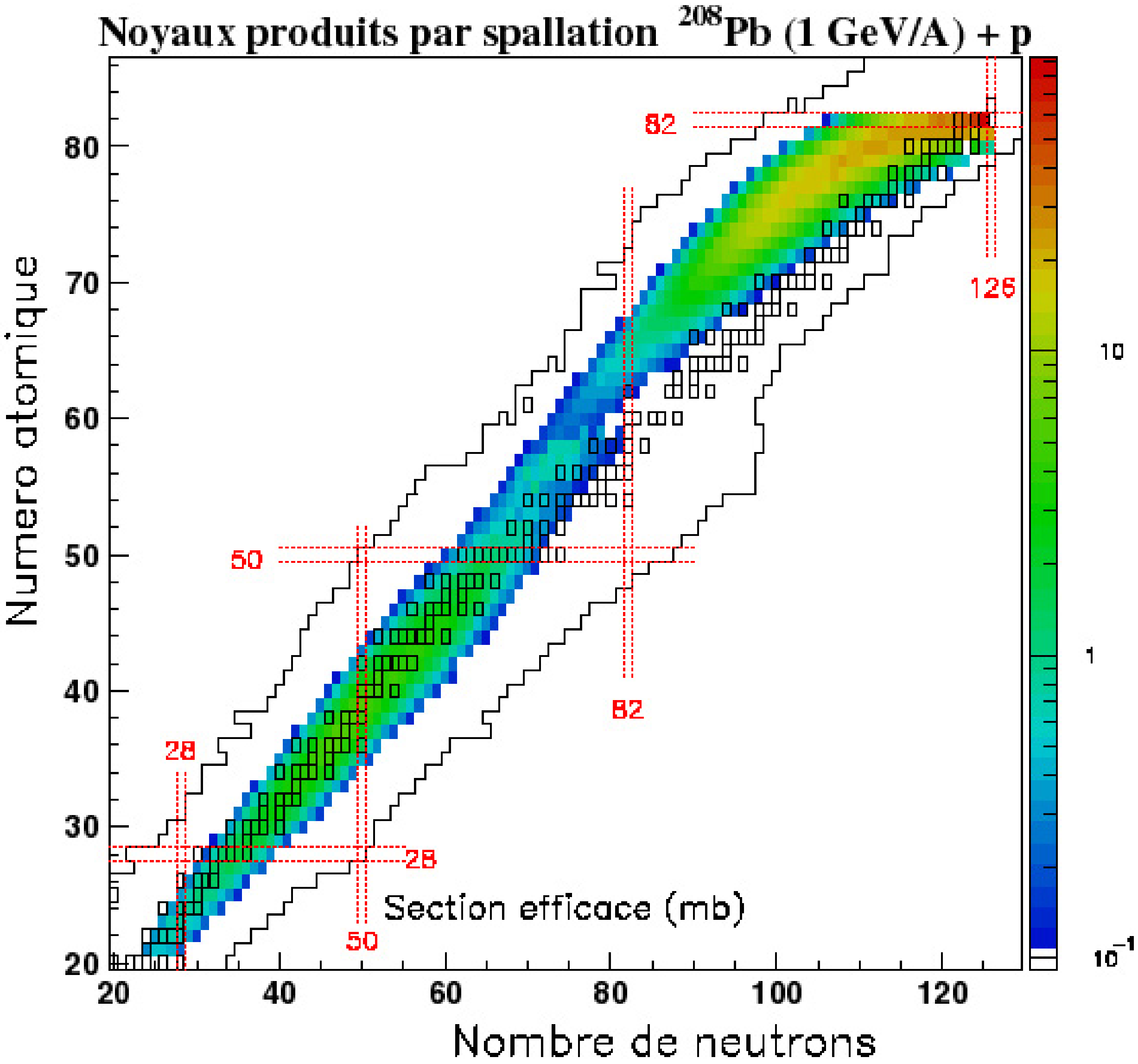
Comparison of several spallation sources

	dpa/y				Helium appm He/y	Hydrogen appm H/y
	Neutrons (E < 20 MeV)	Neutrons (E > 20 MeV)	Protons	total		
JAERI (5 MW)	39.45	6.89	21.16	67.5	2,270	
SNS (1 MW)	~ 12.5	~ 1.4	~ 8.9	22.8	1,014	10,840
ESS (5 MW)				~ 60	4,500	70,000
CRT (1 MW/m^2)				18	250	800

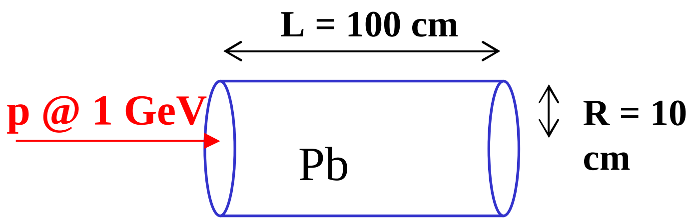
From Watanabe, symposium on Nucl. Data, JAERI (1998)

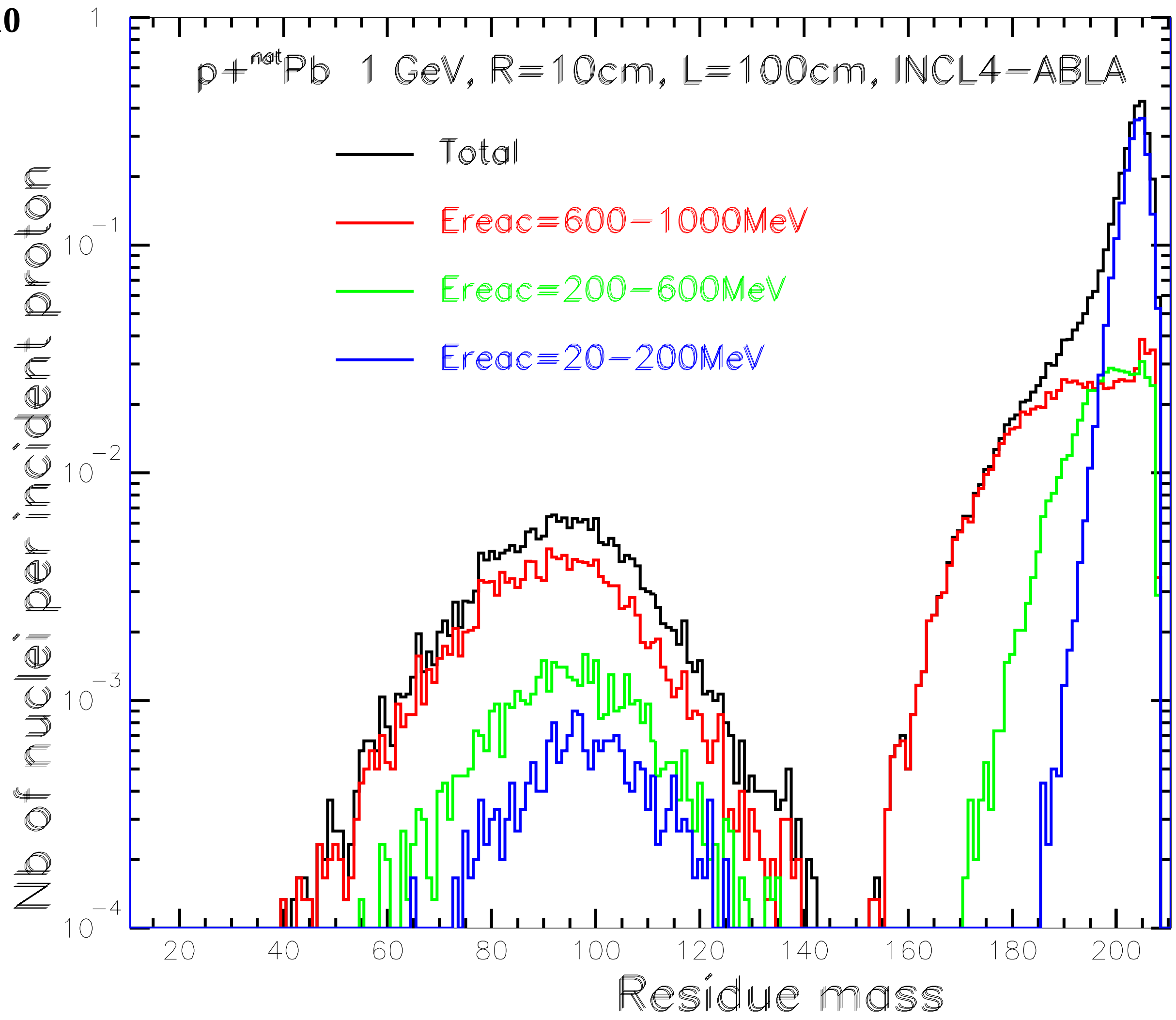
Residues produced in p+Pb reaction at 1 GeV

➢ **Hundreds of different residues produced**



Interactions in a thick target

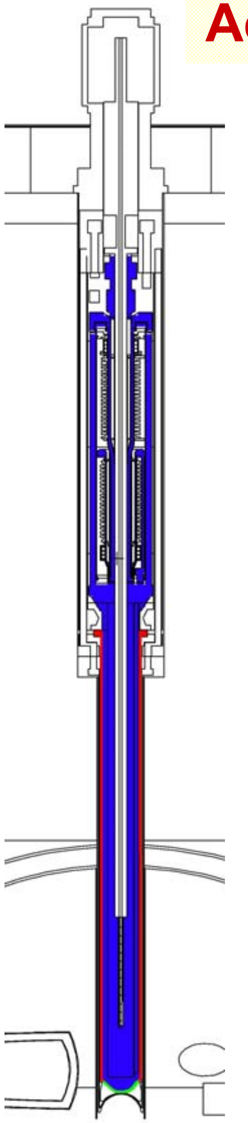


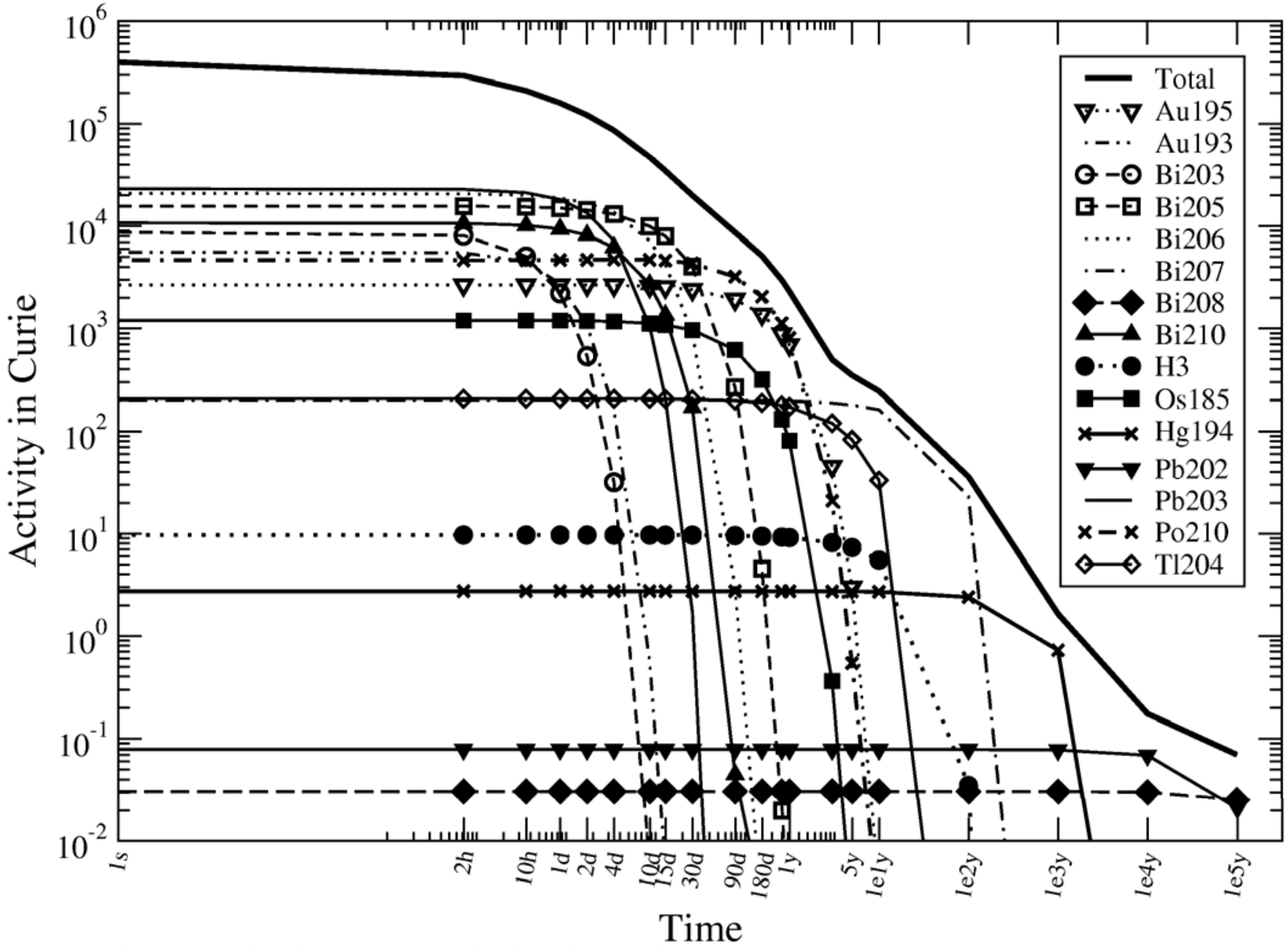


- 3.6 residues per incident protons in average
- Highest mass residue coming mostly from low energy interactions

Activity in a thick target

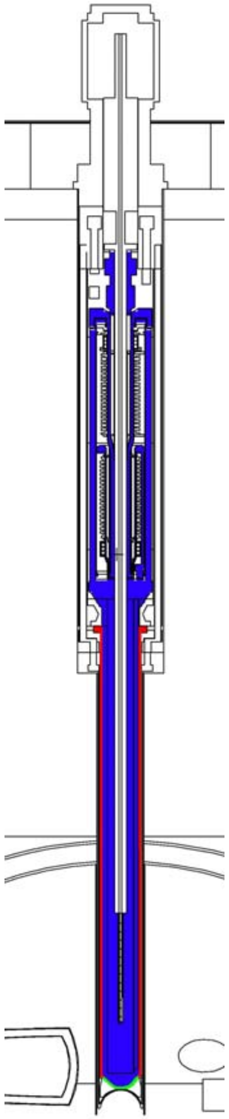
Activity in the MEGAPIE target



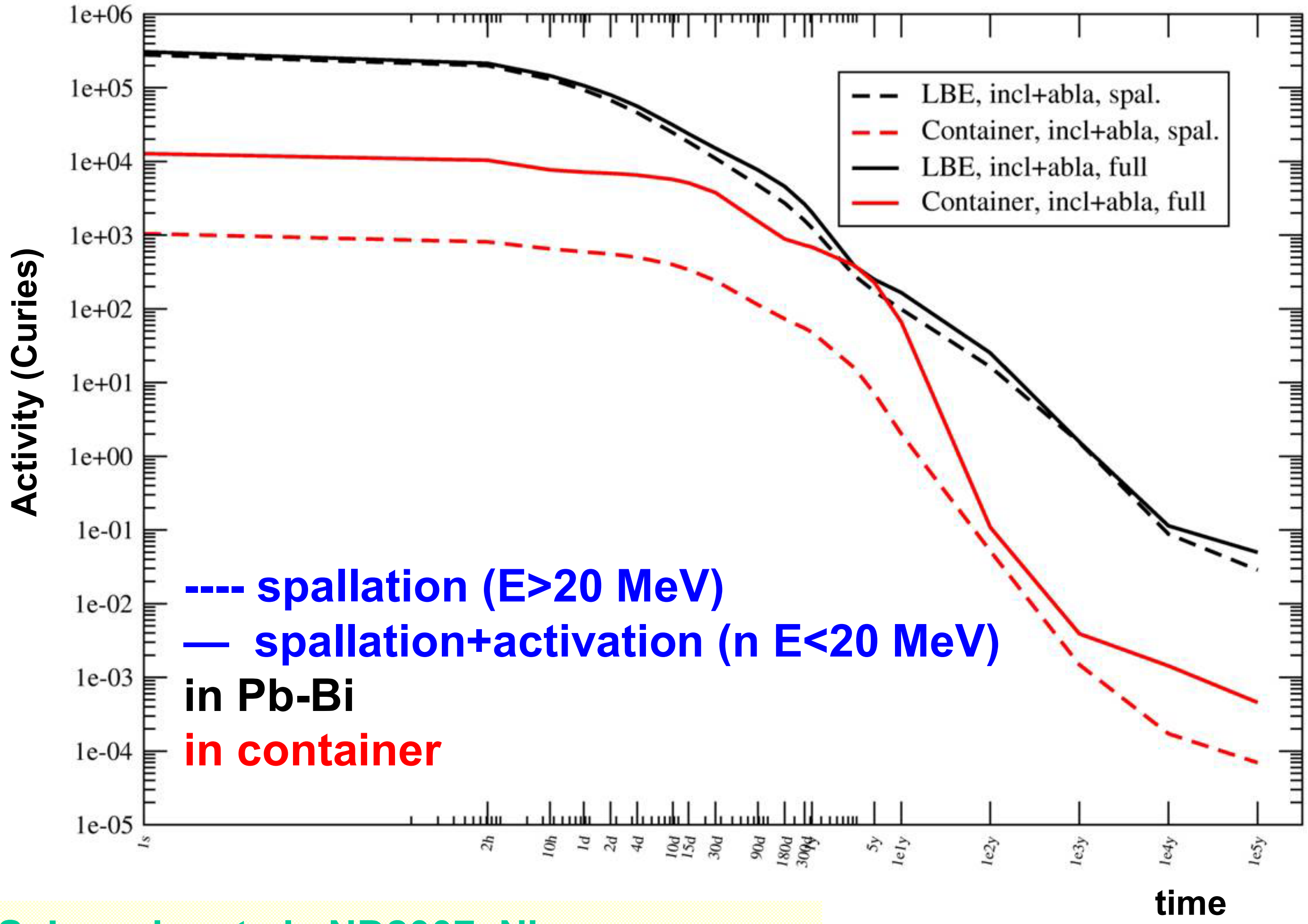


S. Lemaire et al., ND2007, Nice

Activity in a thick target

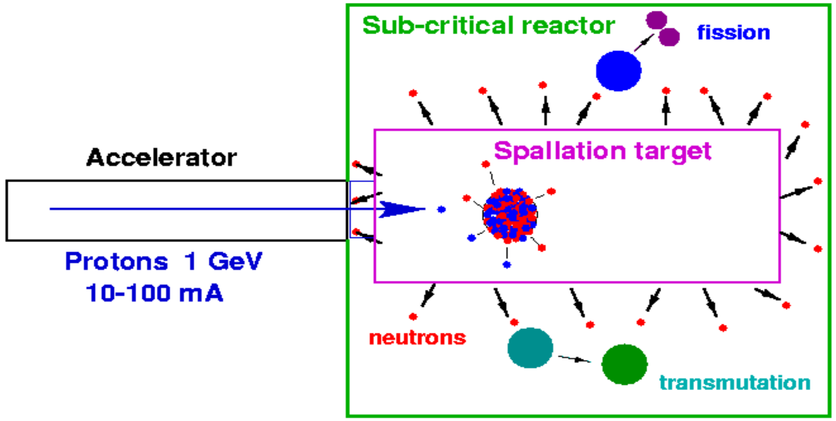


Comparison of activity from spallation and activation



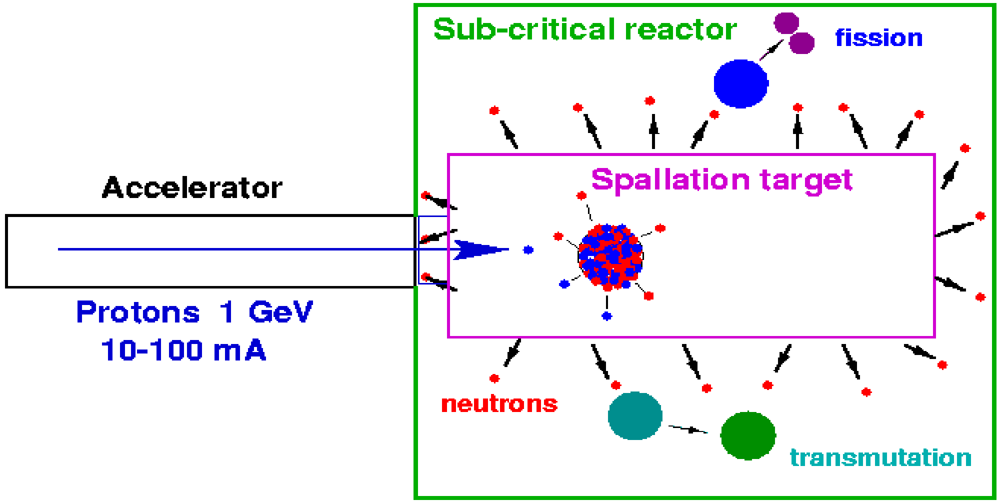
S. Lemaire et al., ND2007, Nice

Nuclear data needed for ADS



- **Neutron production**
  - number ➔ power of the system / needed accelerator intensity
  - energy, spatial distribution ➔ target optimisation, damage in window and structures
  - high energy neutrons ➔ shielding
- **Charged particle production**
  - gas (H_2, He) production ➔ embrittlement, swelling
  - energy ➔ DPA, energy deposition

Nuclear data needed for ADS



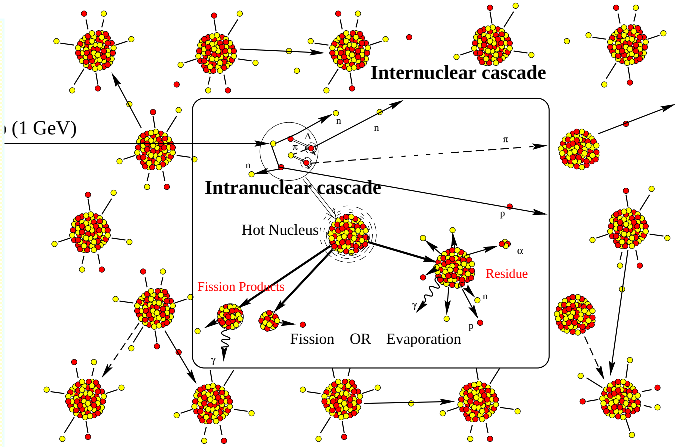
- **Residual nuclide production**
  - ➢ element distribution → corrosion, change in metallurgical properties
  - ➢ isotope distribution → activity (short lived isotopes), radiotoxicity (long lived isotopes), decay heat, delayed neutrons
  - ➢ recoil energies → DPA in window and structures, energy deposition

Simulation tools for Spallation Source design

- **Monte-Carlo transport codes**

➔ propagation of all particles created in elementary interactions

(MCNPX, FLUKA…)

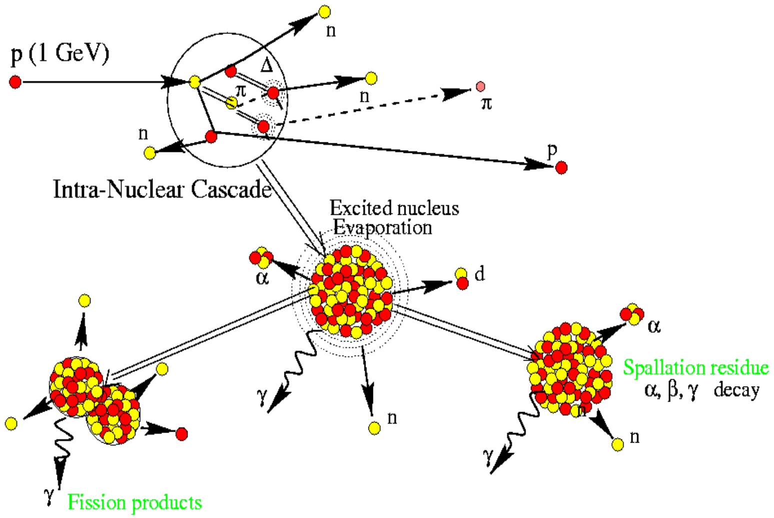


➢ **Above 150-200 (20) MeV :** nuclear physics models (Intra-Nuclear Cascade (+ Pre-eq) + evaporation-fission) ➔ cross-sections, properties of emitted particles directly used by the transport codes

➢ **Below 150-200 (20) MeV :** evaluated data libraries but not all isotopes up to 200 MeV

Models for spallation reactions

Two step mechanism
(Serber 1947)



- **Intra-Nuclear Cascade**

  sequence of independent *N-N* collisions

  $\lambda\!\!\!^{-}_{\text{de Broglie}} = \hbar c/p \ll \Lambda$ **mean free path**

  fast process (≈ 30 fm/c)

  => Heating of the nucleus - thermalisation

- **De-excitation by evaporation or fission**

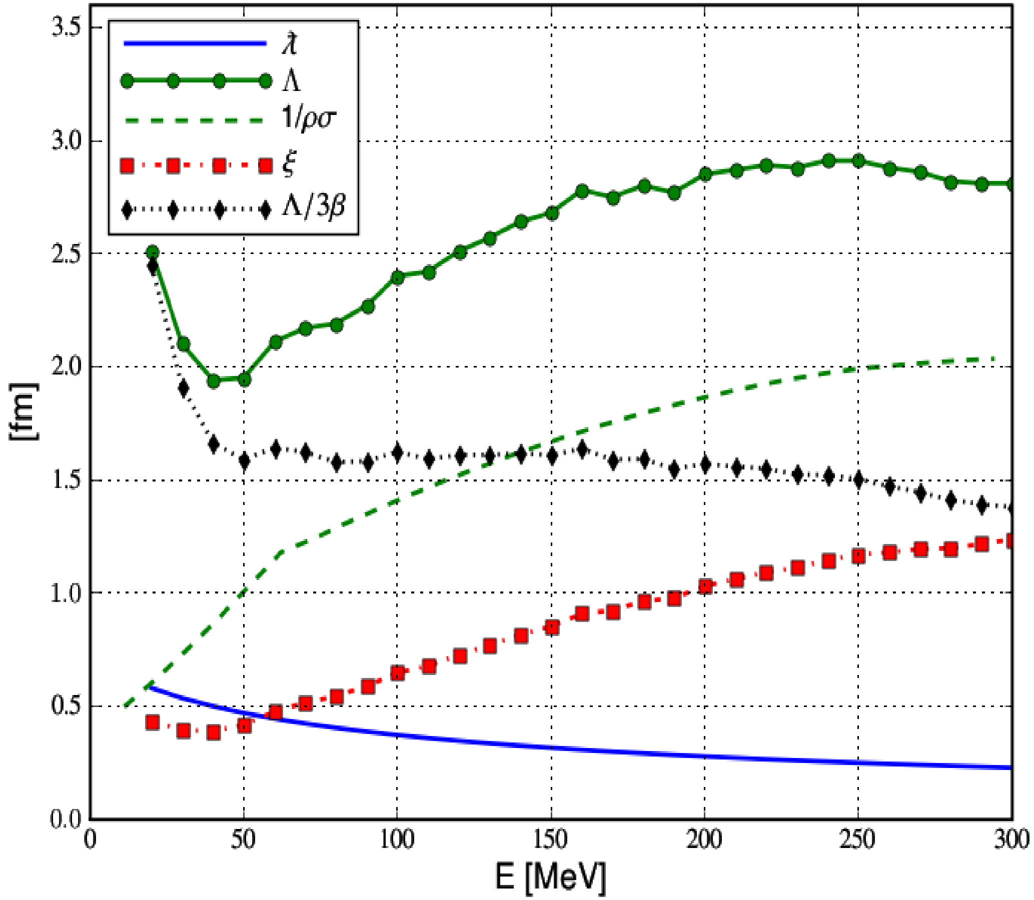
  statistical evaporation models

  slow process (hundreds of fm/c)

Intra-Nuclear Cascade models

Basic assumptions

- **Classical trajectories:**
  De Broglie wave length
  $\lambda\!\!\!^{-} \ll$ d inter-nucleon distance (d~1 fm)
- **Independent collisions:**
  $\lambda\!\!\!^{-} \ll \Lambda$ mean free path between collisions (= $1/\rho\sigma_{NN}$ + Pauli)
- **many scatterings:**
  $R \gg \Lambda$

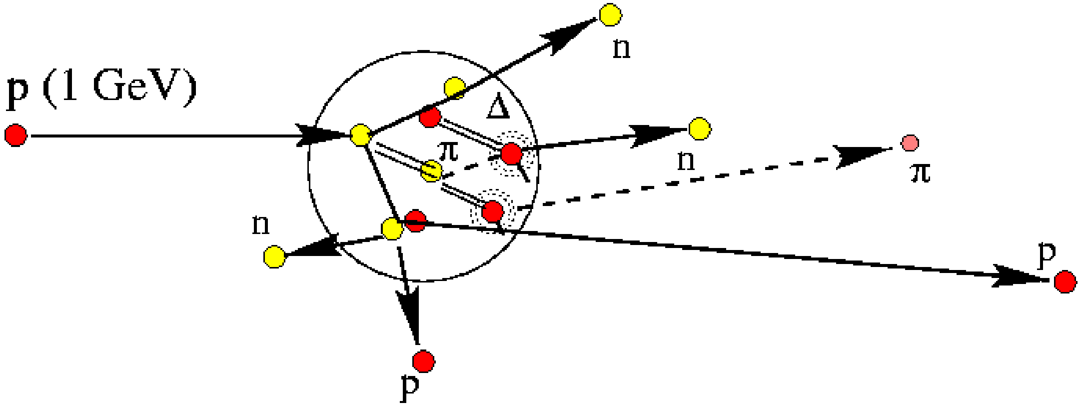


Central collision proton on ^{208}Pb

$\xi = \Lambda / 10\lambda\!\!\!^{-}$

(From Yariv et al., proceedings ND2007, Nice)

Intra-Nuclear Cascade models



Common features

- linear trajectory between collisions
- nuclear potentiel
- free *N-N* cross-sections
- inelastic collisions

  N+N → N+Δ → N+ N+π
- Pauli blocking

Main available INC models

- **Bertini** (Phys. Rev. 131 (1963) 1801)
- **Isabel** (Yariv and Frankel, Phys. Rev. C20 (1979) 2227)
- **Liège → INCL4** (A.Boudard et al., PR C66 (2002) 044615)
- **CEM** (Mashnik, AIP Conf. Proceedings 768, 1188 (2005))

Differences between the different INC models

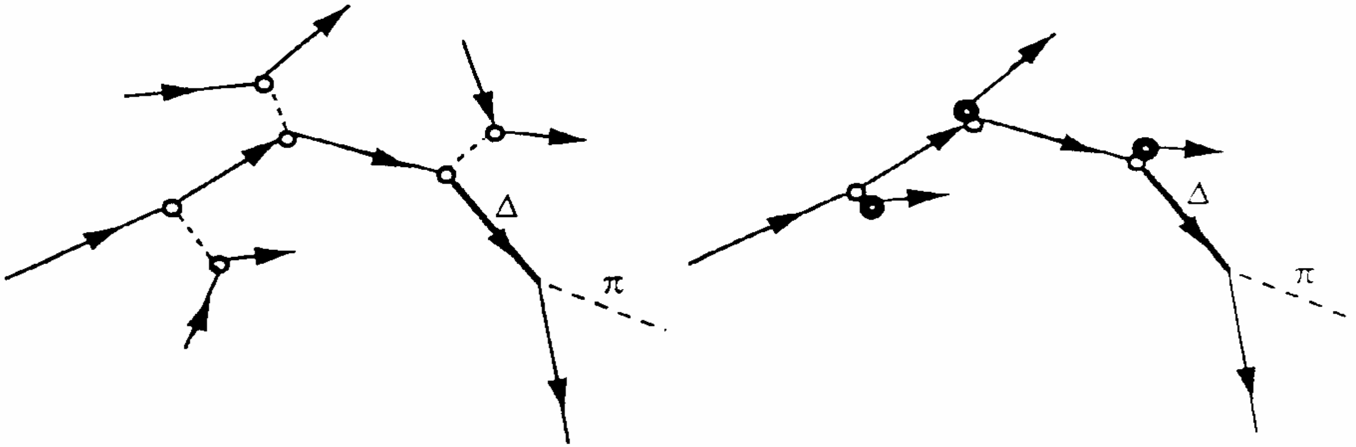
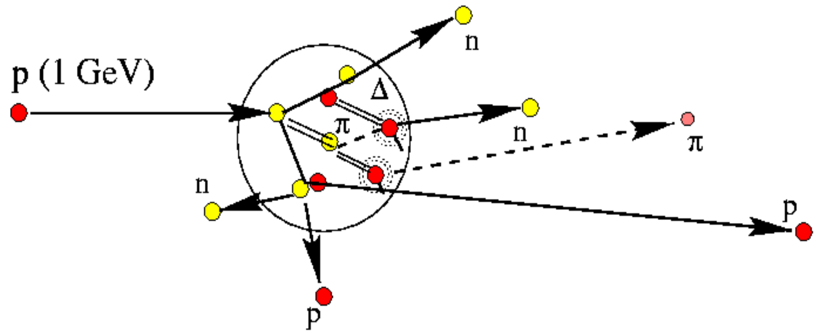


Fig. 3 : Schematic representation of the INC models of the first type (left) and of second type (right). In the latter case, nucleons promoted from the continuum are indicated by heavy dots.

	Bertini	Isabel	INCL4
Medium	continuous	continuous	particles
Cascade propagation	collided particles	time steps	time steps
Collision criterium	mean free path	mean free path	minimum distance of approach
Stopping criterium	energy	energy	time
Surface	diffuse (3 density regions)	diffuse (16 density regions)	diffuse (Wood-Saxon)
Pauli blocking	strict	globally statistic	locally statistic

Intra-Nuclear Cascade



Determines the number and direction of the high energy particles

- shielding against energetic neutrons
- inter-nuclear cascade propagation

for lead INC neutrons = 15% total nb but carry 80% of the energy

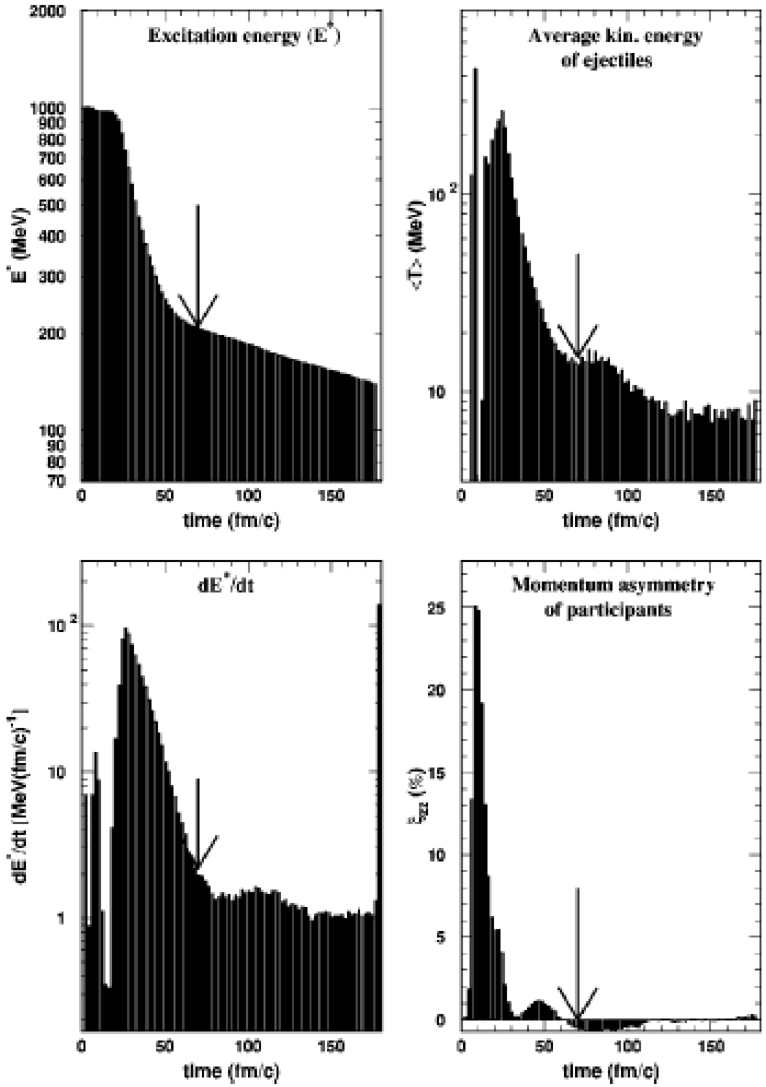
Determines initial conditions for evaporation-fission

- Excitation energy
- Z, A of the pre-fragment
- Angular momentum

The Liège INC model (INCL)

The INCL4 version

- **no really free parameters:**
  - ➥ stopping time fixed by consideration on the variation rate of several observables
    - ➢ results insensitive to a variation of ± 5fm/c
  - ➥ Potential = 45 MeV (E_F+S)
    - ➢ could be slightly varied



Evaporation models

Weisskopf-Ewing formalism

Detailed balance principle:

A → (A-a) + a equivalent to (A-a) + a → A

➥ $\rho_A P_{Aa} = \rho_{(A-a)} P_{(A-a)a}$

ρ_A, $\rho_{(A-a)}$ **densities of nuclear states**

Probability of emission of particle a with energy ε :

➥ $P_a(\varepsilon) = \rho_{(A-a)}(Ef^*)/\rho_A(Ei^*)\ (2s+1)\ (4\pi p^2/h^3)\ \sigma_c(\varepsilon)$

$\sigma_c(\varepsilon)$ **inverse cross-section**

Main available evaporation-fission models

- **Dresner-Atchison** (ORNL Report ORNL-TM-196 (1962))
- **ABLA** (Junghans et al., Nucl. Phys. A629, 635 (1998))
- **GEM** (Furihata et al., Nucl. Instr. and Meth. in Phys. Res. B 171, 251 (2000))

Fission models

Bohr-Wheeler formalism

Competition evaporation/fission governed by partial decay width

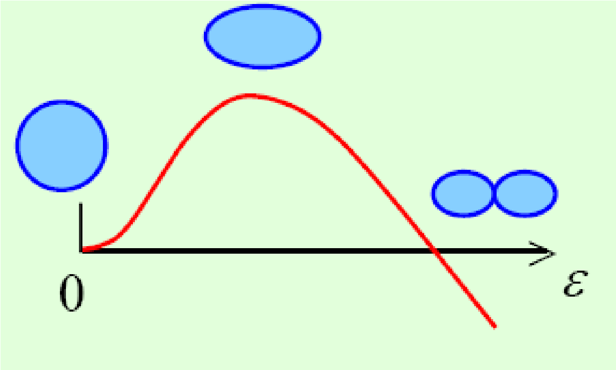
Fission width

➥ $\Gamma_f(E) = (1/2\pi\ \rho_c)\ T_{sad}\ \rho_{sad}\ (E-B_f)$

ρ_c : densities of nuclear states of the fissioning nucleus

T_{sad}, ρ_{sad} : temperature and density at saddle point

B_f : fission barrier dependent on Z^2/A, angular momentum



Results obtained during the last years

- **Large amount of high quality data collected**

  ➥ **Neutron and light charged particle production, isotopic residue distributions, excitation functions**

- **Improvement of nuclear models**

  ➥ **INCL4/ABLA tested against all the available data with the same set of parameters** (A.Boudard et al., PR C66 (2002) 044615)

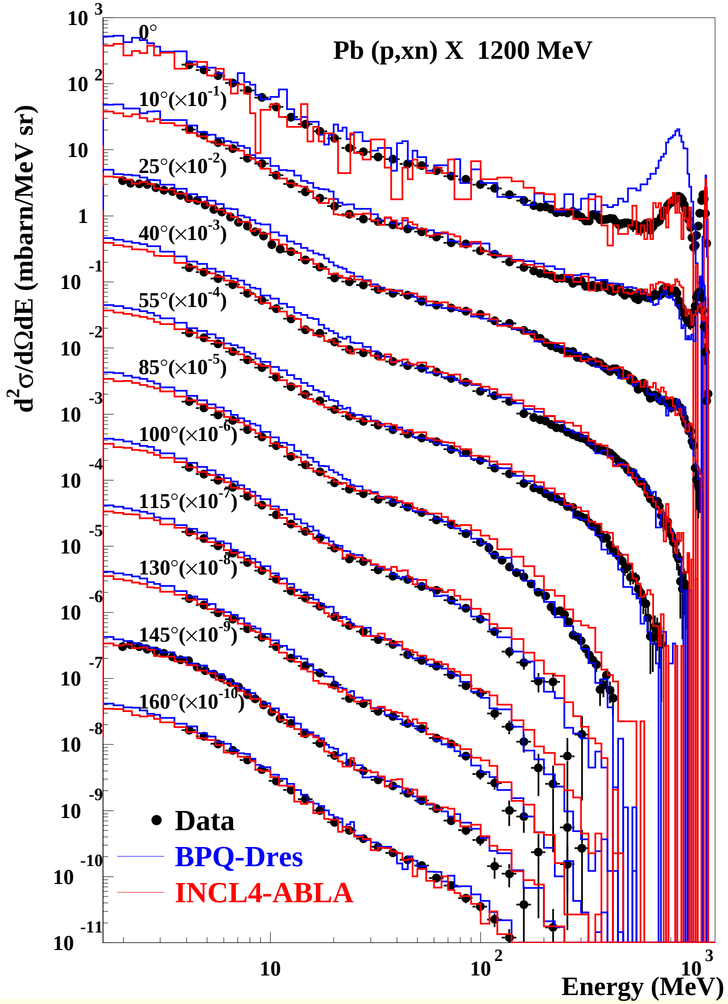
  ➥ **but also FLUKA and CEM**

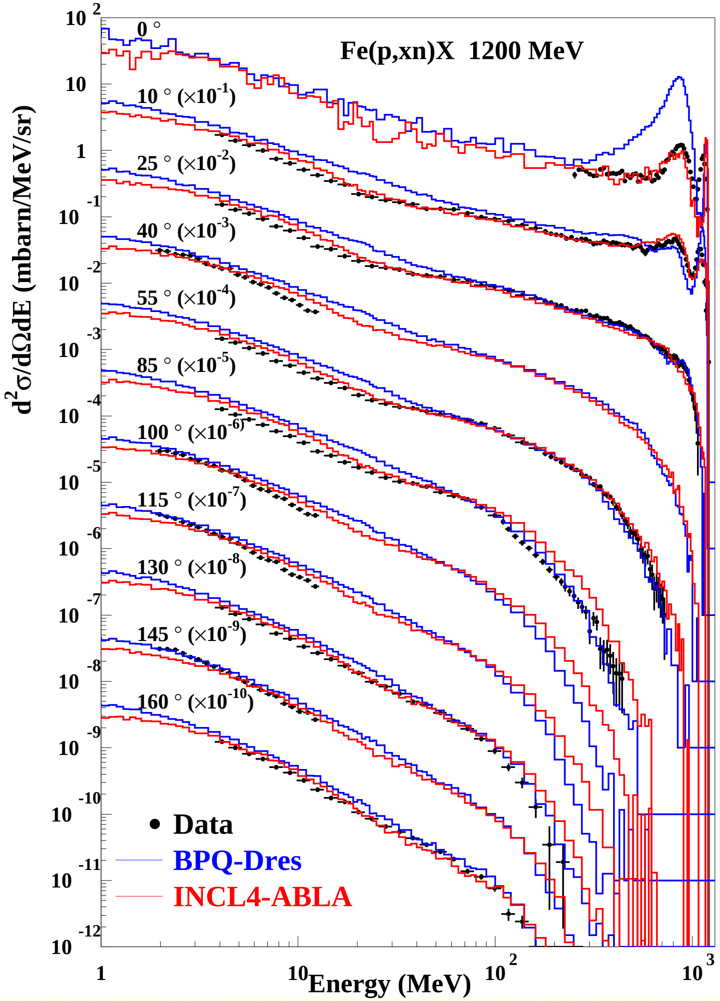
- **Implementation of INCL4/ABLA and CEM into MCNPX, INCL4/ABLA soon in GEANT4**

State-of-the art

- **Neutron production: can be predicted with a 10-20% precision by most of the models**
- **Hydrogen: overall good agreement**

Neutron production



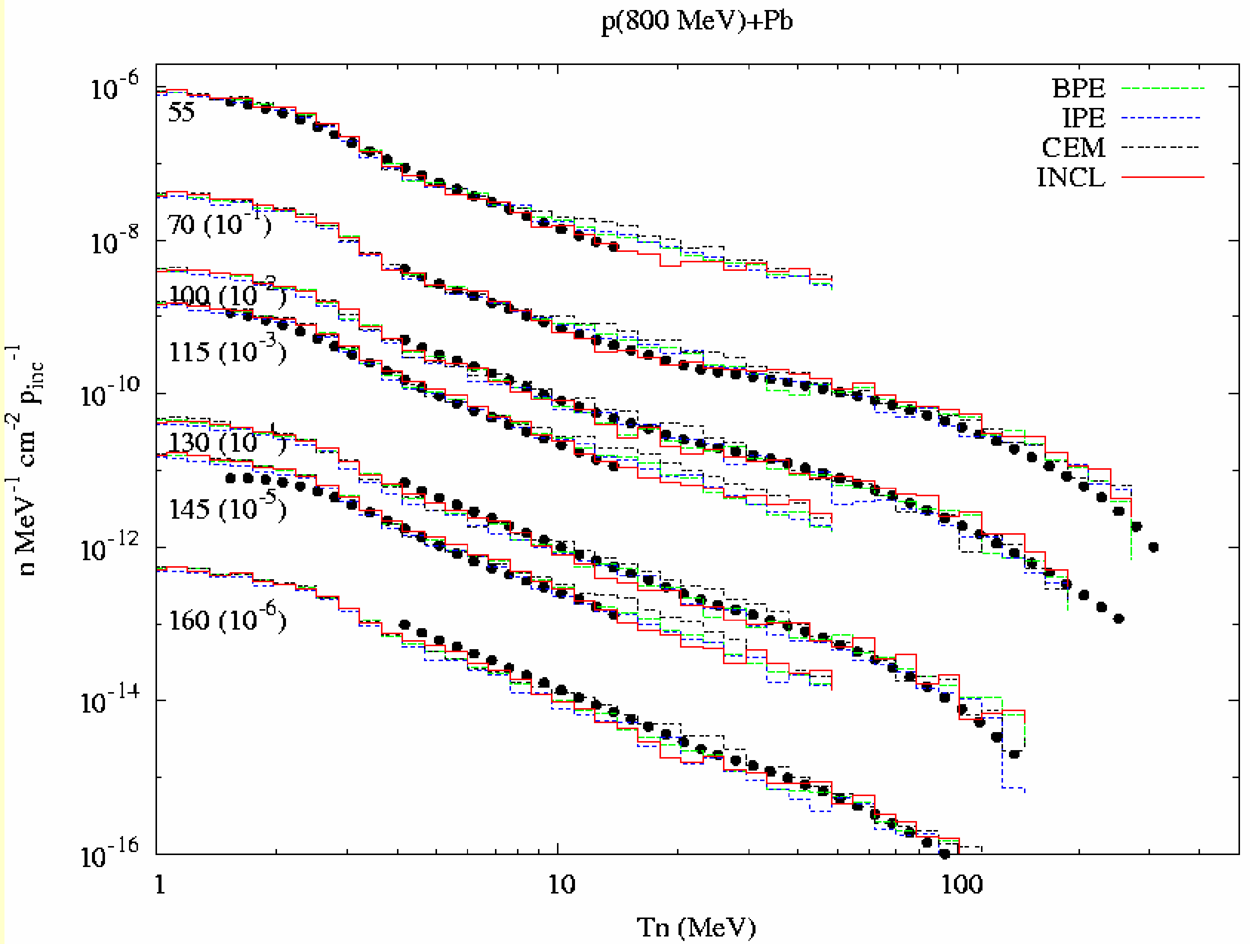


Calculations with INCL4 (A.Boudard et al.) **/ ABLA** (K.H.Schmidt et al.) **and Bertini / Dresner in LAHET3** Data: S.Leray et al., Phys. Rev. C 65 (2002) 044621

Neutron production

- **Energy and angular distribution : general trends well understood**

Differential spectra from a thick Pb target (SATURNE data)



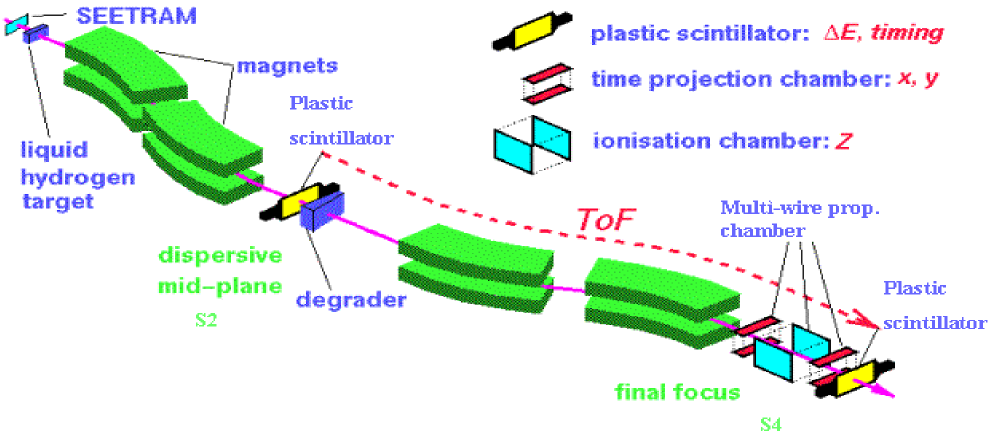
From T. Aoust et al., ND2004, Santa Fe

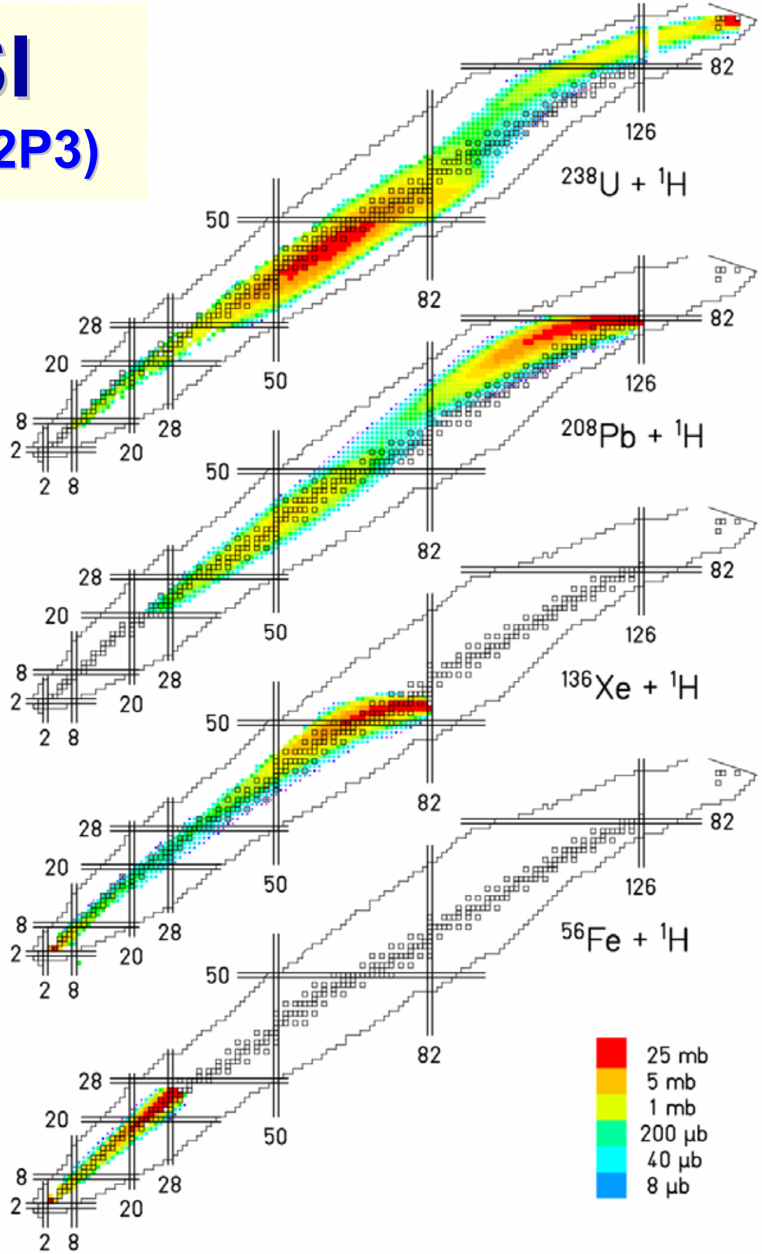
State-of-the art

- Residues: new data obtained with the reverse kinematics methods →considerable progress in reaction modelling
- Models
  - for heavy evaporation residues, generally good very close to the target nucleus ➔ Total activity prediction ok
  - Fission fragments ➔ activity of volatile elements
  - Light evaporation residues: most models generally bad
  - Intermediate mass fragments: all models orders of magnitude wrong

FRS experiments at GSI

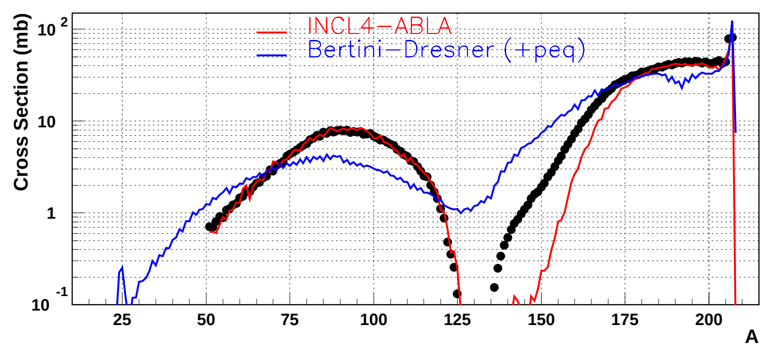
(coll. GSI, Santiago Univ., CEA/DSM, IN2P3)

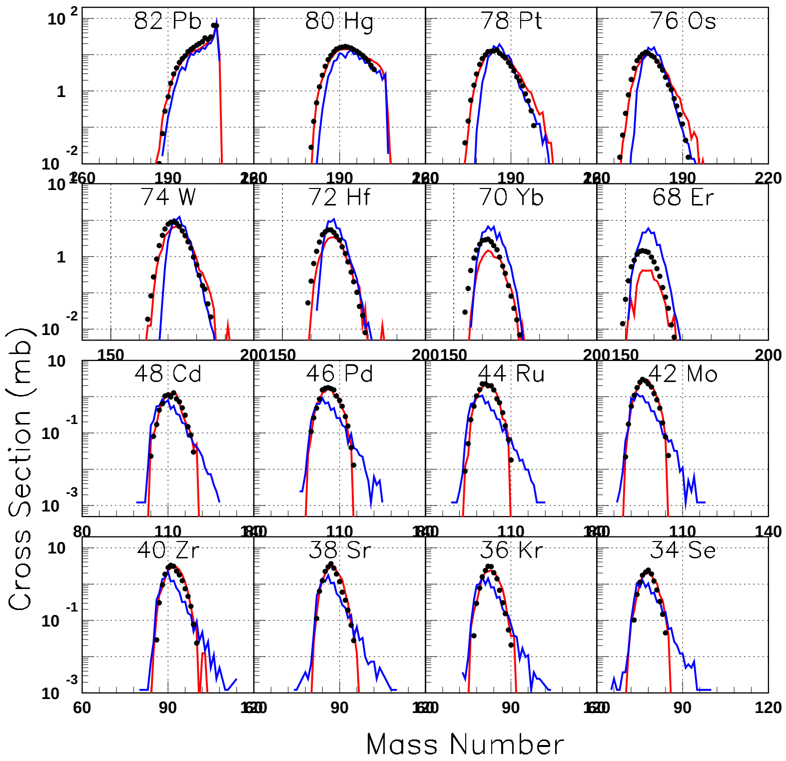




From K.H. Schmidt, proceedings ND2007, Nice (2007)

Residue production: heavy systems

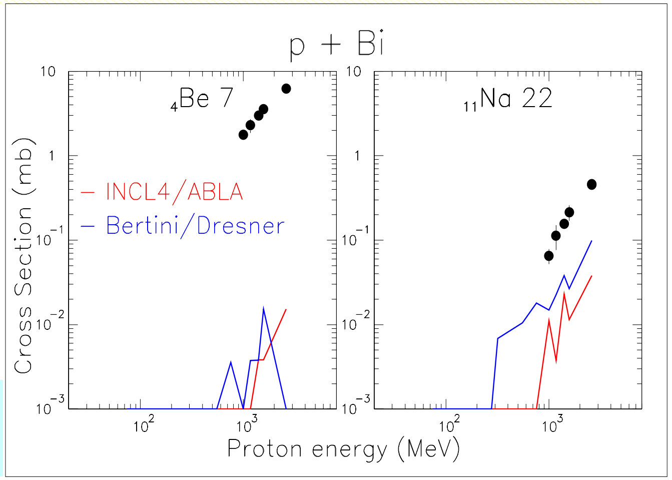




- ➢ INCL4/ABLA agrees much better with GSI data than Bertini/Dresner for fission fragments, very heavy residues and isotopic distribution shape

- ➢ Both fail for light evaporation residues and intermediate mass fragments

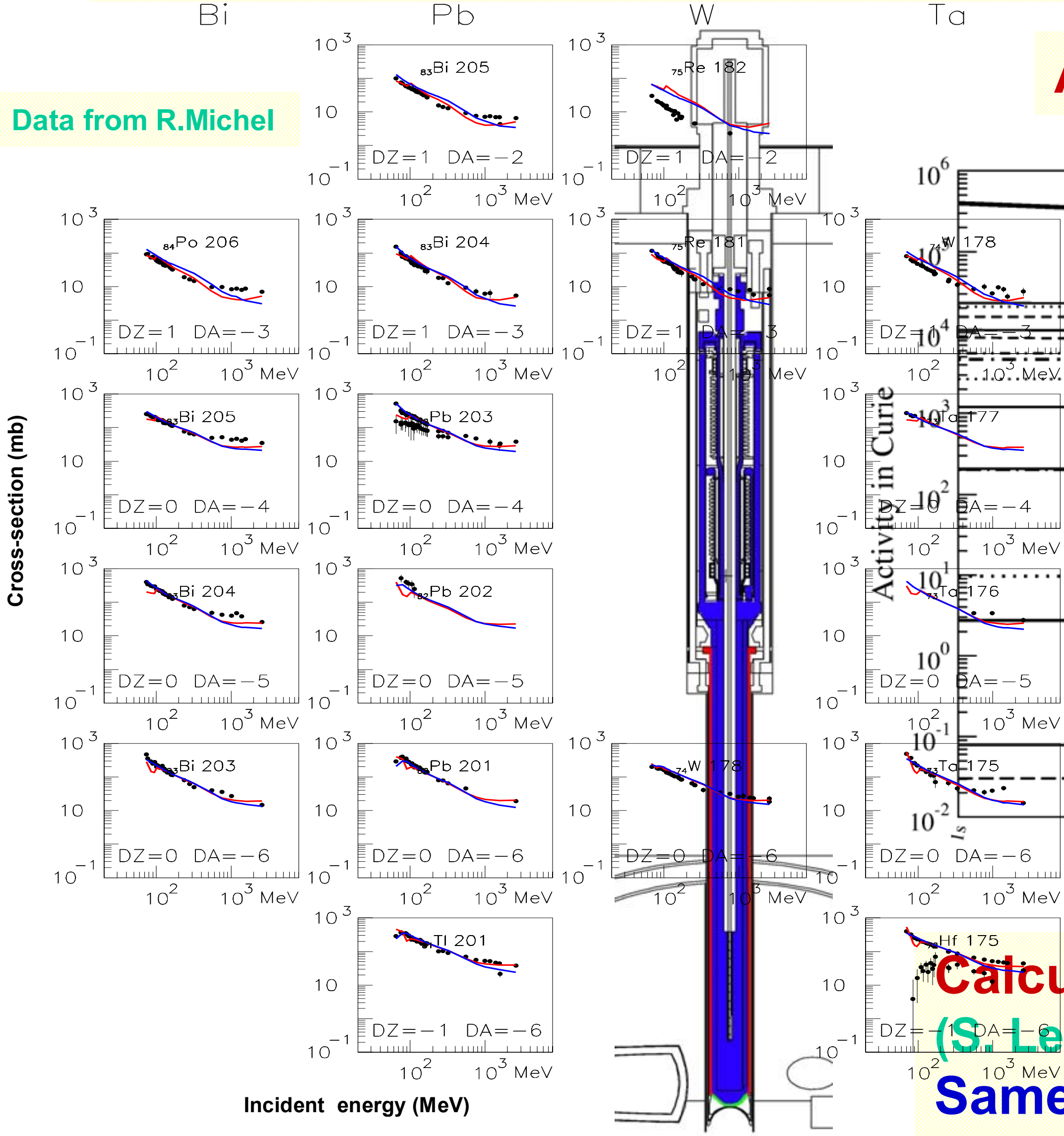
Data from Enqvist et al.



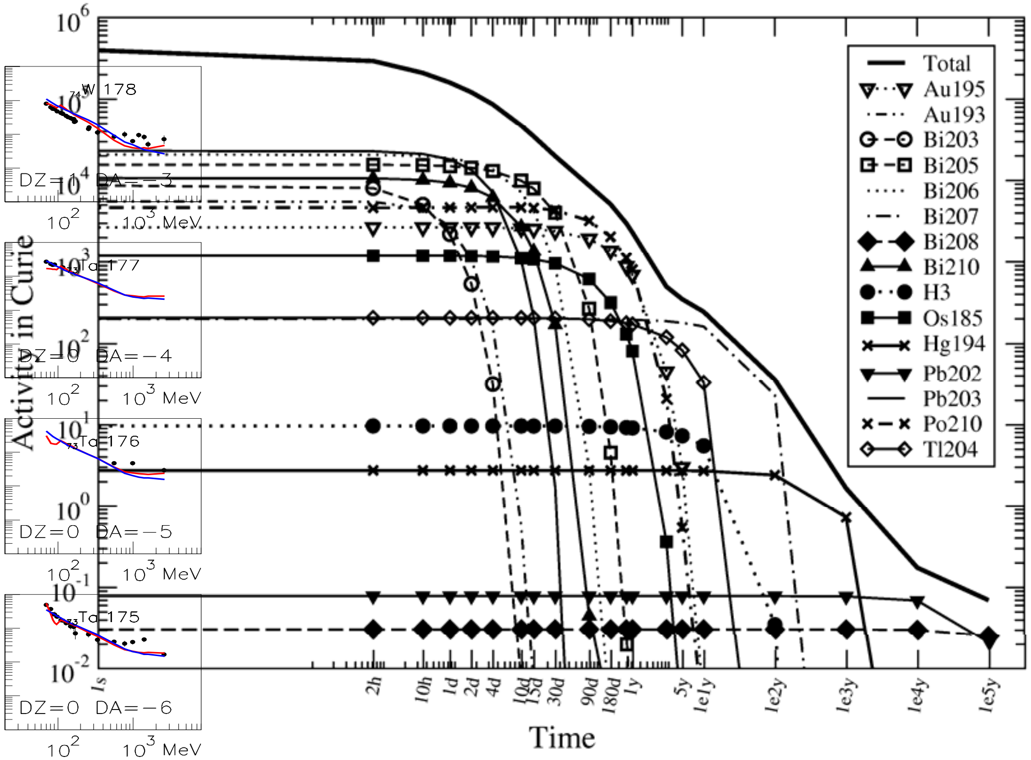
Data from Michel et al.

Residues close to the target

Data from R.Michel



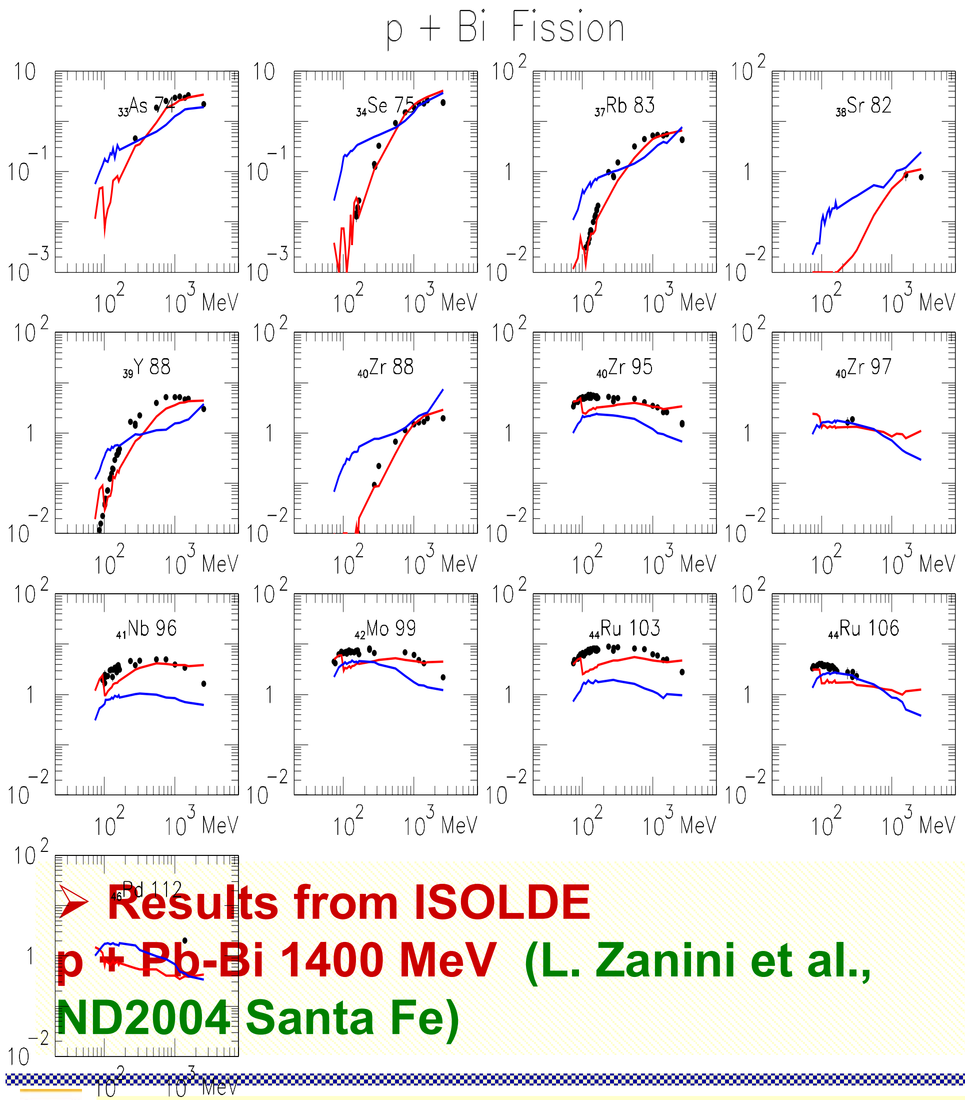
Activity in the MEGAPIE target



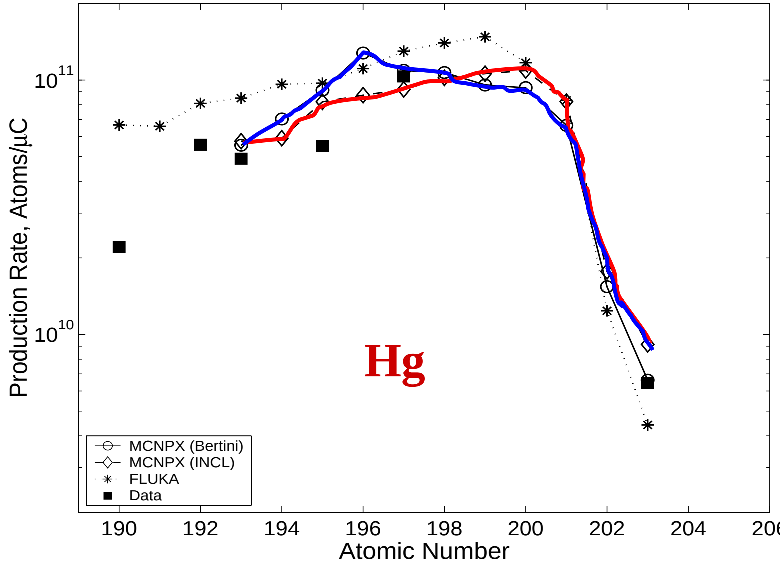
Calculation with INCL4/ABLA
(S. Lemaire et al., ND2007, Nice)
Same results with other models

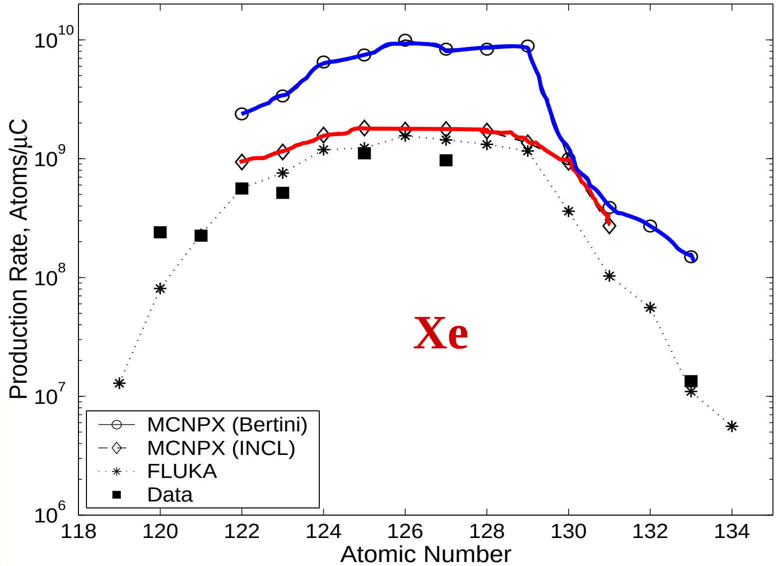
Volatile isotope production

Data from Michel et al.

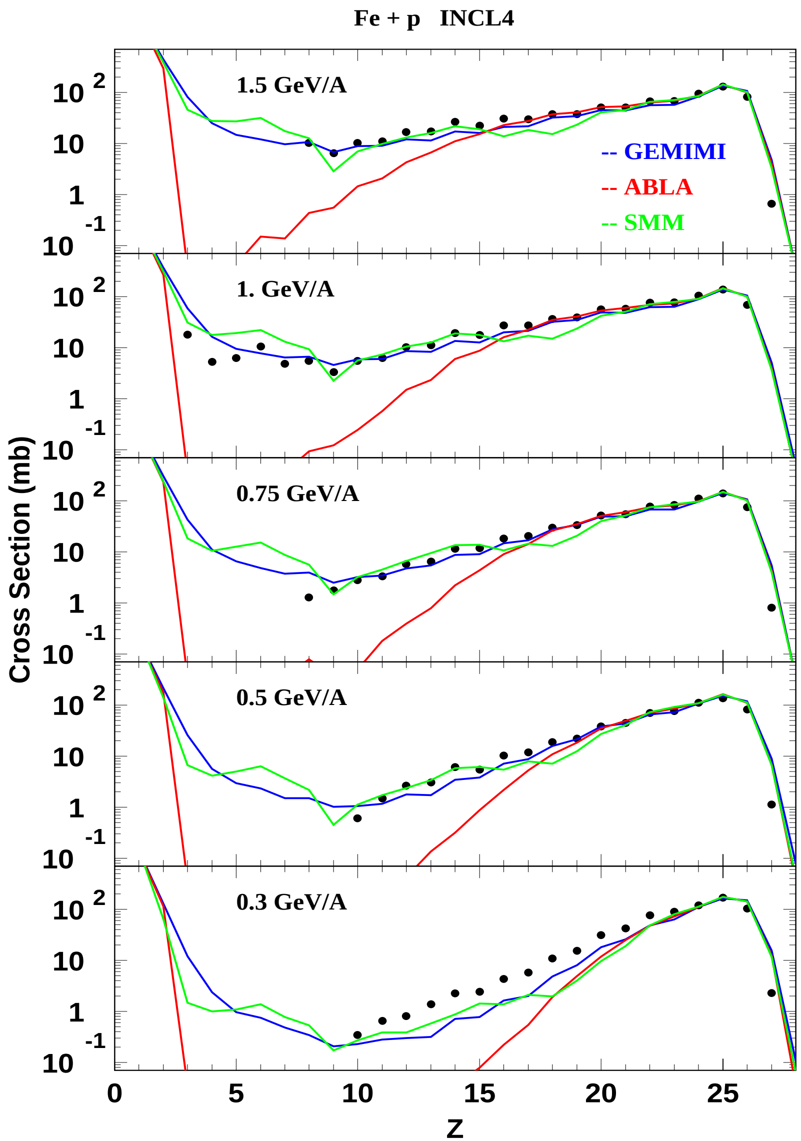


➢ **Results from ISOLDE**
p + Pb-Bi 1400 MeV (L. Zanini et al., ND2004 Santa Fe)





Residue production: light systems



— **INCL4 + ABLA**

— **INCL4 + GEMINI**

which includes an asymmetrical fission mode for light nuclei (Charity et al., NPA 483 (1988) 371)

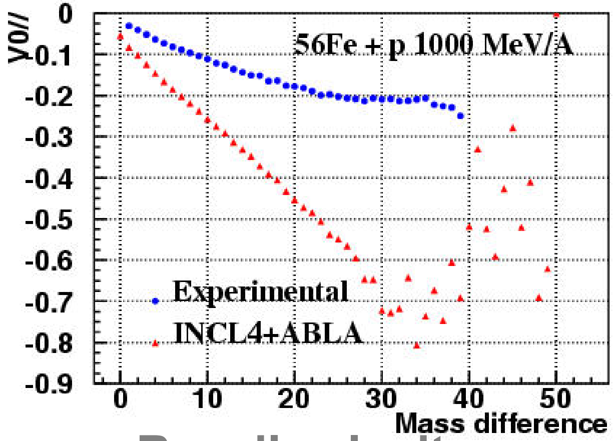
— **INCL4 + SMM**

a multifragmentation model
(A. Botvina et al., NPA 507, 649 (1990))

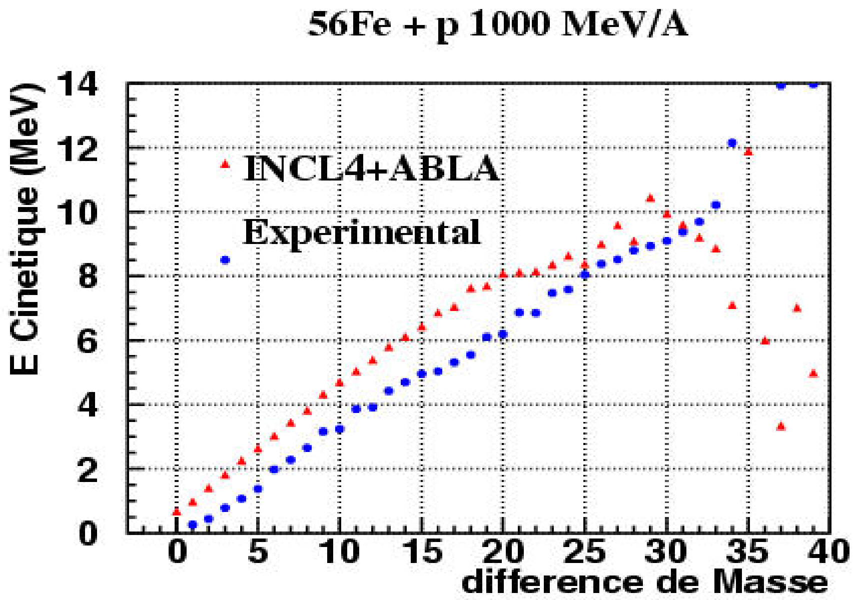
Data from C.Villagrasa et al., PRC 75 (2007) 044603 (additional data for low Zs at 1 GeV Napolitani et al. PRC 70 (2004) 054607)

Residue kinetic energies

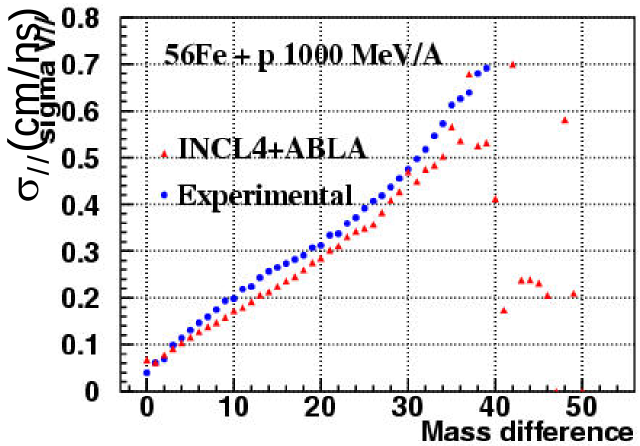
(cm/ns)



Recoil velocity



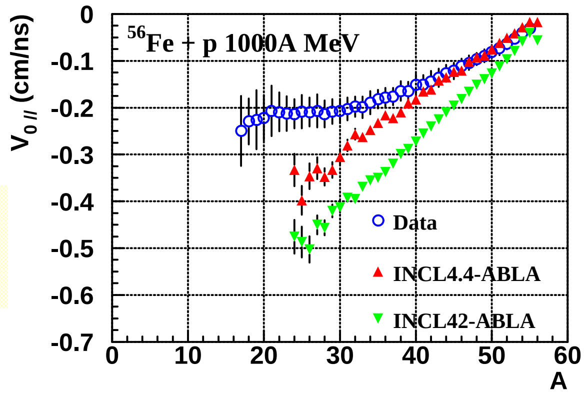
Kinetic energy



Width of the velocity distribution

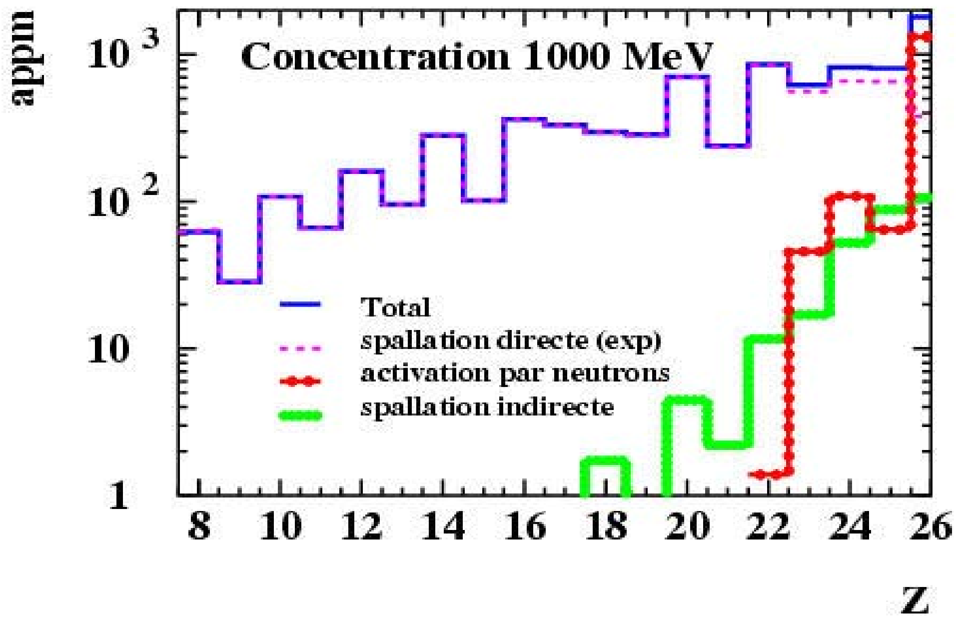
$$E_K = \frac{1}{2} mA \left(v_{0//}^2 + 3\sigma_{//}^2 \right)$$

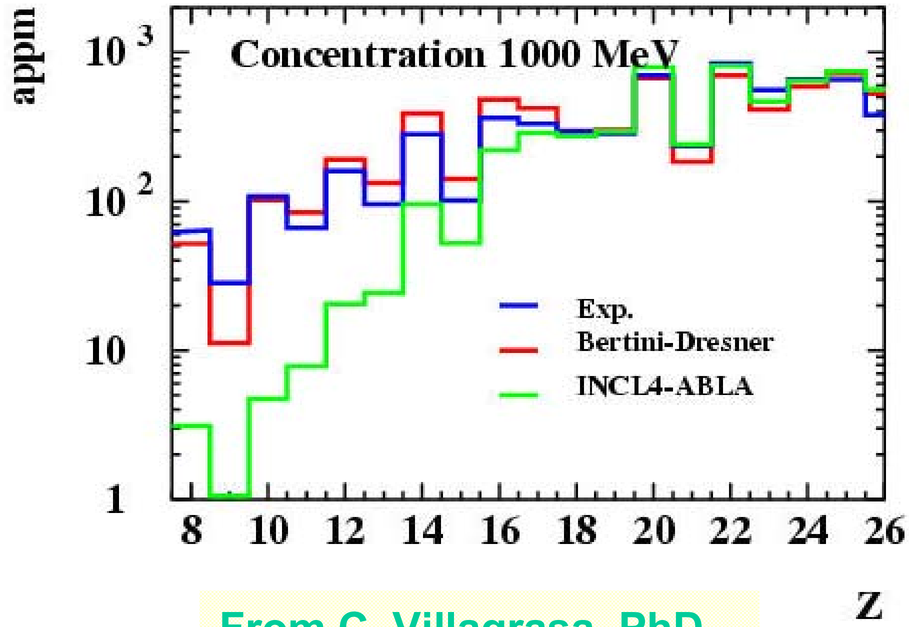
From C. Villagrasa, PhD Thesis



Impurety production in a Fe window

Protons 1GeV, I= 0.1 mA (31,8 μA/cm2), 1 year





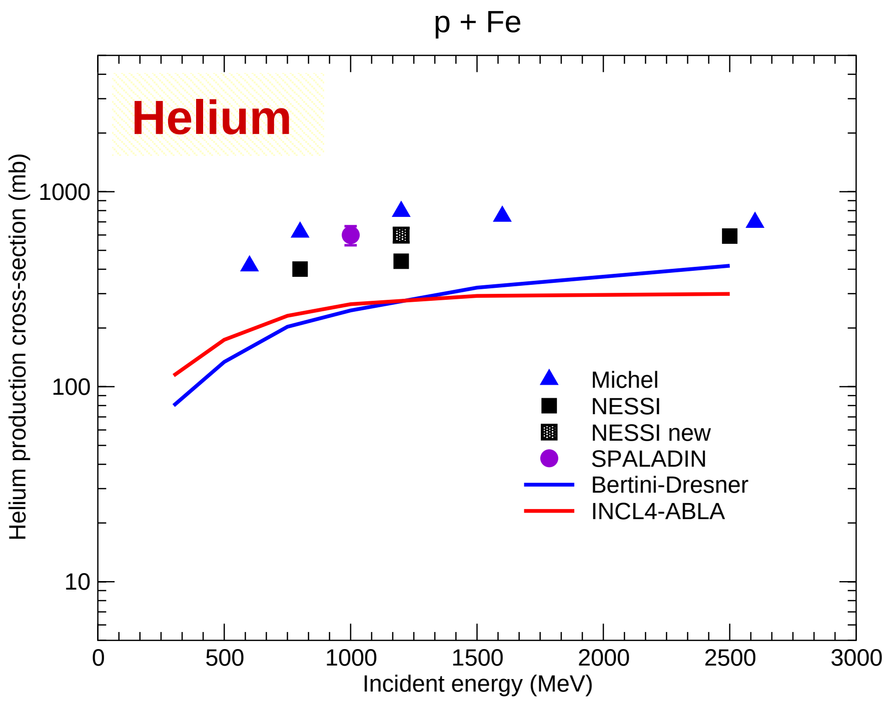
From C. Villagrasa, PhD Thesis

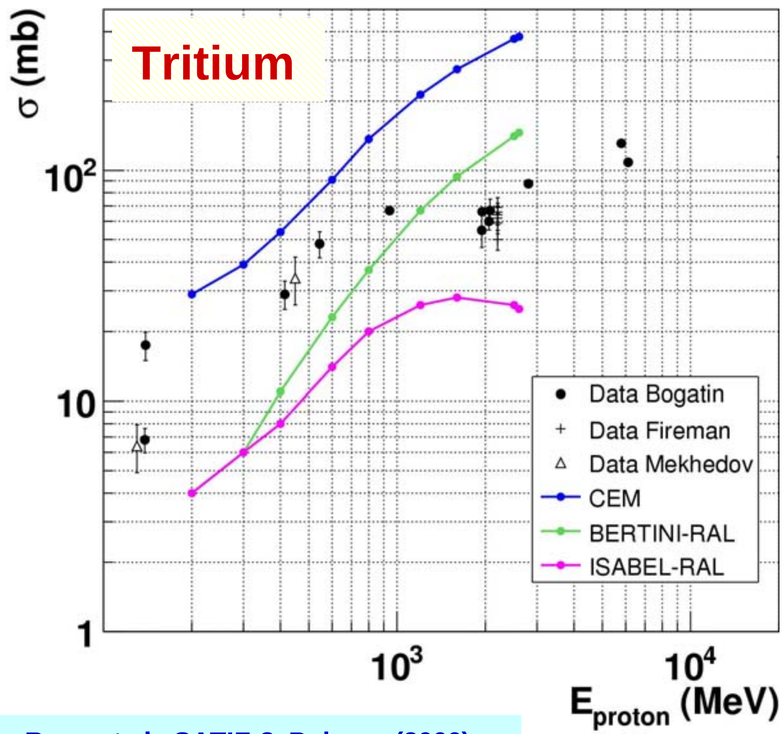
- INCL4/ABLA not good for light residues

State-of-the art

- Neutron production: can be predicted with a 10-20% precision by most of the models
- Hydrogen: overall good agreement
- Residues: INCL4/ABLA much better then Bertini/Dresner
  - for heavy evaporation residues, both good very close to the target nucleus ➔ Total activity prediction ok
  - Fission fragments ➔ activity of volatile elements
  - Light evaporation residues: generally bad
  - Intermediate mass fragments: orders of magnitude wrong
- **Light charged particles: no satisfactory prediction with the models implemented in MCNPX**

Gas production in Fe

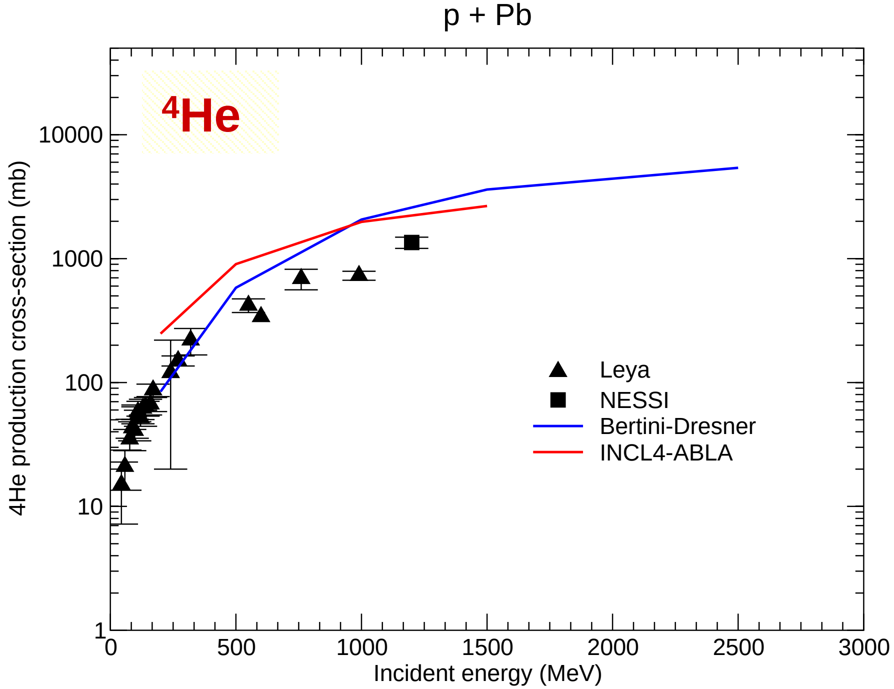


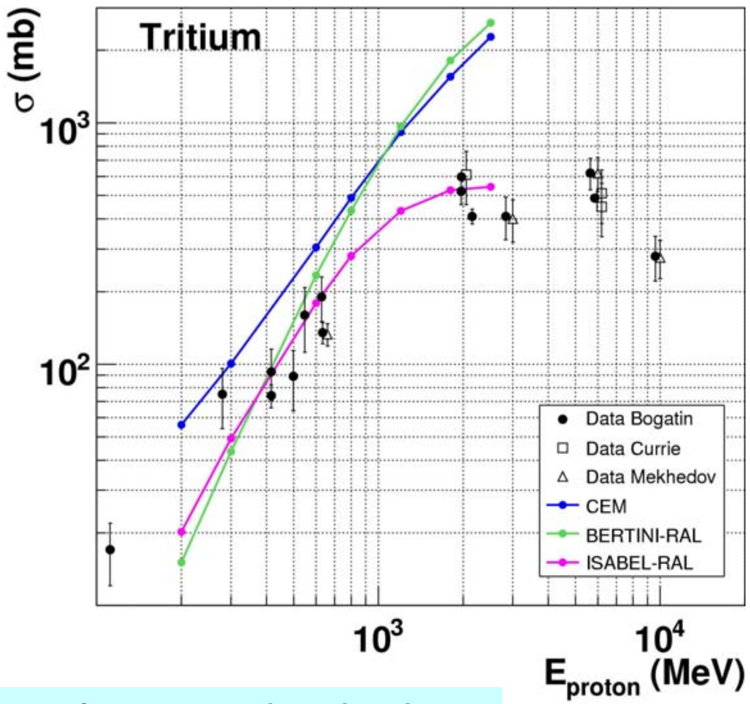


From Rapp et al., SATIF-8, Pohang (2006)

- **INCL4/ABLA does not produce tritium**
- **No good model for gas prediction in MCNPX**

Gas production in Pb

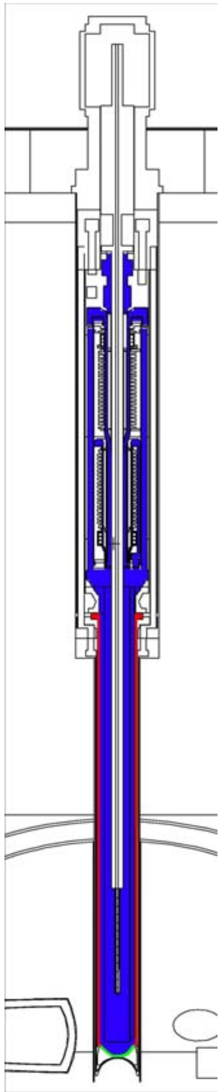




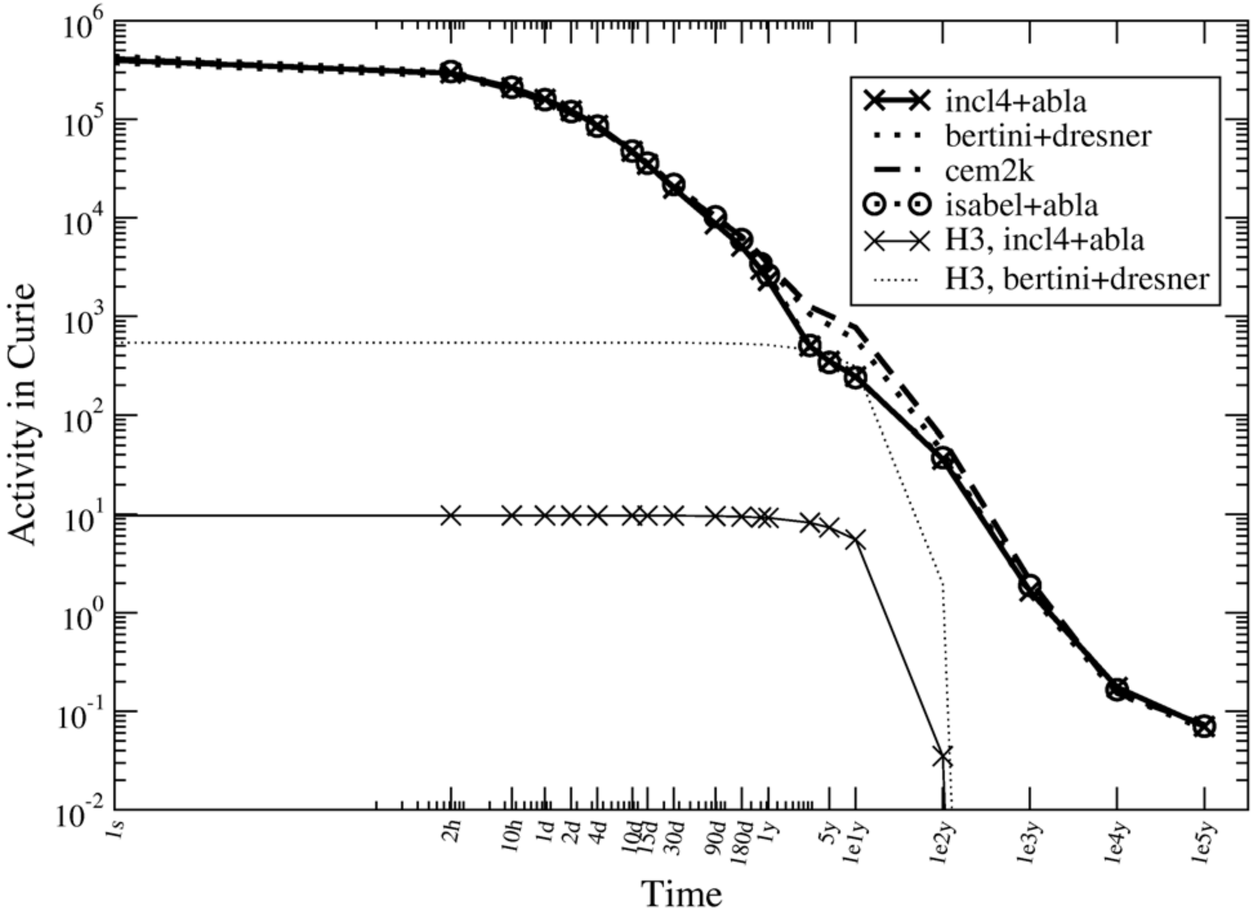
From Rapp et al. , SATIF-8, Pohang (2006)

- INCL4/ABLA does not produce tritium
- No good model for gas prediction in MCNPX

Tritium activity in the MEGAPIE target



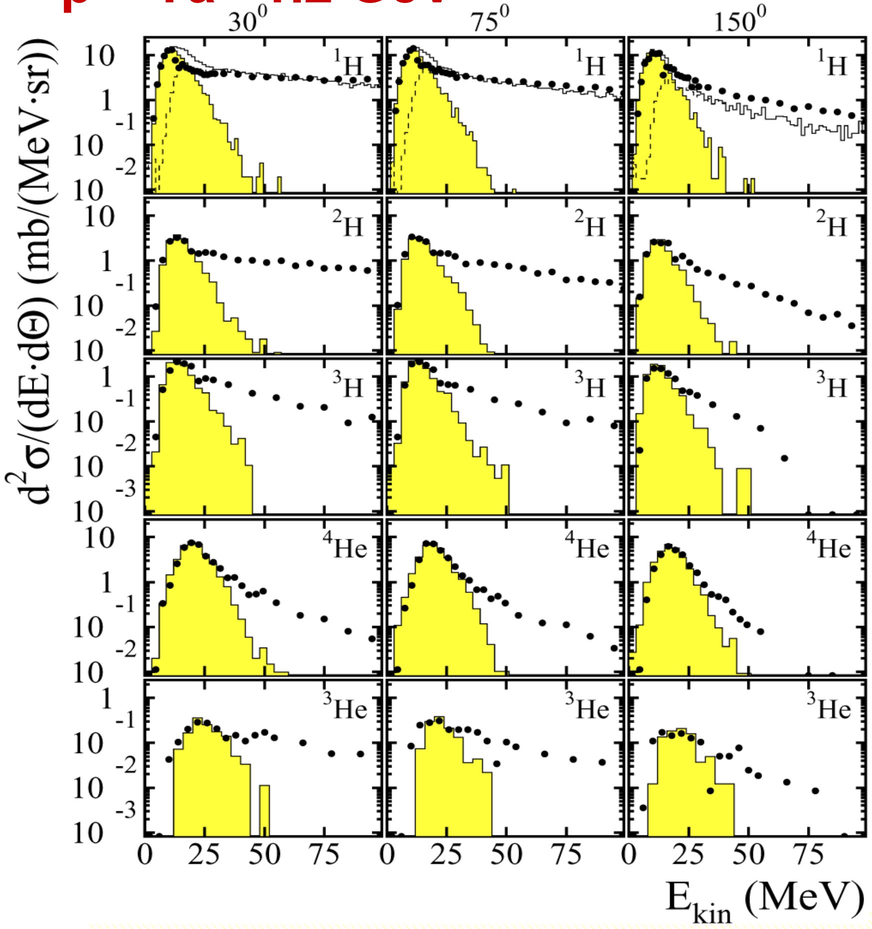
Total activity in the Pb-Bi

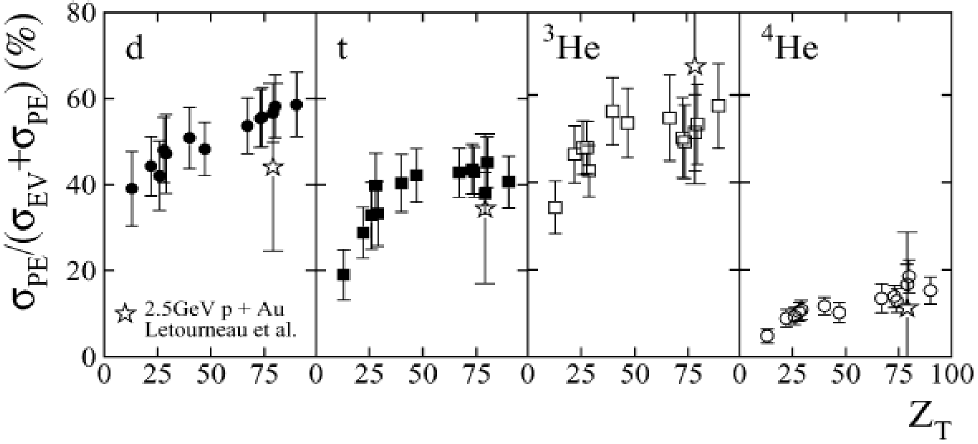


From S. Lemaire et al., ND2007

Light charged particle production

p + Ta 1.2 GeV

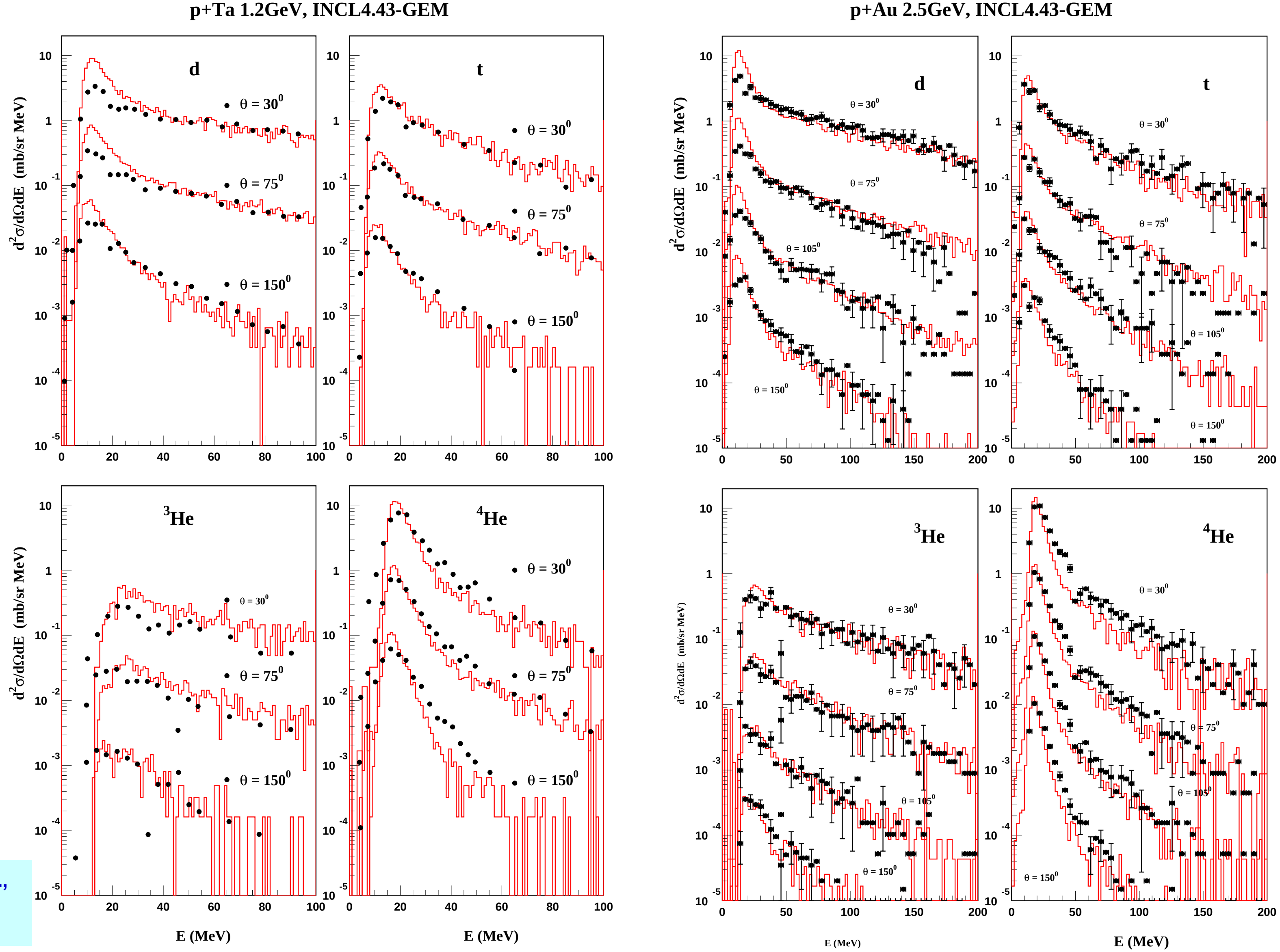




From Herbach et al., Nucl. Phys. A 765 (2006) 426

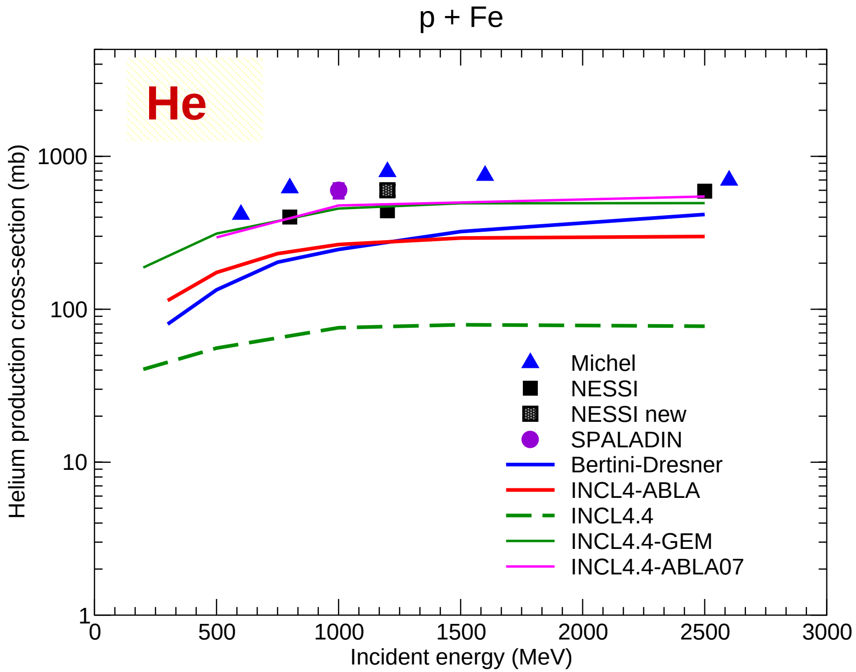
➥ **important non-evaporative contribution in d, t, ^{3}He spectra**

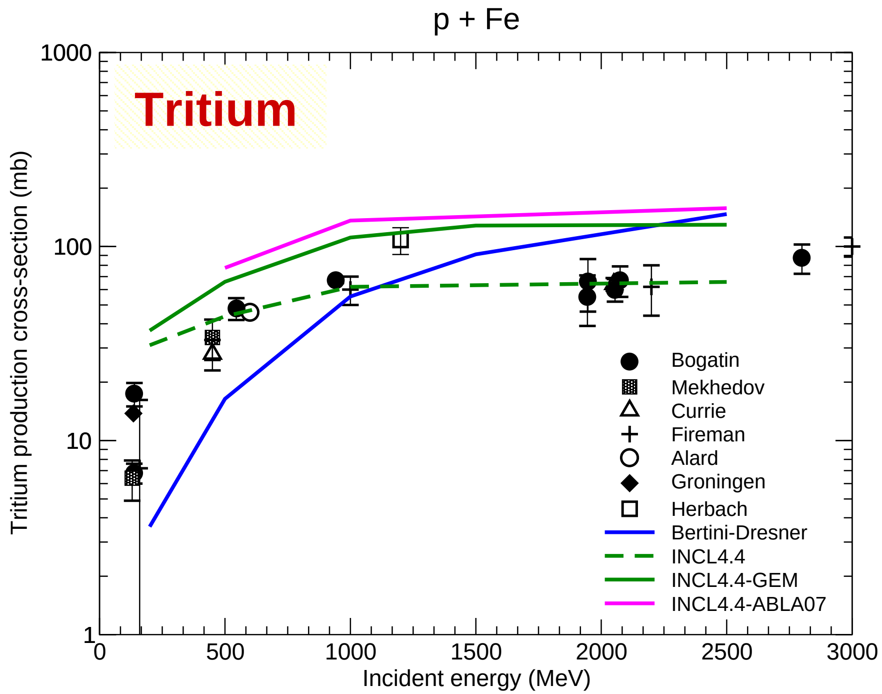
Cluster emission



Data: Herbach et al., Nucl. Phys. A 765 (2006) 426

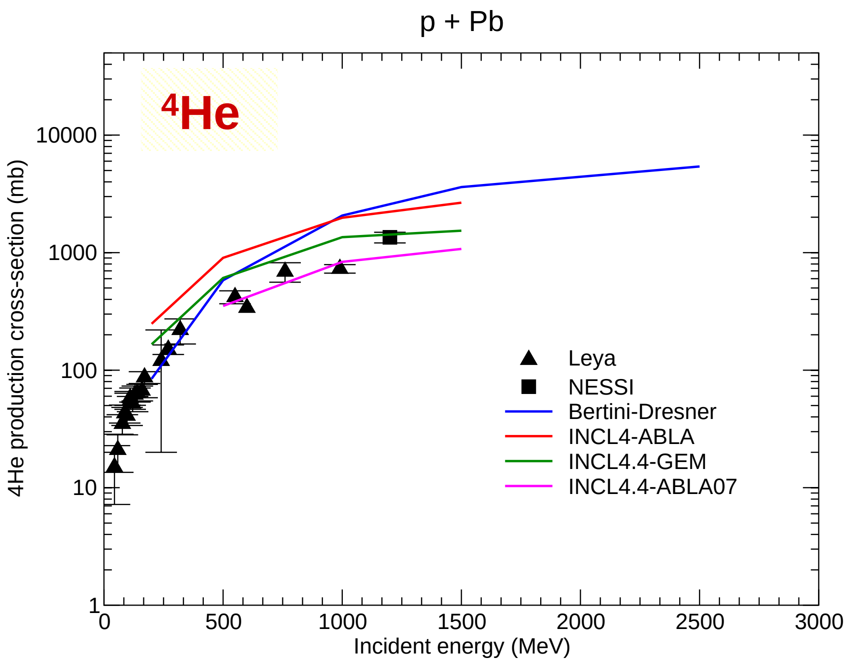
Gas production in Fe

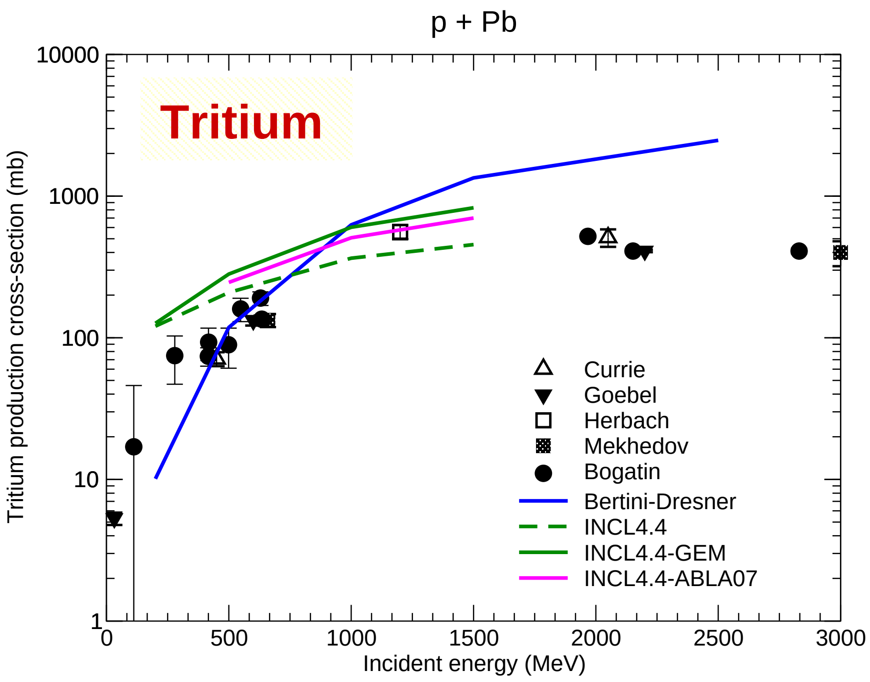




- **INCL4.4-ABLA07 now produces tritium**
- **situation improved compared to models presently in MCNPX**

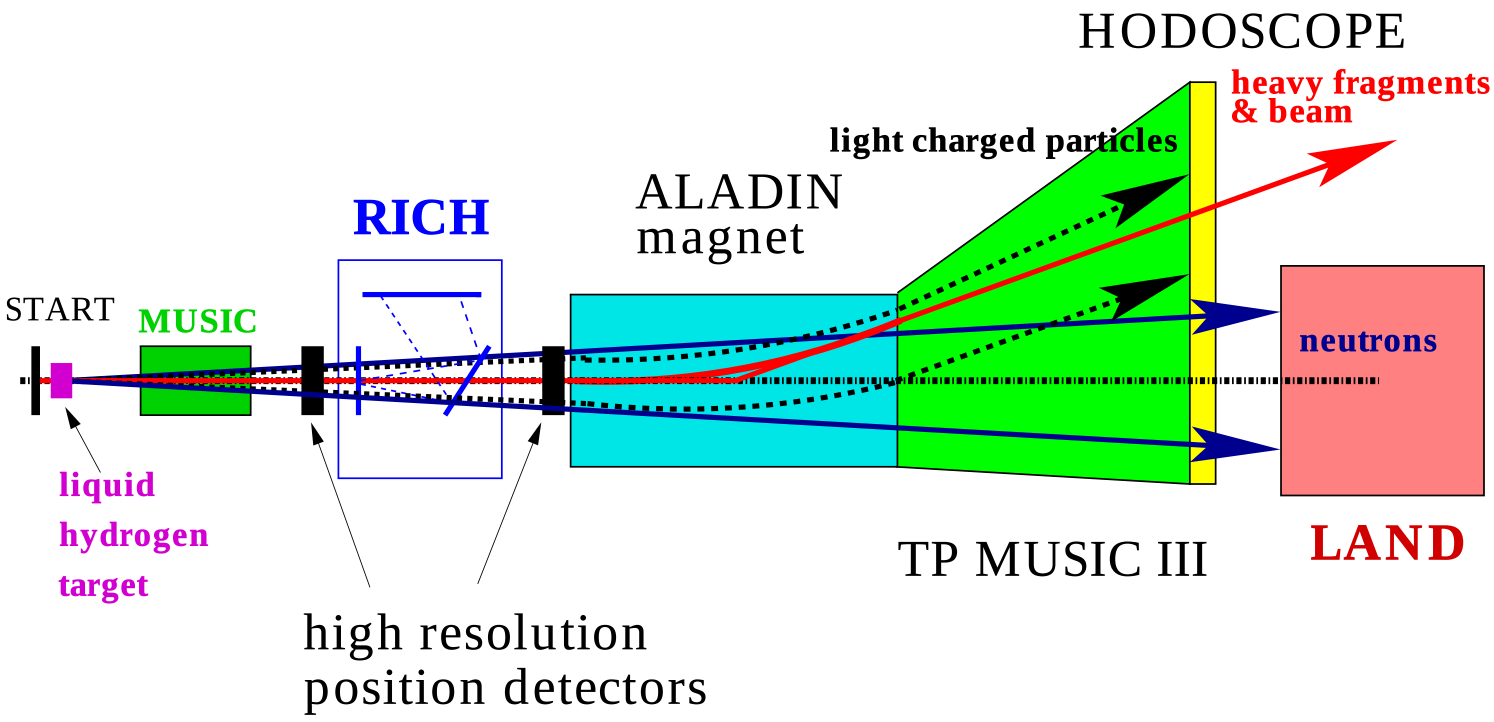
Gas production in Pb





- **INCL4.4-ABLA07 now produces tritium**
- **situation improved compared to models presently in MCNPX**

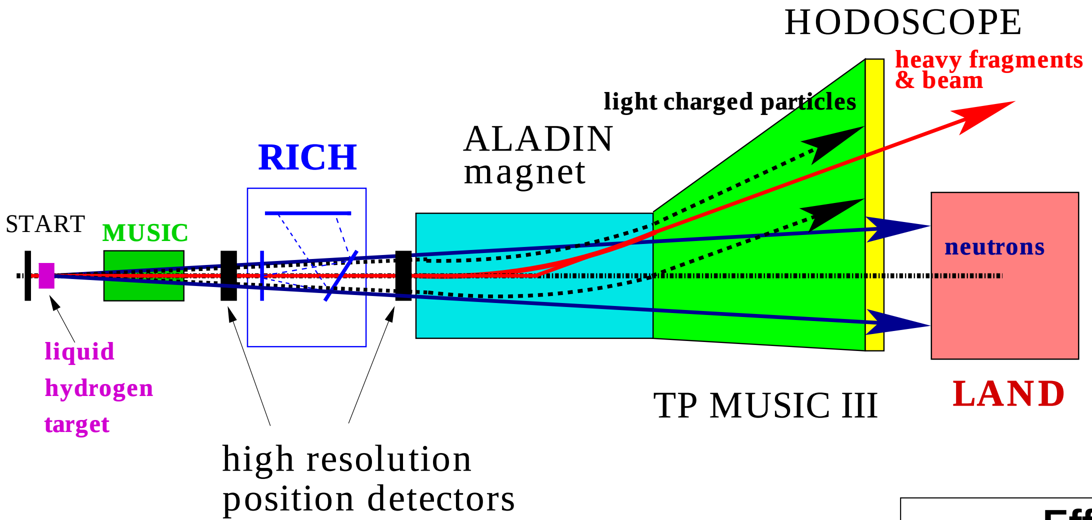
The SPALADIN experiment at GSI: Fe(1 AGeV)+p



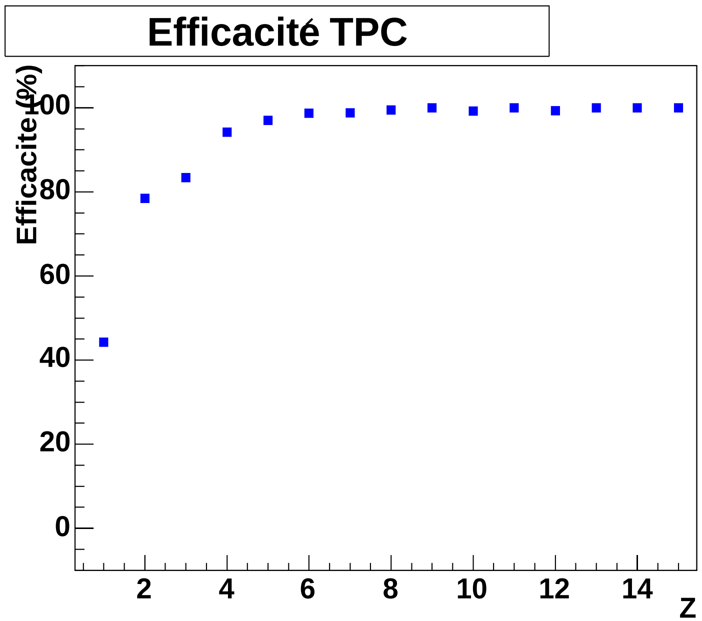
- **Reverse kinematics**

- **Measurement of all fragments simultaneously with light charged particles and neutrons from evaporation**

The SPALADIN experiment at GSI



Acceptance	Cascade	Evaporation
neutrons	11 %	64 %
protons	14 %	43 %
He	36 %	92 %
Z ≥ 3	> 97 %	



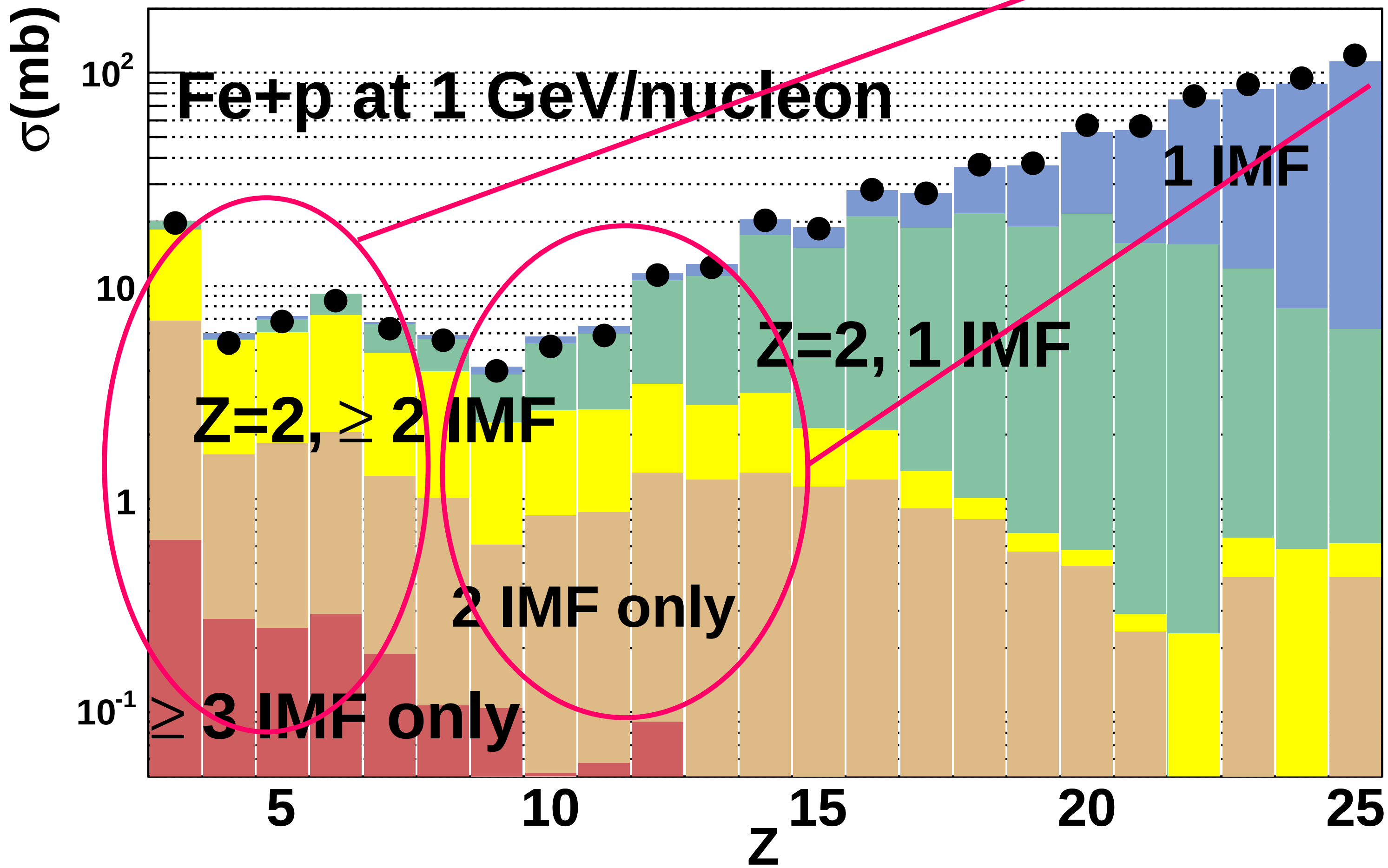
SPALADIN experiment

Def: IMF= Z≥3

IMF emission is dominant

Contributions to the cross sections

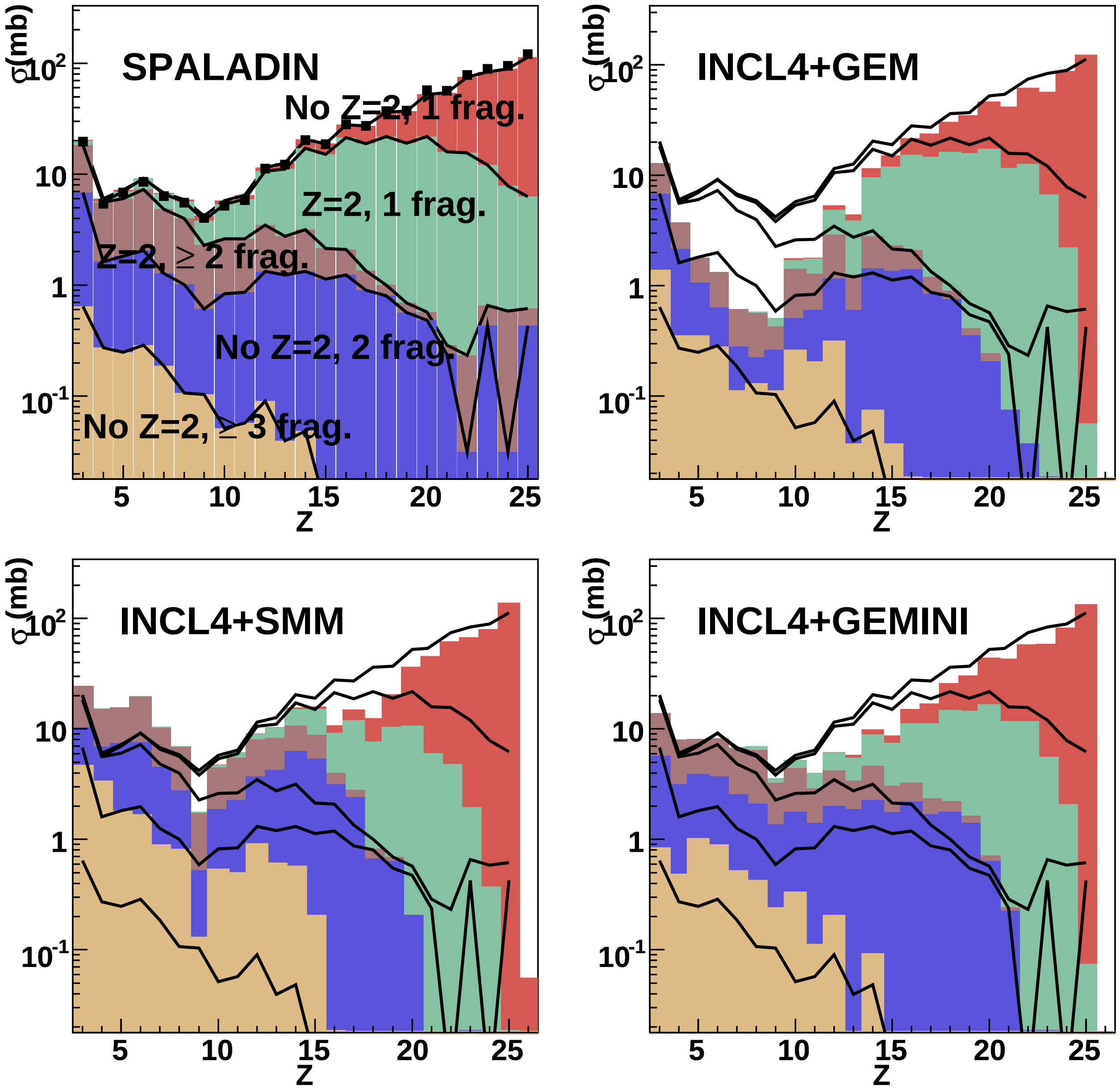
Z=2 emission is dominant



From
E. Le Gentil,
PhD Thesis

SPALADIN

Fe (1 AGeV+p)



Comparison to models:

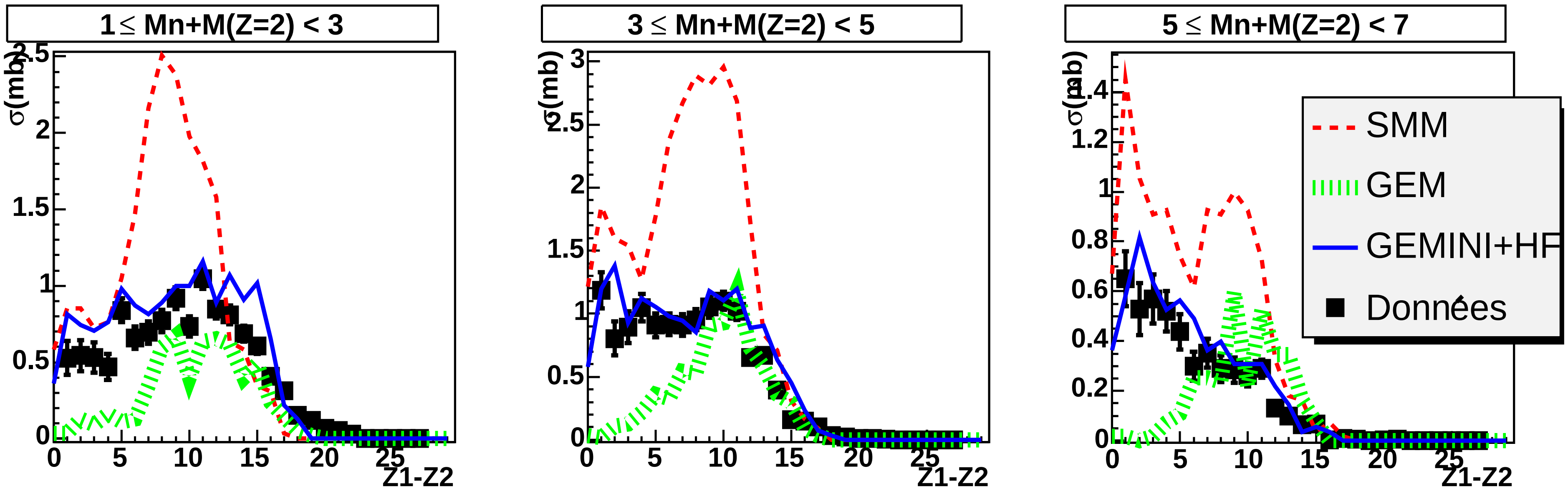
INCL4 + different de-excitation models

Calculations filtered through GEANT4

SPALADIN experiment

Events with 2 fragments (Z≥3) for different bins of particle multiplicity:

Difference between the charges of the two heaviest fragments



From E. Le Gentil, PhD Thesis
arXiv:0708.1127

SPALADIN

➢ The simultaneous measurements of fragments and LCP allows

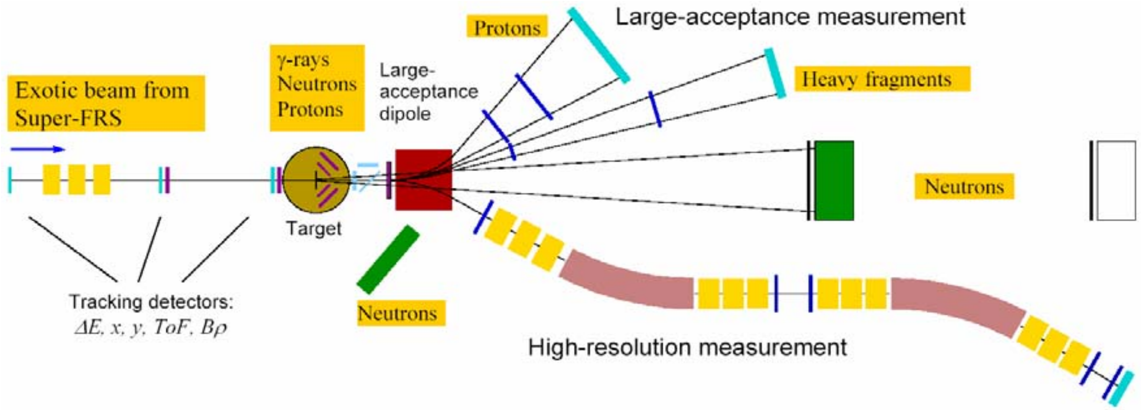
↪ to decompose the total reaction cross-section into different reaction channels

↪ to study the de-excitation mechanism as a function of E* (at moderate E*)

➢ IMF production and correlations in p+Fe at 1 GeV can be explained totally with the transition state model

➢ Near future with SPALADIN:
Si+p, Xe+p, fission

➢ Longer term future :
U+p at FAIR/R3B



Conclusion

- Specific features of spallation reactions: high energy particles, huge number of produced residues, high gas production

- Necessity of good physics models validated on good experimental data to be implemented in simulation codes

- Present predictions of currently used models acceptable for neutron production and heavy residues, only new models good for fission residues, problems for helium and light residues

- Work in progress (model improvement and more constraining experiments) should lead to better prediction of helium, tritium, IMF and light residue production