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The physics of the spallation (target)

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Introduction: content and general ideas

- Two lectures, one on physics and one on applications :
  - General description of spallation process
    - Models
    - Comparison with experimental data
  - Application to spallation targets
    - Few chosen examples

- Global bias from my past and current work
  - Models (INCL)
  - Targets (MEGAPIE)

- I will never use the word « subcritical » since I only concentrate on the target (the surrounding core does not exist… for me!!!)

- Acknowledgements: Alain Boudard (CEA), Sylvie Leray (CEA), Luca Zanini (PSI)

Introduction: spallation physics

- General characteristics and observables

- Strategy:
  - observables for the range 20 MeV-200MeV
  - models beyond 200 MeV

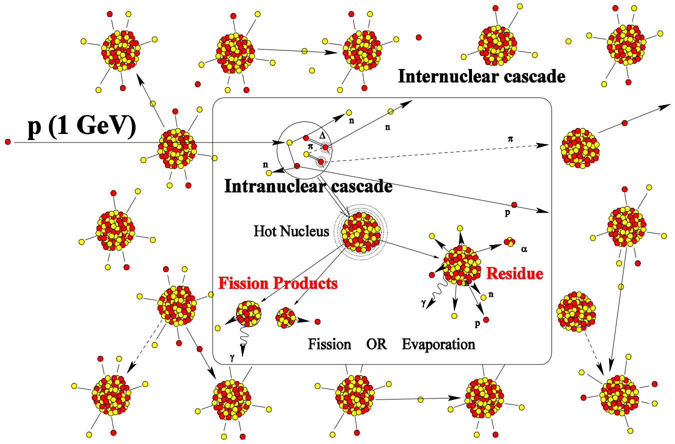
- Modelling of the spallation physics
  - Two or three steps
  - Low energy models

- Experimental information:
  - Large list of observables
  - Comparison with model predictions

- What we have and what we still need…

Spallation: definition and history

- Spallation definition (*G.T. Seaborg, PhD thesis, 1937*)
  - Process between a light particle (p,n) with an energy of at least 100 MeV with an “heavy” nucleus leading to emission of light particles and leaving an heavy residue
  - NOT a reaction!!! But an *ensemble* of nuclear reactions
    - Huge variety of final states



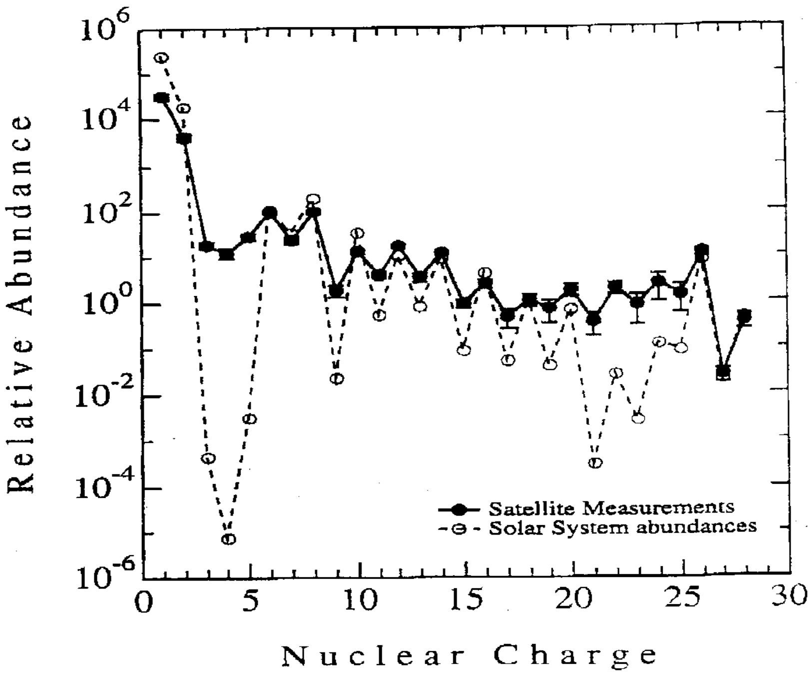
- History:
  - observation of particle cascades in cosmic rays interactions
    G. Rossi, ZP82 (1933) 151
  - first accelerators: many nucleons emitted by the target nucleus
    Cunningham, PR72 (1947) 739
  - two step mechanism
    Serber, PR72 (1947) 1114

Spallation: observables

- Observables needed for the design of a target:
  - Neutron production
    - Number ➔ power of the system / needed accelerator intensity
    - Energy and spatial distribution ➔ target
    - High energy neutrons ➔ shielding
  - Charged particle production
    - Gas production (H_2, He) ➔ embrittlement
    - Energy distributions ➔ Energy deposition, dpa
  - Residual nuclei production
    - Element distribution ➔ corrosion, change in metallurgical properties
    - Isotope distribution ➔ activity (short lived isotopes), radiotoxicity (long lived isotopes), decay heat
    - Recoil energies ➔ dpa in structures, energy deposition

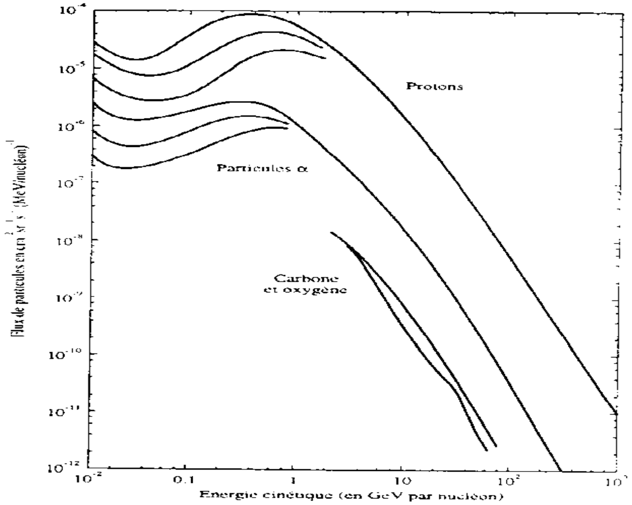
Spallation: applications in different fields

- Astrophysics
  - Secondary reactions of cosmic rays in interstellar medium
    - explanation of abundance of isotopes
    - decide among models for galactic nucleosynthesis
    - origin of cosmic rays
  - Composition of meteorites



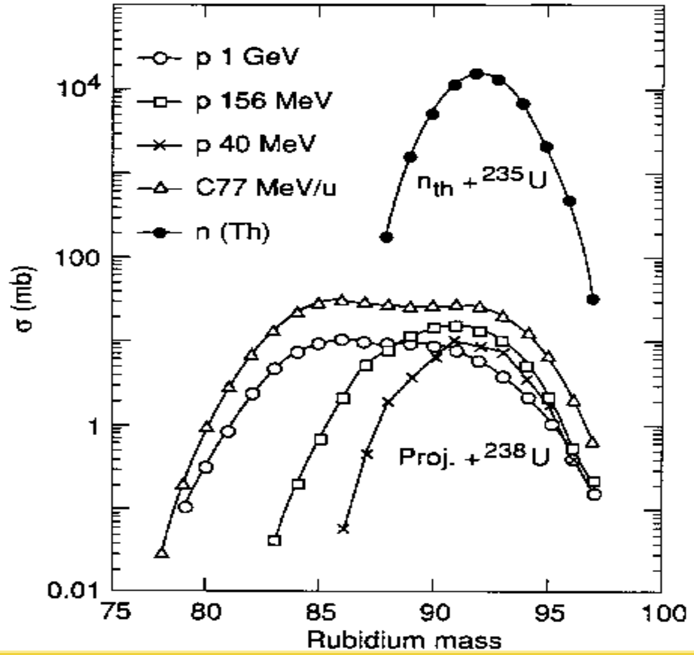
Spallation: applications in different fields

- Space instruments
  - Cosmic ray bombardment of the spacecraft and instruments
    - Radiation damage on electronics
    - Radioprotection of space crew
    - Noise due to secondary gammas, neutrons and spallation residues
      - Ex.: spectrometer of the INTEGRAL mission devoted to high resolution γ-ray astronomy



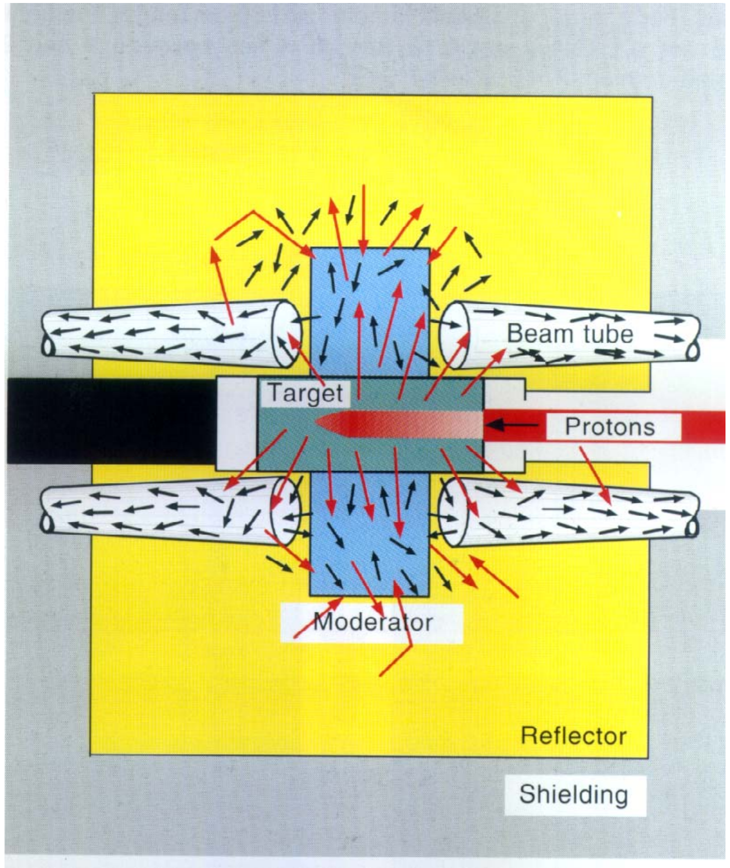
Spallation: applications in different fields

- Rare isotope production and RIB
  - Direct methods
    - 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
    - produce tritium and radioisotopes for medicine

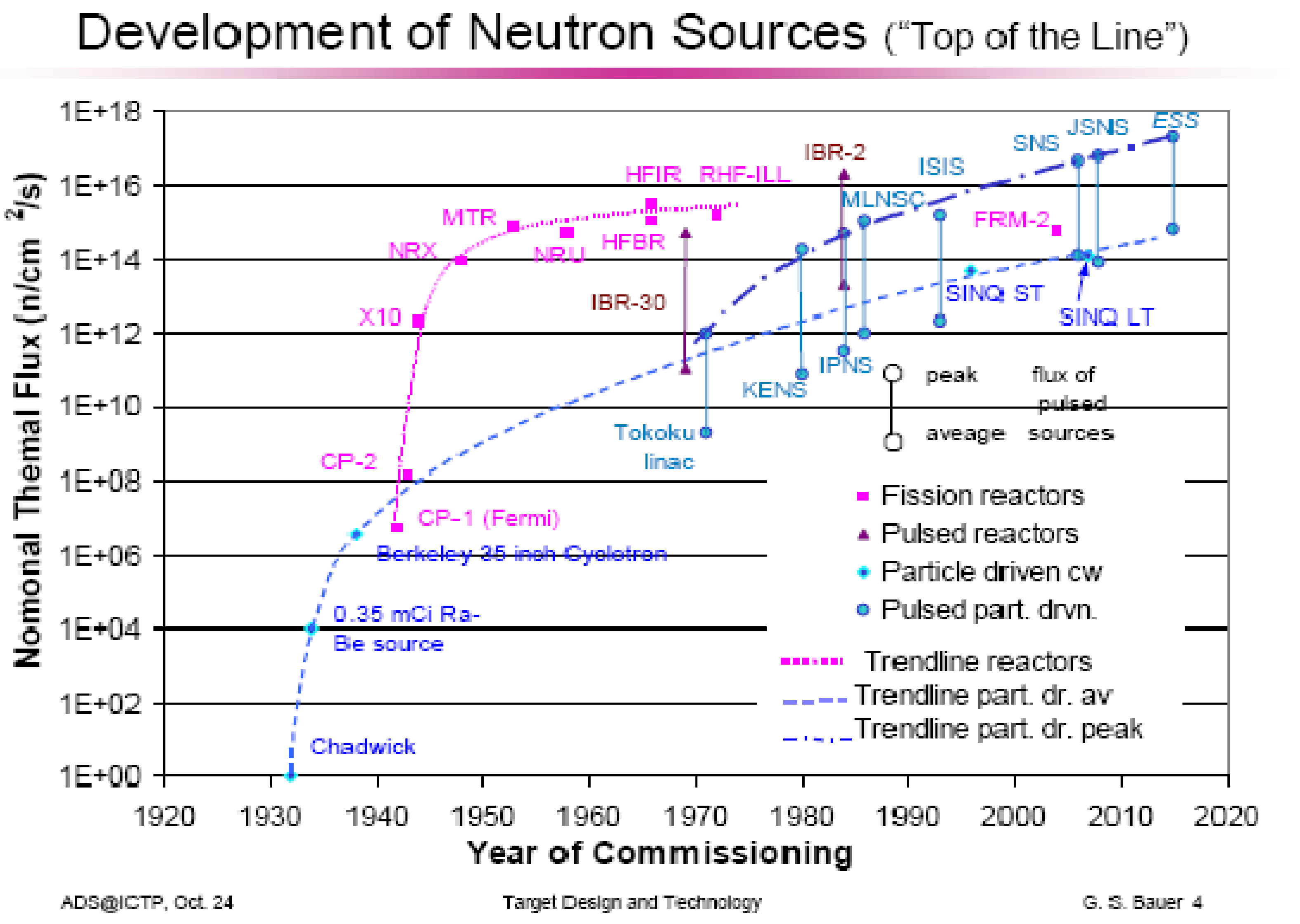


Spallation: applications in different fields

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



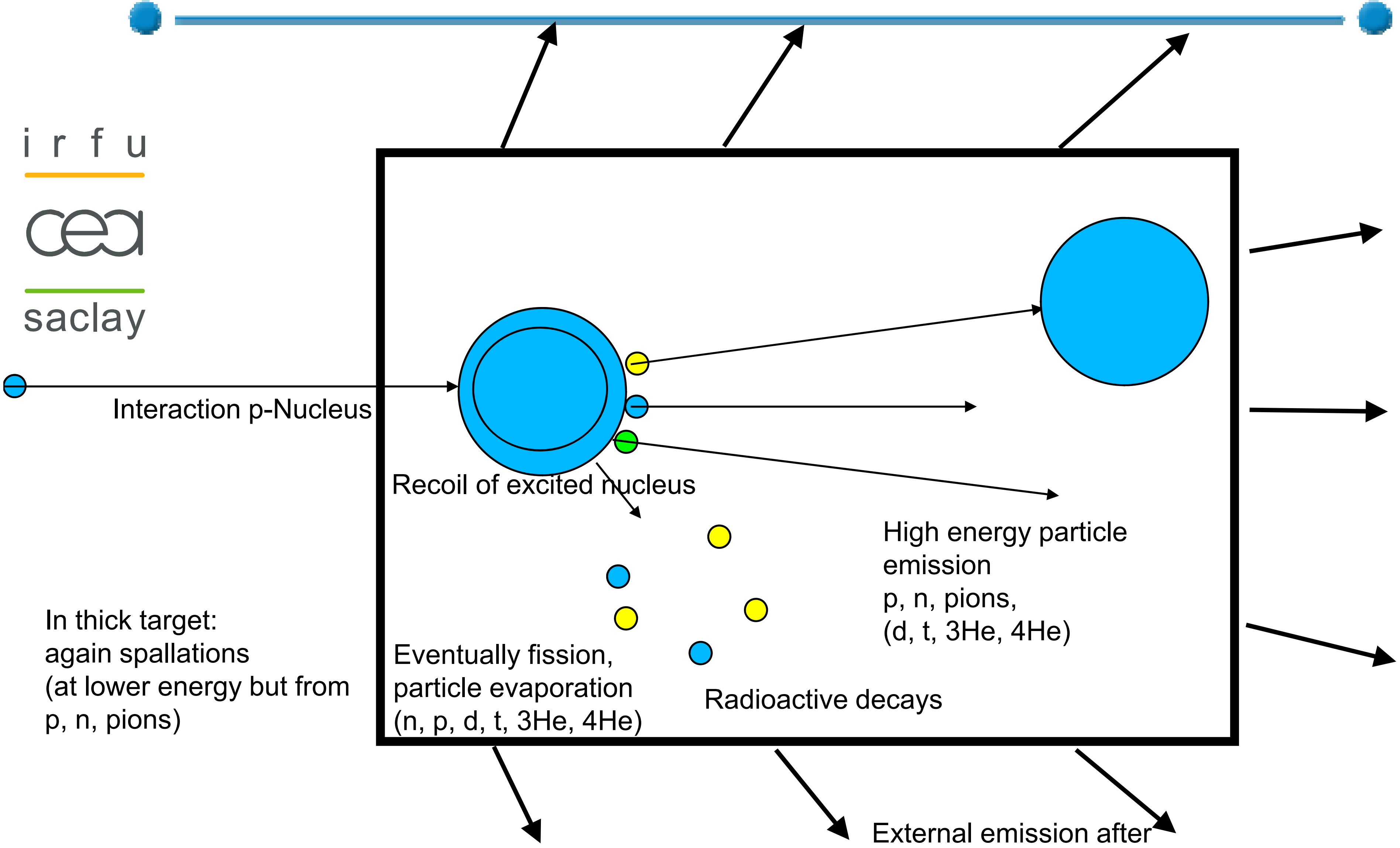
Neutron sources in the world



Development of Neutron Sources ("Top of the Line")

ADS@ICTP, Oct. 24   Target Design and Technology   G. S. Bauer 4

The spallation process as a cartoon….



Interaction p-Nucleus

Recoil of excited nucleus

High energy particle
emission
p, n, pions,
(d, t, 3He, 4He)

In thick target:
again spallations
(at lower energy but from
p, n, pions)

Eventually fission,
particle evaporation
(n, p, d, t, 3He, 4He)

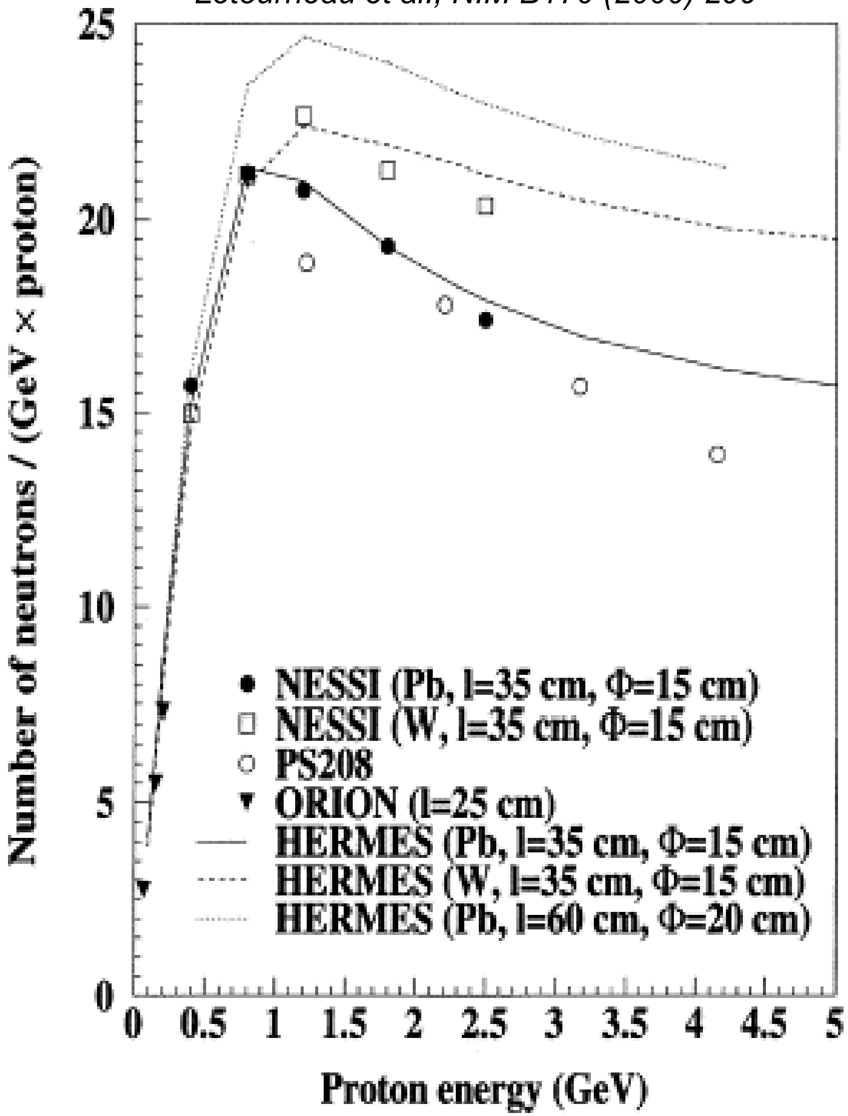
Radioactive decays

External emission after
diffusion-absorption
(transport)

Spallation neutron production

- In heavy metal target (Pb, W, Ta) around 20 neutrons per incident proton and GeV
- Maximal efficiency around 1GeV BUT…
  - Very dependent on geometry and optimization…

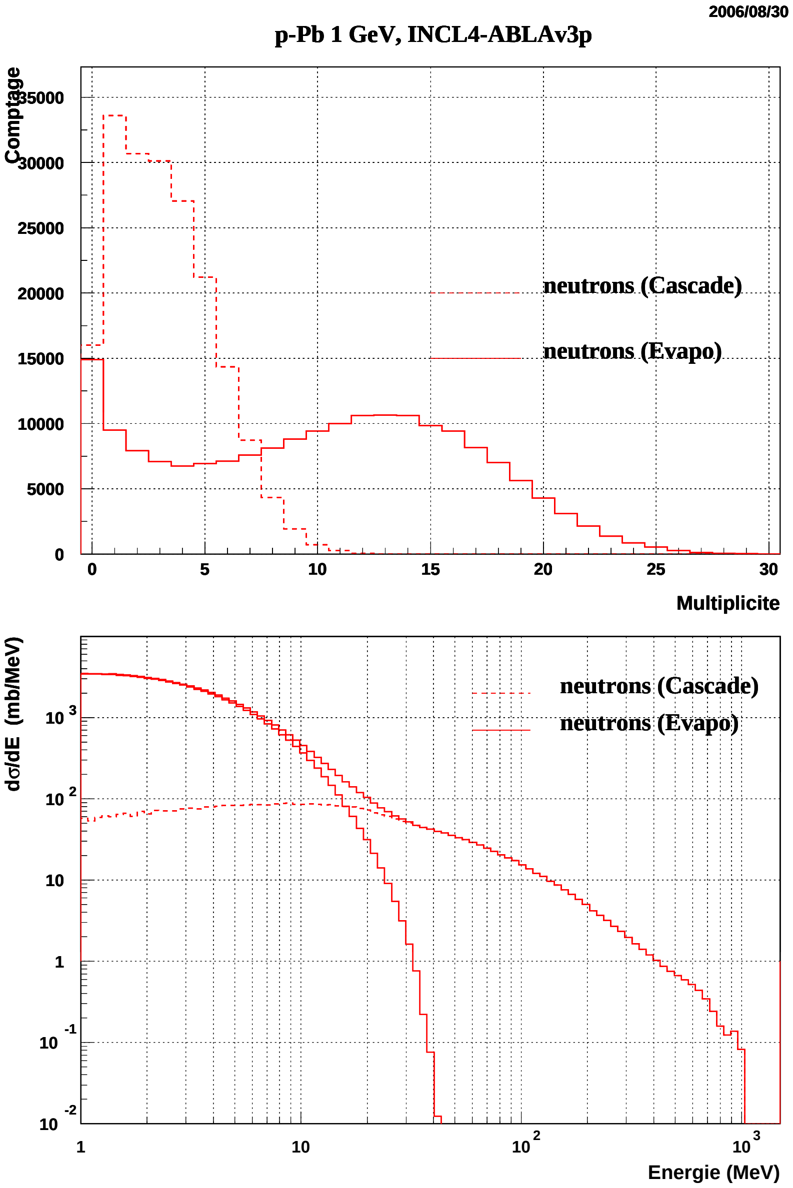
Letourneau et al., NIM B170 (2000) 299



Spallation characteristics: neutron spectrum

Neutrons come from:

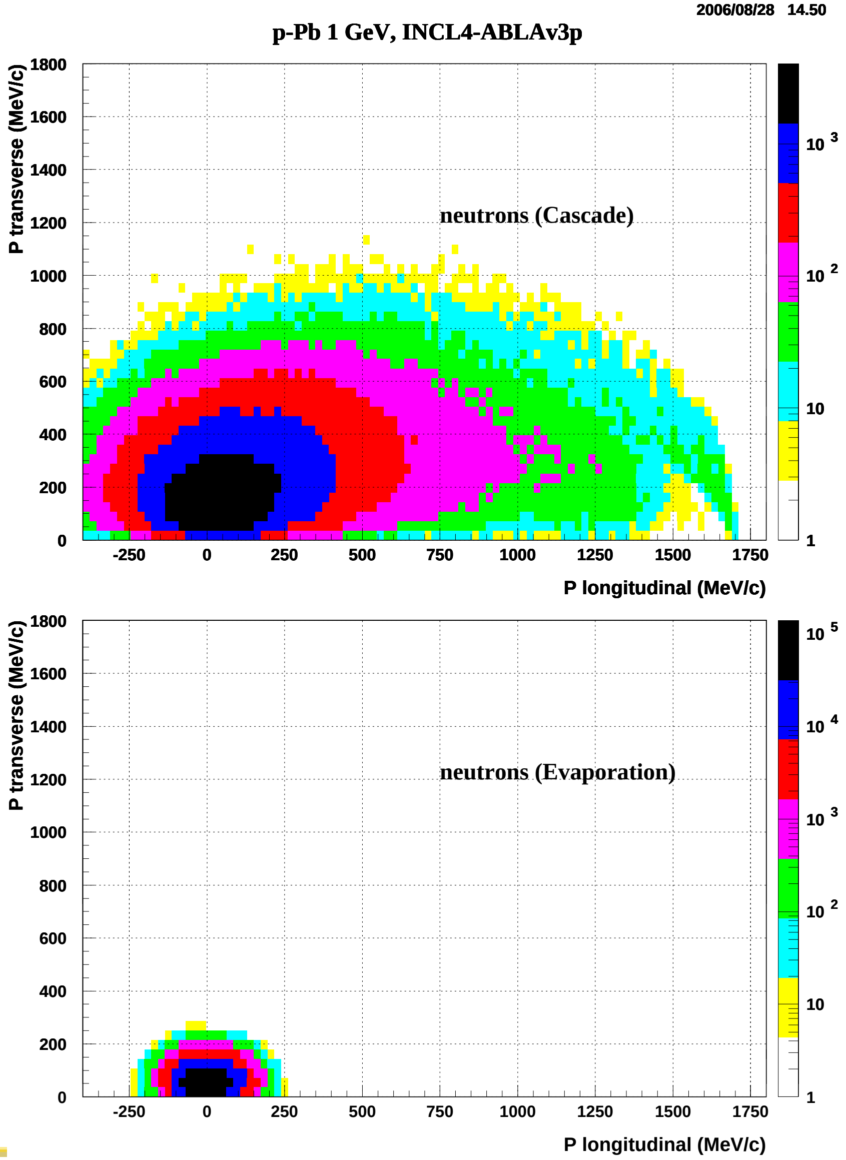
- Cascade
  - High energy
  - Low multiplicity
- Evaporation
  - $E_n < 20$ MeV
    - High cross section
  - High multiplicity



Spallation characteristics: n angular distrib.

Neutrons from:

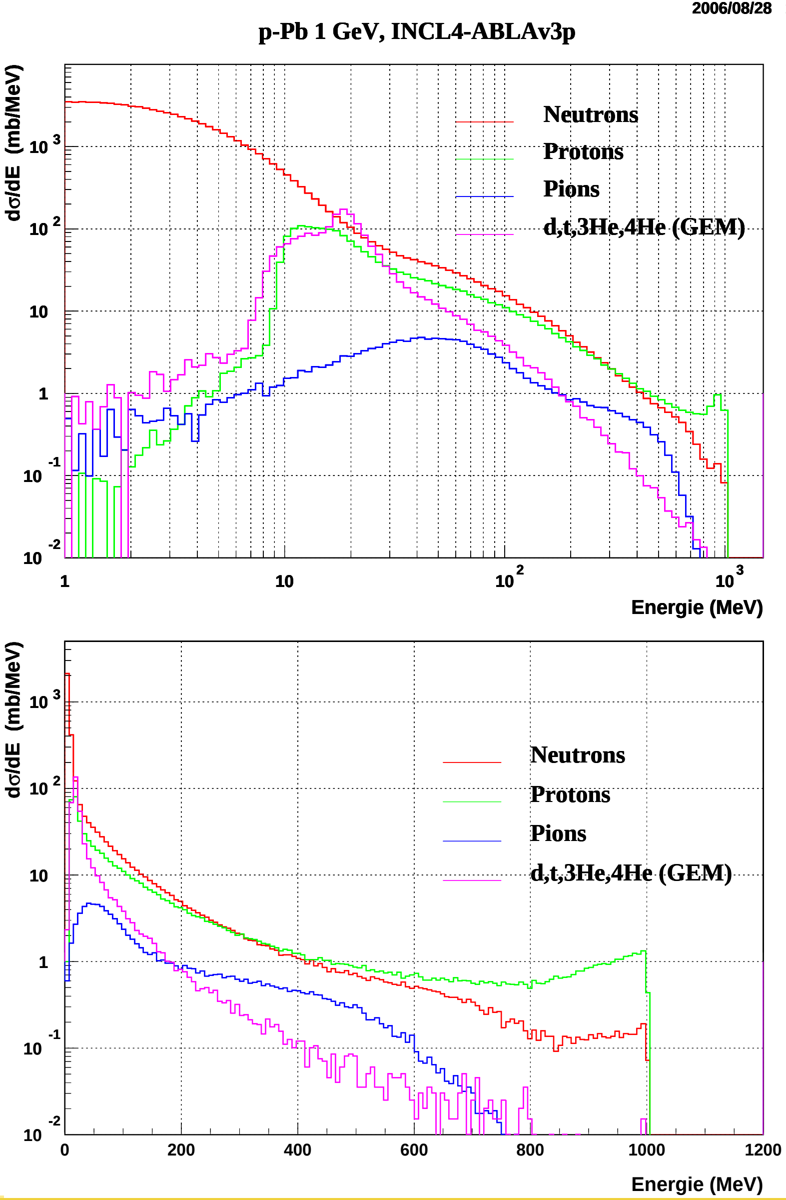
- Cascade
  - Forward emission
- Evaporation
  - Isotropic emission



Spallation characteristics: particle spectra

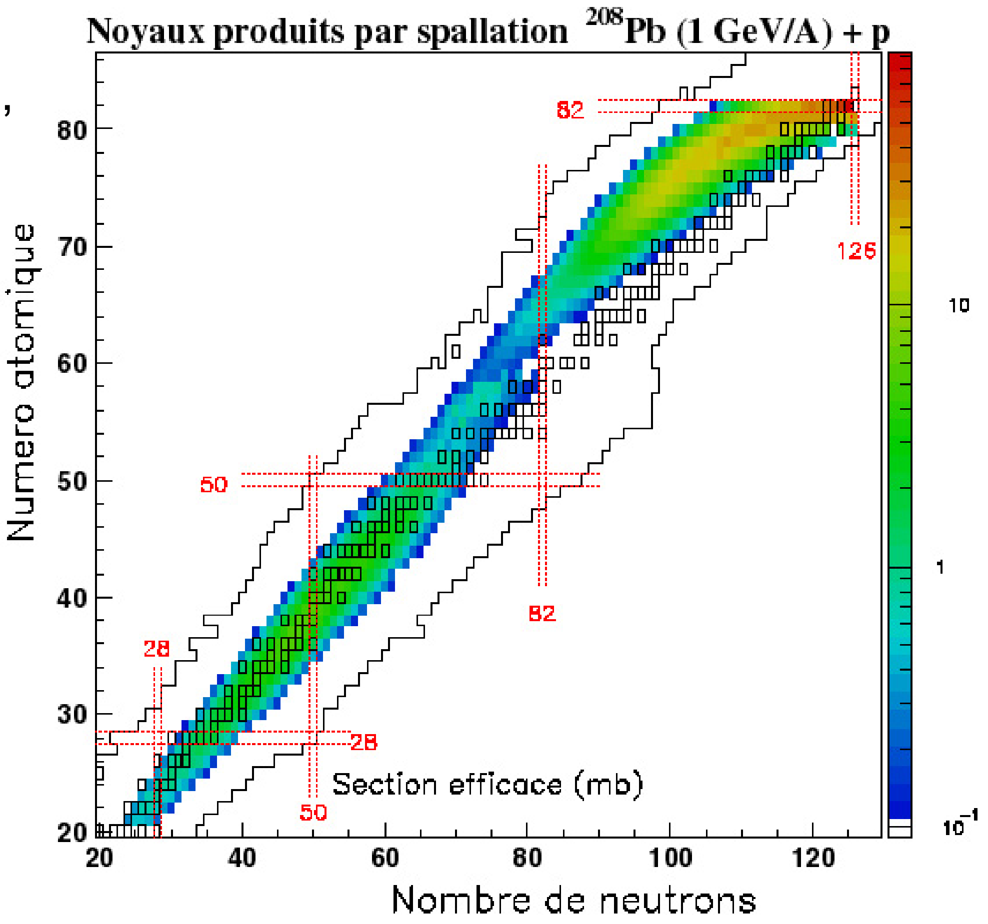
- Neutrons
  - Predominant at low energy (not sensitive to the Coulomb barrier)
- Protons
  - Predominant at high energy
- Light charged particles (LCP)
  - Important between 10 and 100 MeV
- Pions
  - Non negligible between 100 MeV and 1 GeV
- Cascade particles have lower multiplicity BUT they mainly carry the beam energy

Type	Mean energy (MeV)	Fraction in cascade
n	355	85 %
p	364	98 %
π	58	100%
lcp	69	80%
Remnant (E*)	137	

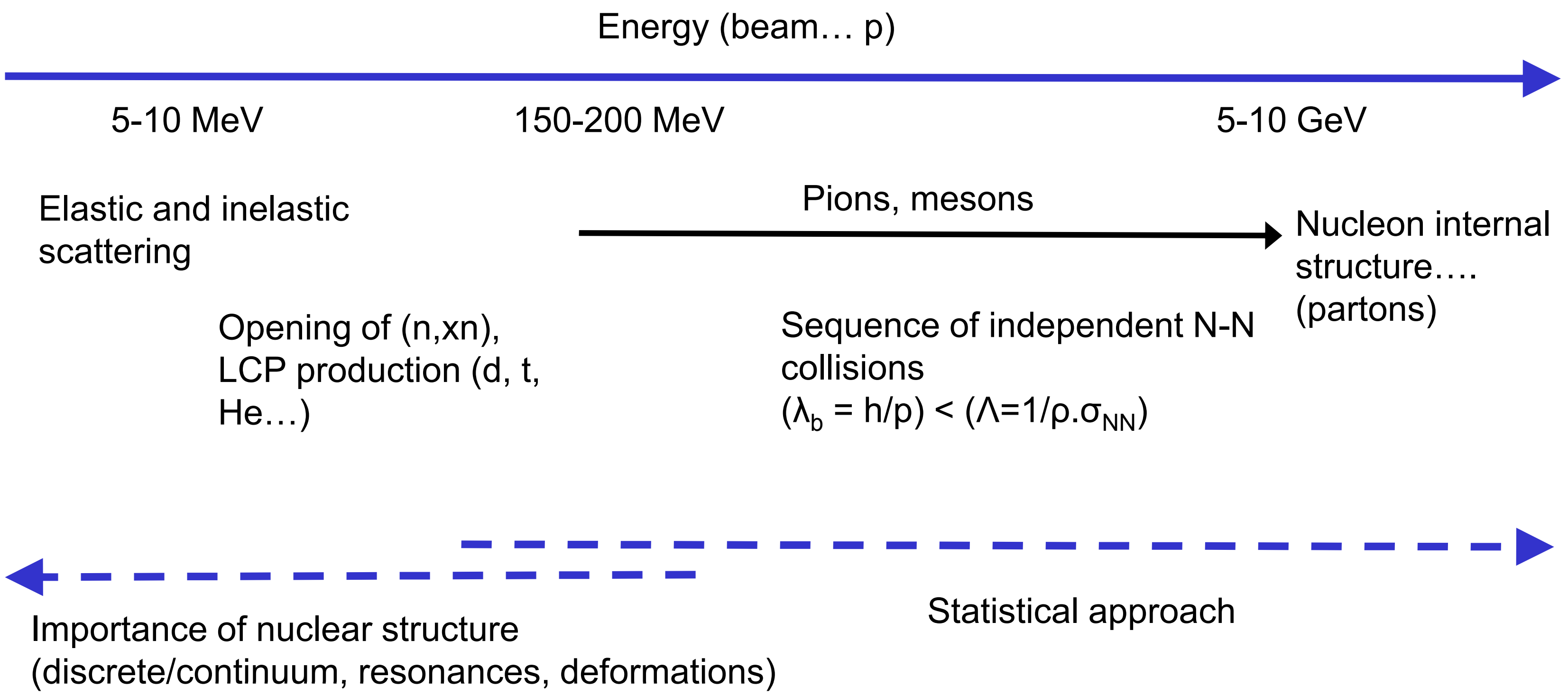


Spallation characteristics: residues production

- Hundreds of different residues are produced by
  - Evaporation (high mass, near the target mass)
  - Fission (lighter mass)



Modeling of spallation reactions



Energy (beam… p)

5-10 MeV

150-200 MeV

5-10 GeV

Elastic and inelastic scattering

Pions, mesons

Nucleon internal structure…. (partons)

Opening of (n,xn), LCP production (d, t, He…)

Sequence of independent N-N collisions $(\lambda_b = h/p) < (\Lambda=1/\rho.\sigma_{NN})$

Importance of nuclear structure (discrete/continuum, resonances, deformations)

Statistical approach

Optical model, DWBA, coupled channels

Pre-equilibrium models (config. particle-hole, excitons)

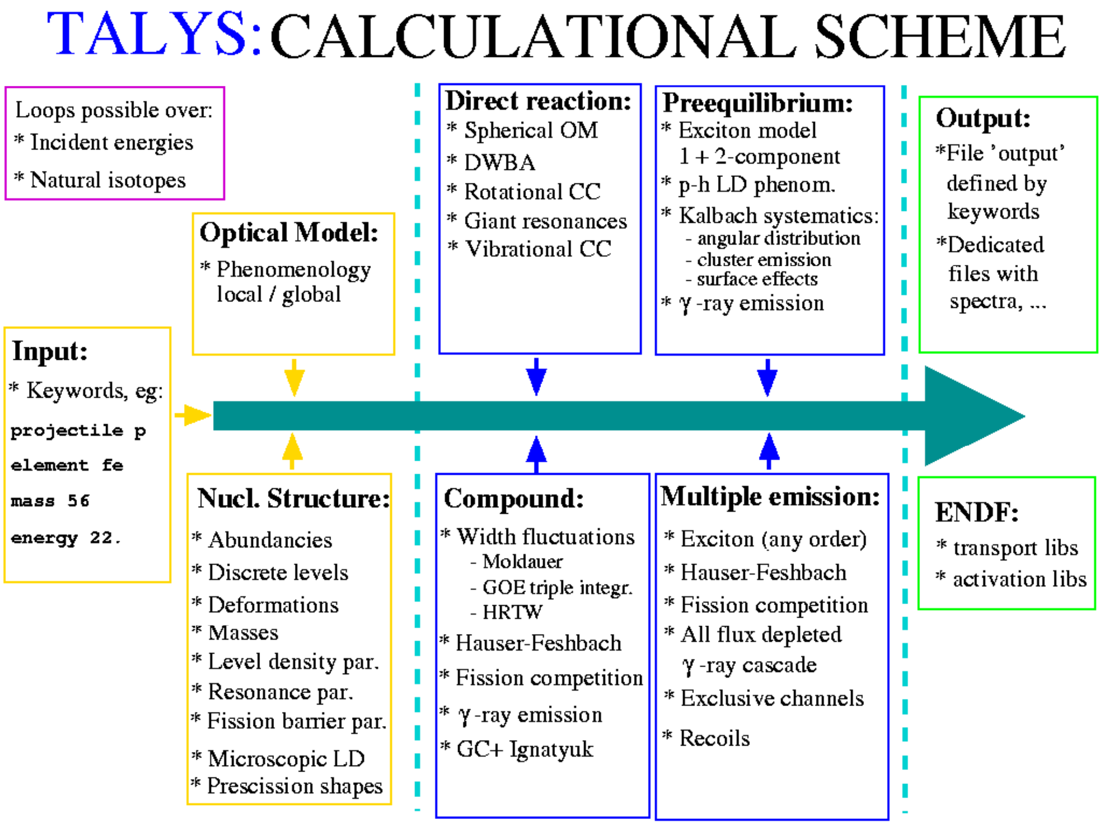
Limits are not well defined: a lot of overlapping

Intra-nuclear cascade + de-excitation

(Coherent diffusion: Glauber-KMT)

Modeling of spallation reactions

Ep < 200 MeV, code type: TALYS *(A. Koning, JP Delaroche et al.)*



TALYS: CALCULATIONAL SCHEME

Loops possible over:
- Incident energies
- Natural isotopes

Optical Model:
- Phenomenology local / global

Input:
- Keywords, eg:

```
projectile p
element fe
mass 56
energy 22.
```

Nucl. Structure:
- Abundancies
- Discrete levels
- Deformations
- Masses
- Level density par.
- Resonance par.
- Fission barrier par.
- Microscopic LD
- Prescission shapes

Direct reaction:
- Spherical OM
- DWBA
- Rotational CC
- Giant resonances
- Vibrational CC

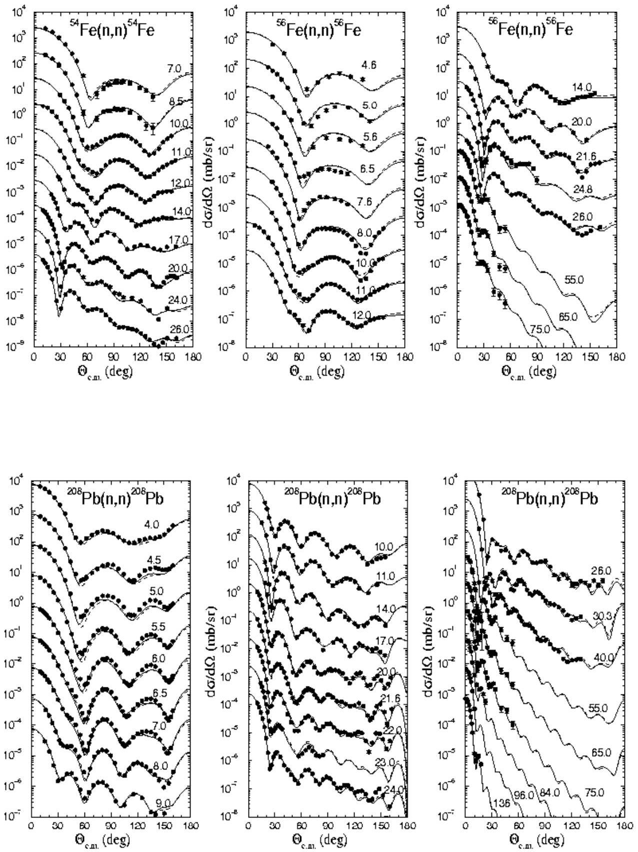
Compound:
- Width fluctuations
  - Moldauer
  - GOE triple integr.
  - HRTW
- Hauser-Feshbach
- Fission competition
- γ -ray emission
- GC+ Ignatyuk

Preequilibrium:
- Exciton model 1 + 2-component
- p-h LD phenom.
- Kalbach systematics:
  - angular distribution
  - cluster emission
  - surface effects
- γ -ray emission

Multiple emission:
- Exciton (any order)
- Hauser-Feshbach
- Fission competition
- All flux depleted γ -ray cascade
- Exclusive channels
- Recoils

Output:
- File 'output' defined by keywords
- Dedicated files with spectra, ...

ENDF:
- transport libs
- activation libs

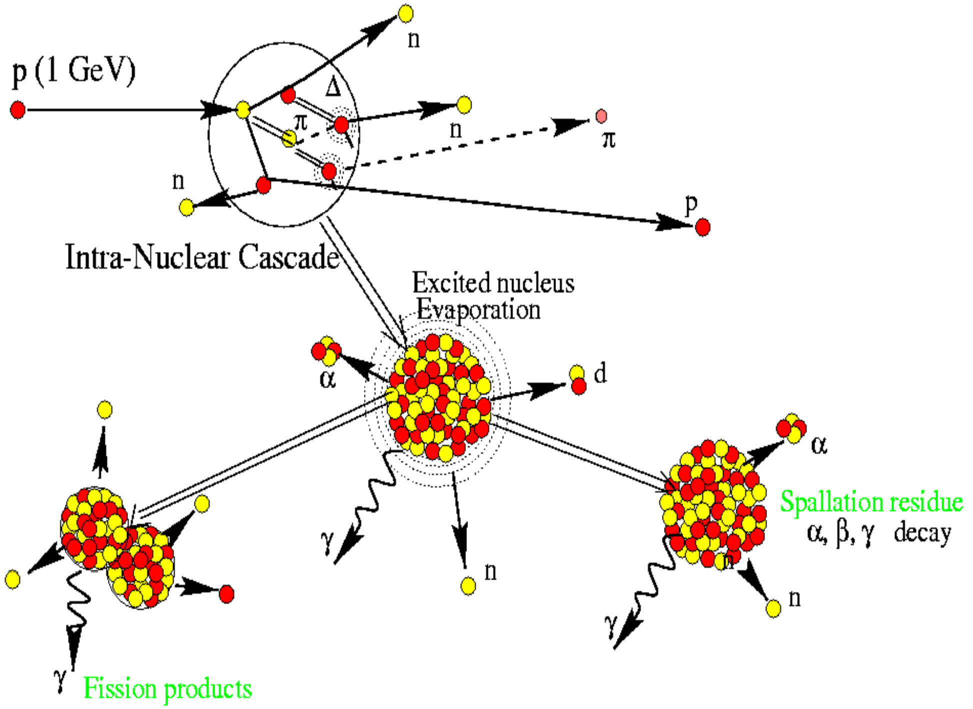


Lots of input, parameter fitting, phenomenological approach
- Very good on elastic scattering, (also (n,xn) ou (n,xp), Koning, Duijvestijn)
- More difficult on compound production (LCP)

GNASH: older code but same type *(P. Young et al. Los Alamos)*

Modeling of spallation reactions

- Two step mechanism:
  - Intra-Nuclear Cascade
    - Sequence of independent N-N collisions
    - $\Lambda_b = hc/p \ll \lambda = 1/\rho\sigma_{NN}$ (mean free path)
    - Fast process (≈30 fm/c)
  - De-excitation
    - Competition between evaporation and fission
    - Statistical models
    - Slow process (hundreds of fm/c)



- Three step mechanism
  - INC
  - Pre-equilibrium
  - Evaporation/fission

Modeling of pre-equilibrium

Exciton = 1 particle - hole

« never come back »: towards more complexity

Ingredients:

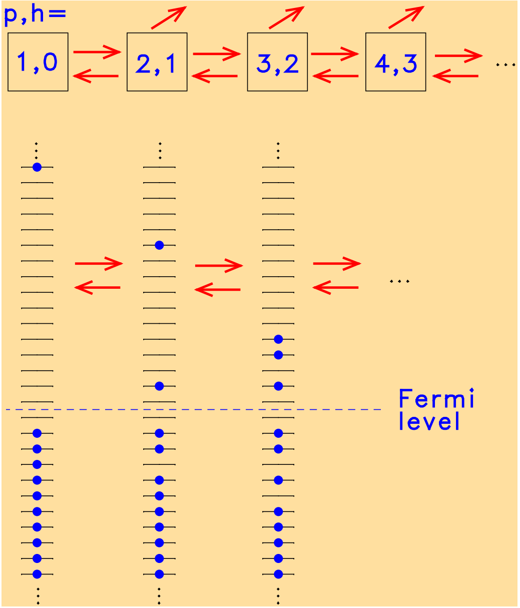
- Transition between configurations
- Level density (statistical description, Gilbert-Cameron)
- Emission probability (Weisskopf-Ewing)
  - Direct emission (1 param.)
  - Compound emission (2 param.)

  Parameters are fitted on data

  (Kalbach systematic)

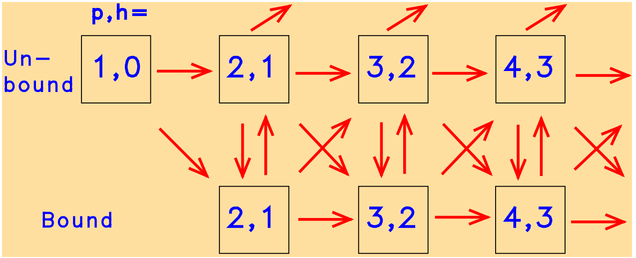
J. Griffin,Phys. Rev. Lett. 17 (1966) 478

(C. Kalbach, Phys. Rev. C33 (1986) 818)



- Twofold differentiation: proton-neutron (shell and pairing effect taken into account)

- There are a lot of extensions
- This part is “naturally” taken into account in INC-EVAP models (but not energy levels)



(bound exciton configurations)

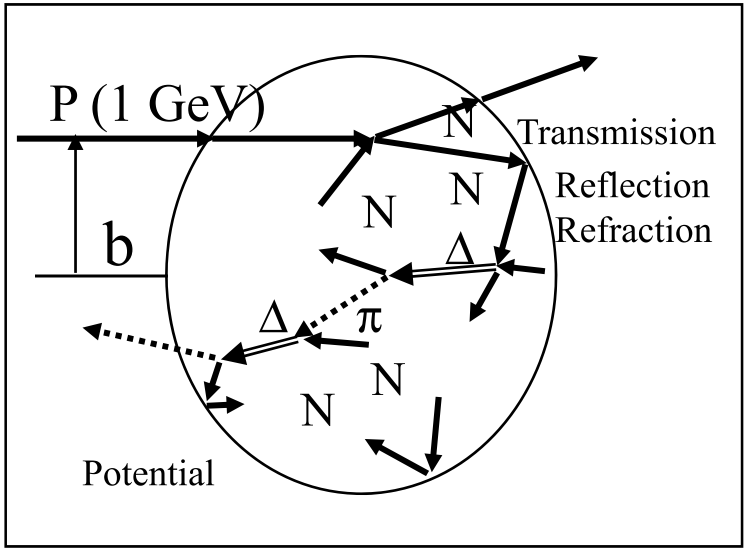
Modeling of intra-nuclear cascade (INC)

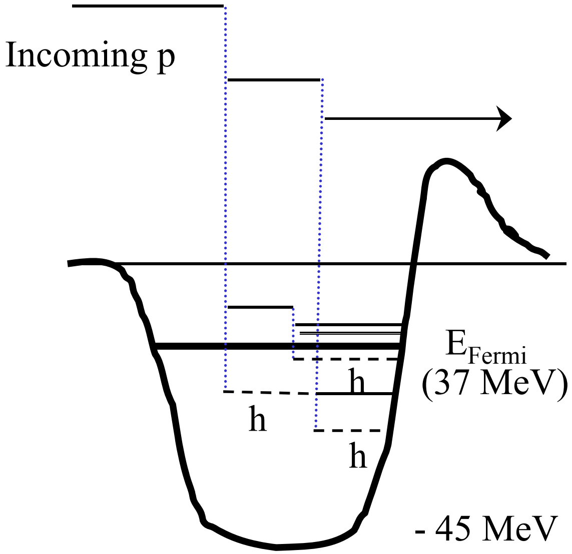
Ingredients:

- Realistic nuclear density (r,p space)
- Realistic NN interaction
  - $\sigma_{NN}(E)$, $d\sigma/d\Omega(\theta)$
  - Elastic
  - Pion production
- Pauli blocking
- Particles are “followed” in space (and time)
- N participants-spectators

  (participant beam + N interacting)
- Endpoint criteria (time or energy)

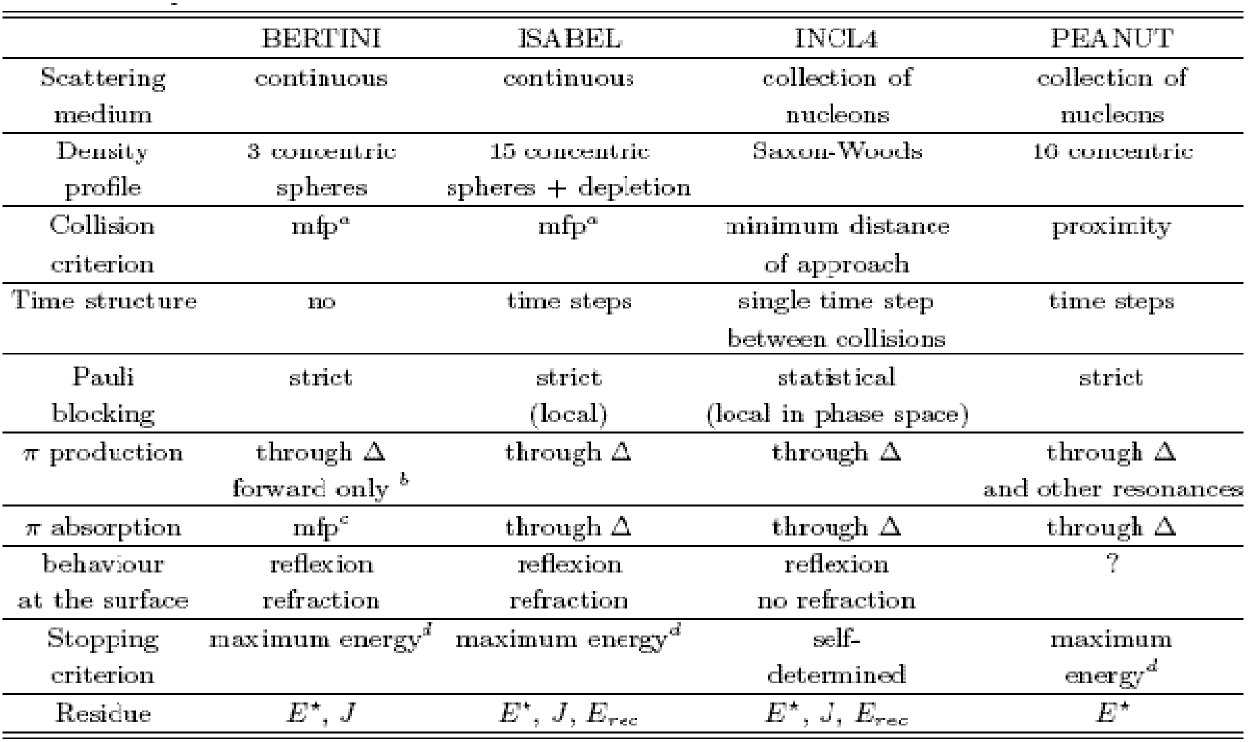
- The model leads to the production of particles and a residual nucleus (A’, Z’, E*, J, P_{recoil}





Modeling of intra-nuclear cascade (INC)

(from J. Cugnon)



	BERTINI	ISABEL	INCL4	PEANUT
Scattering medium	continuous	continuous	collection of nucleons	collection of nucleons
Density profile	3 concentric spheres	15 concentric spheres + depletion	Saxon-Woods	16 concentric
Collision criterion	mfp^a	mfp^a	minimum distance of approach	proximity
Time structure	no	time steps	single time step between collisions	time steps
Pauli blocking	strict	strict (local)	statistical (local in phase space)	strict
π production	through Δ forward only ^{b}	through Δ	through Δ	through Δ and other resonances
π absorption	mfp^c	through Δ	through Δ	through Δ
behaviour at the surface	reflexion refraction	reflexion refraction	reflexion no refraction	?
Stopping criterion	maximum energy^d	maximum energy^d	self-determined	maximum energy^d
Residue	E^*, J	E^*, J, E_{rec}	E^*, J, E_{rec}	E^*

(in LAHET-MCNPX)

(in FLUKA-GEANT)

BERTINI: H.W. Bertini et al. Phys. Rev 131 (1963) 1801

ISABEL: Y. Yariv et Z. Fraenkel Phys. Rev. C 24 (1981) 488

INCL4: J. Cugnon et al. Nucl. Phys. A620 (1997) 475; A. Boudard et al. Phys. Rev. C66 (2002) 44615

PEANUT: A. Fasso, A. Ferrari et al Monte-Carlo Conf 2000 edited by A. Kling et al (Springer-Verlag, Berlin)

✓CEM2k (S. Maschnik et al. Los Alamos) : in LAHET, important pre-equilibrium + cascade

✓BRIC (H. Duarte CEA DIF) : derived from INCL, movement equations + refraction cross section in NN medium

Modeling of de-excitation: evaporation

Excited nucleus… a bit,... but not too much!

> Nucleon emission threshold
(high energy level density)

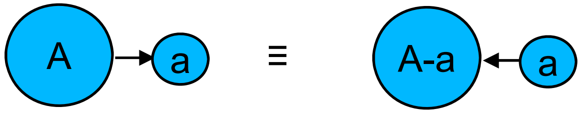
< E* ~ 3 MeV/u

Statistical treatment: emission independent from energy levels (only level density is important)

Explosion (multi-fragmentation) of the nucleus
Sequential emission is no longer valid!!!!

From QCD T-inversion invariance:
(detailed balance principle)

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



ρ: level density
P_{Aa}: probability for A to emit a
$P_{(A-a)a}$: probability for A-a to absorb a

1) Evaporation probability of particle a, energy ε, momentum p and spin s (*Weisskopf-Ewing*) :

$$\mathbf{P_a(\varepsilon) = \rho_f(Ef^*)/\rho_i(Ei^*)\ \ (2s+1)\ (4\pi p^2/h^3)\ \sigma_c(\varepsilon)}$$

2) *Hauser-Feshbach* put explicitly the angular momentum l (of a) and some transmission coefficients $T_l(\varepsilon)$ calculated from the optical model

Ingredients: $s_c(e)$ (capture cross section) and ρ(A,E) (level density)

Modeling of de-excitation: evaporation

Level density:

$$\rho(E^*, A) = \frac{\sqrt{\pi}}{12} \frac{e^{2\sqrt{aE^*}}}{a^{1/4}(E^*)^{5/4}}$$

From static treatment of Fermi gas

$E^* = a T^2$

T is the temperature,
E* is the excitation energy

a: Level density parameter…. A very long history… and literature!!!

$a = f(A,E^*)$

It should « partially » take into account nuclear effects (pairing, shells, magic numbers) and *E** evolution

The limit for high *E** is: $a \sim A/8 \div A/13$

The most common parametrization is GCCI (Gilbert-Cameron-Cook-Ignatyuk)

Inverse cross sections:

Geometrical model, fit on data or explicit calculation

Main difficulty: Fusion-Absorption for an excited nucleus!

Modeling of de-excitation: fission

Atchison (RAL code, default in LAHET/MCNPX ~1980) *(ORNL only for Z>90)*

$Z > 70$: competition limited to n evaporation (Weisskopf with simplified *a*)

$Z^2/A < 35$: symmetric fission (fission fragments mass distribution)

$Z^2/A > 35$: symmetric + asymmetric fission

Mainly based on empirical data on actinides fission at low energy (thermal)

K.H. Schmidt (J. Benlliure, B. Jurado @ GSI, ABLA code): time evolution of fission channel width

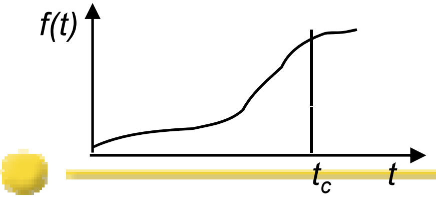
$$\Gamma_f^{BW} = \frac{1}{2\pi\rho_c(E)} T_{sad}\,\rho_{sad}\,(E - B_f)$$

Bohr-Wheeler: Temperature (T_{sad}) and level density (ρ_{sad}) at the saddle point calculated right above the fission barrier (B_f)

$$\Gamma_f^{K} = K(\beta)\Gamma_f^{BW}$$

Kramer- Grangé: Dissipative process giving a reduction parameter $K(\beta)$, where β is the viscosity, derived from Fokker-Planck equations

$$\Gamma_f^{K} = K(\beta)\Gamma_f^{BW} f(t)$$

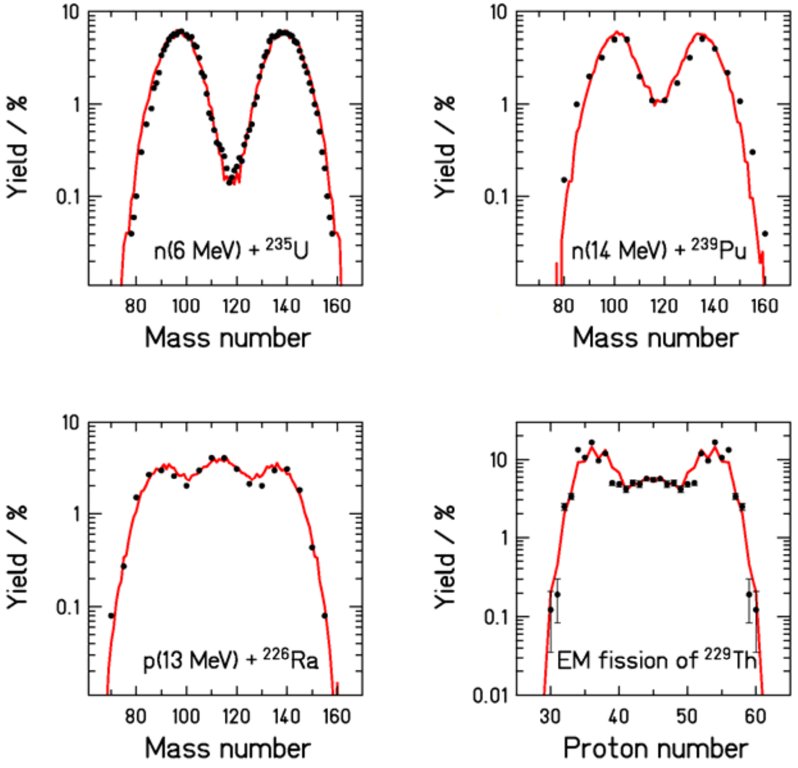


B. Jurado et al. (*Phys. lett. B 533 (2003) 186*): dynamical competition between fission and evaporation given by a transition function: $t_c \sim 1.7\ 10^{-21}$ s

Modeling of de-excitation: fission fragments

Level density above the fission barrier (statistical approach)

Barrier defined by 3 terms giving 3 FF structures:
1. Symmetric (liquid drop model)
2. Asymmetric N=82 (empirical)
3. Asymmetric N=90 (empirical)



ABLA: the most detailed model for fission at spallation energies
Parameters based on experimental data ➔ Still difficulties on Ta-W

Modeling of de-excitation: extreme cases

- Light nuclei (A < 15-20, E* ≈ 50 MeV/u):
  - Small level density
  - E* ≈ binding energy
  - Breaking in ONE STEP: Fermi breakup
  - All possible configurations are weighed by the phase space
    - The nucleus *A* is decomposed on *n* components, A_i, with weight *W*

$$W = \frac{c}{A_1!\ldots A_n!}\left(\frac{Vol}{h^3}\right)^{n-1}\int d\vec{p}_i\,\delta(\Sigma\,\vec{p}_i)\,\delta(E^* - S - \sum t_i)$$

$$A = \sum_1^n A_i$$

- High excitation energy (E* > 3 MeV/u):
  - Breaking in ONE step : Multifragmentation
  - Violent expansion up to a freeze-out volume (density ~ 1/3-1/6 ρ_0)
  - Weighting of possible configurations (high temperature: Boltzmann low)

$$W = \frac{c}{A_1!\ldots A_n!}\prod_1^n e^{-\frac{E_i}{T}} g_i \frac{Vol(2\pi m_i T)^{3/2}}{h^3}$$

- Evaporation like a very asymmetric fission:
  - Transition state model
  - Alternative to classical evaporation, extended to light ion emission
  - Capture cross section is replaced by a barrier

Modeling of de-excitation: the codes

- Dresner:
  - It is the oldest
  - Too high Coulomb barriers
  - Evaporation à la Weisskopf (up to ^{4}He) + Fission à la Atchison
- GEM
  - Revised (and modernized) version of Dresner-Atchison
  - Evaporation à la Weisskopf (up to A=24)
  - Revised masses, pairing, fission param., capture X sect., Coulomb barriers
- ABLA
  - Evaporation à la Weisskopf (only for p, n, ^{4}He!!!!!!!)
  - Fission VERY complex and detailed
  - Very active community on development (extended evapor., multifragm., dynamic fission)
- GEMINI
  - Evaporation à la Hausser-Feshbach (for $Z < 2,4$)
  - Transition state model (for $Z > 2,4$)
- SMM
  - Evaporation à la Weisskopf (up to A<18)
  - Multifragmentation

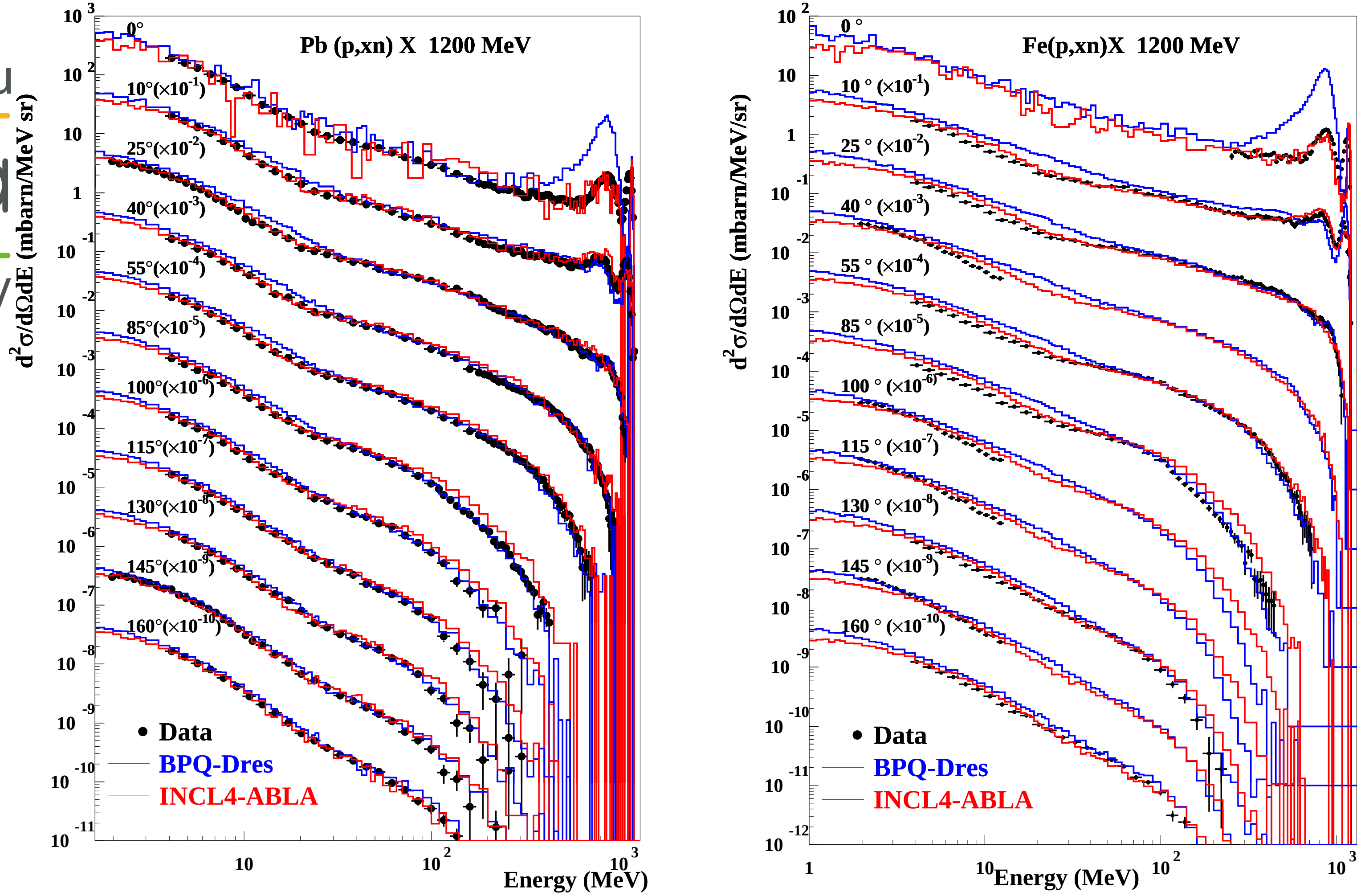
Comparison between models and data

- Large amount of high quality data has been collected
  - Neutron and LPC production
  - Isotopic residue distributions
  - Excitation functions

- Improvements on nuclear models
  - INCL4/ABLA tested against all the available data with the same set of parameters
  - Important improvements also in CEM and FLUKA
  - Implementation of INCL4/ABLA and CEM into MCNPX
  - Implementation of INCL4/ABLA in GEANT4

Neutron production

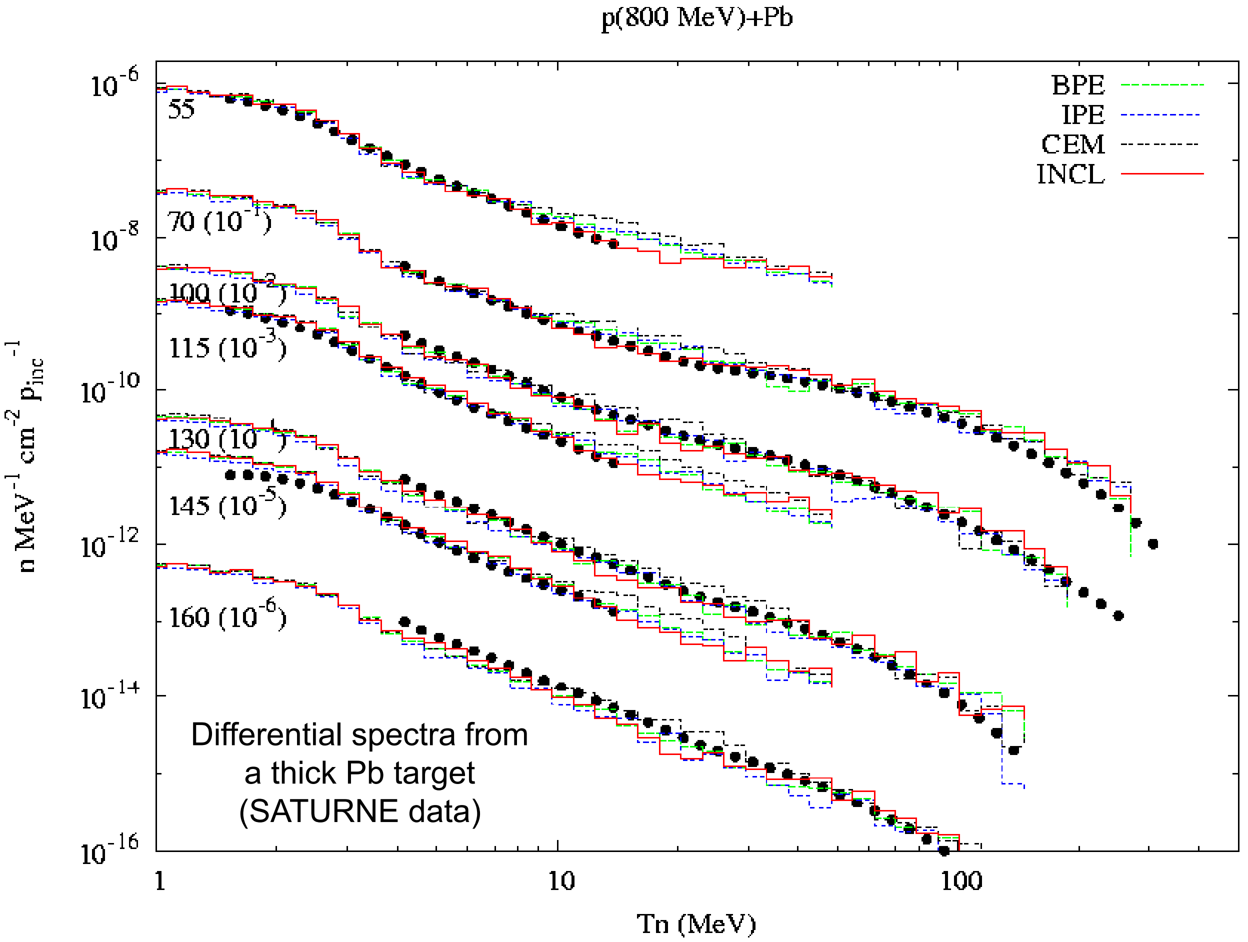
S.Leray et al., Phys. Rev. C 65 (2002) 044621



Neutron production can be predicted with a 10-20% precision by most of the models

Neutron production

T. Aoust et al., ND2004, Santa Fe

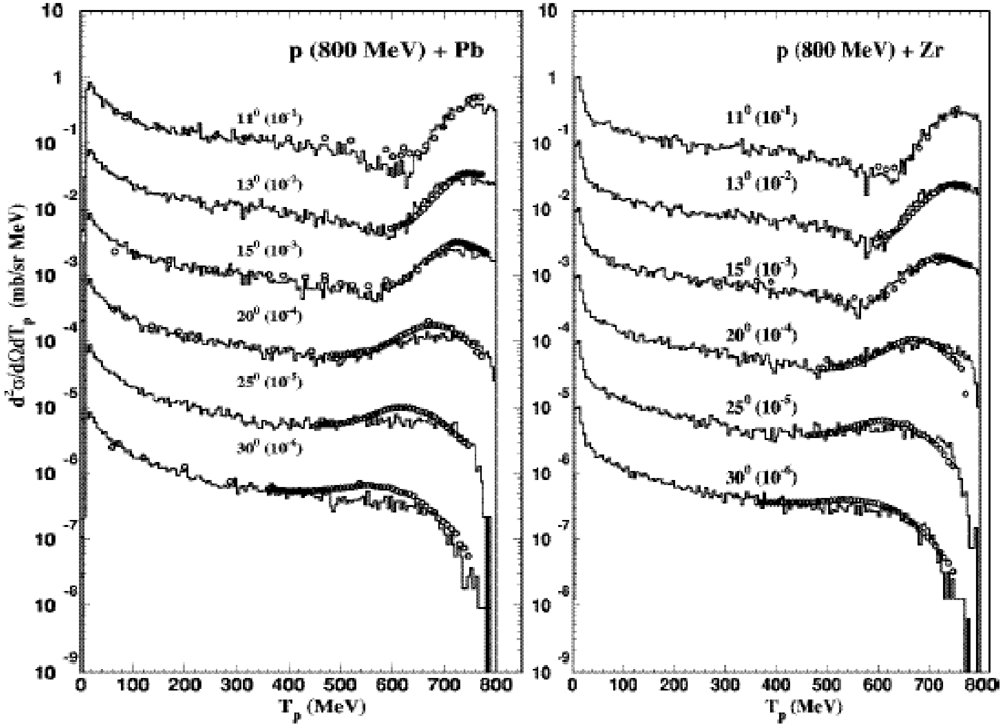


Differential spectra from
a thick Pb target
(SATURNE data)

Energy and angular distribution are well reproduced

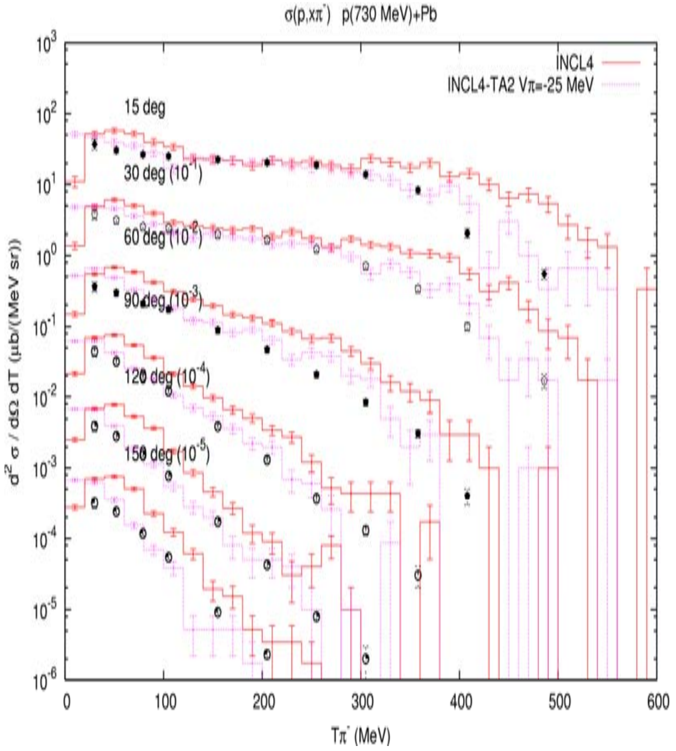
Proton and pion production

R. Chrien et al, Phys. Rev. C21 (1980) 1014 *J. McGill et al Phys. Rev. C29 (1984) 204*



Protons

D. Cochran et al, Phys. Rev. D6 (1972) 3085

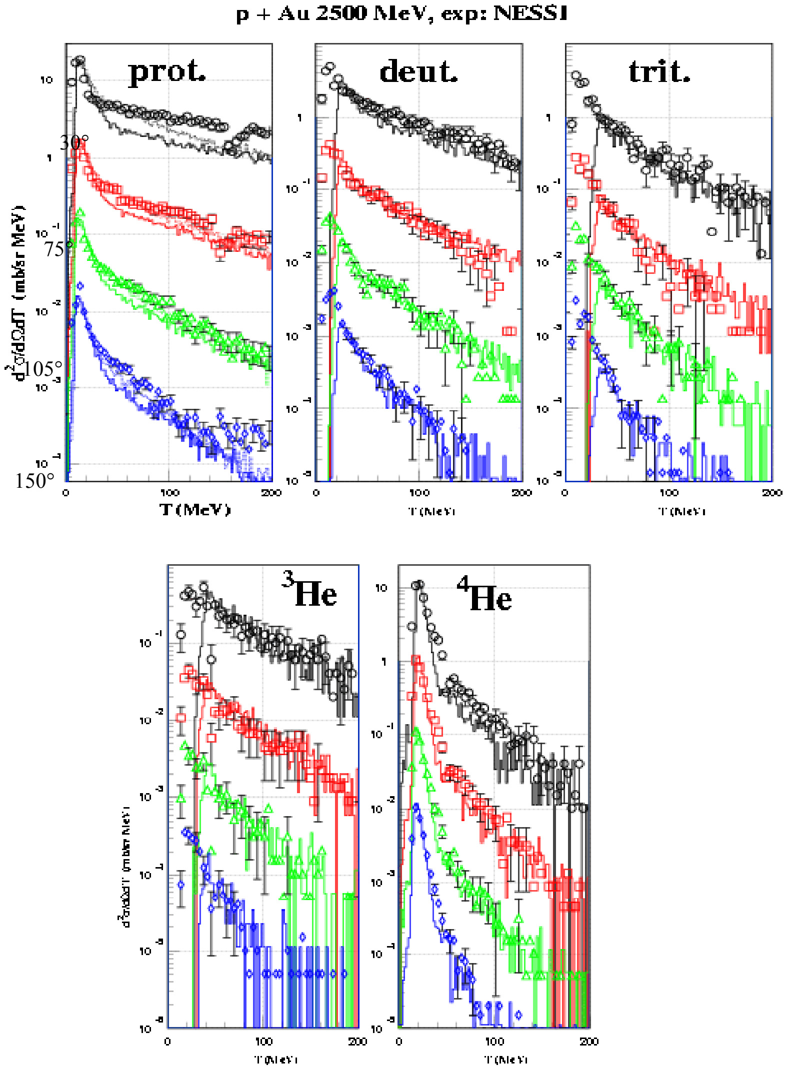


$\pi+$

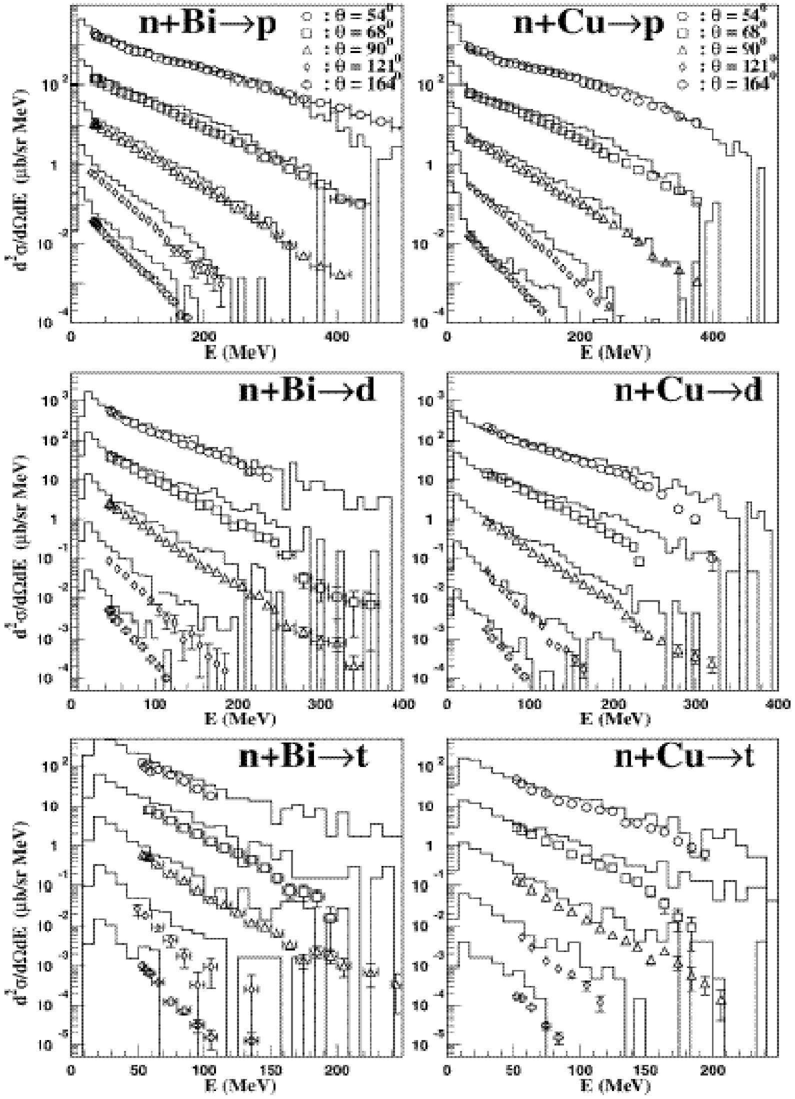
Quasi-elastic peak well reproduced but need to add of a pion potential

LCP production

A. Letourneau et al, Nucl. Phys. A712 (2002) 133



J. Franz et al, Nucl. Phys. A472 (1987) 733, Nucl. Phys. A510 (1990) 774



n (542 MeV)

A comment on LCP production

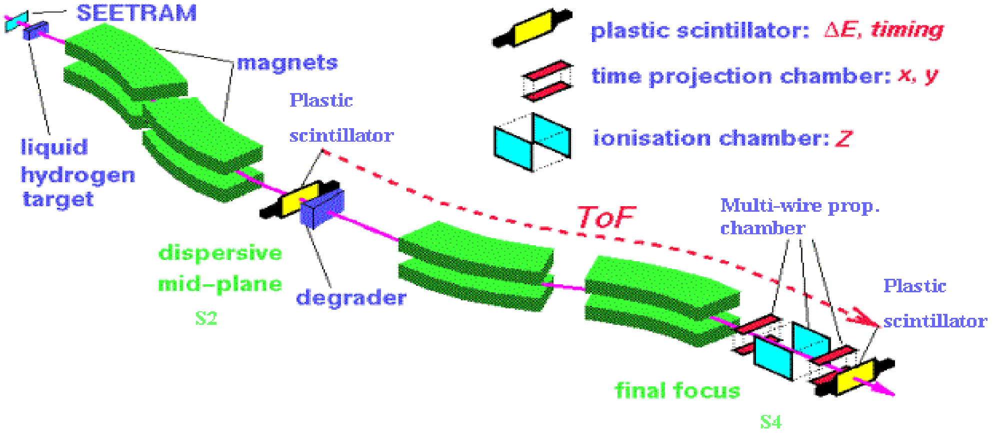
- In the cascade:
  - Extension out of standard description (N-N interactions)
  - In INCL4: hypothesis of cluster formation at the surface given by
    - Distance parameter (from R0): r = 1.75 fm
    - Phase space parameter $\Delta r \Delta p < 387$ fm*MeV/c

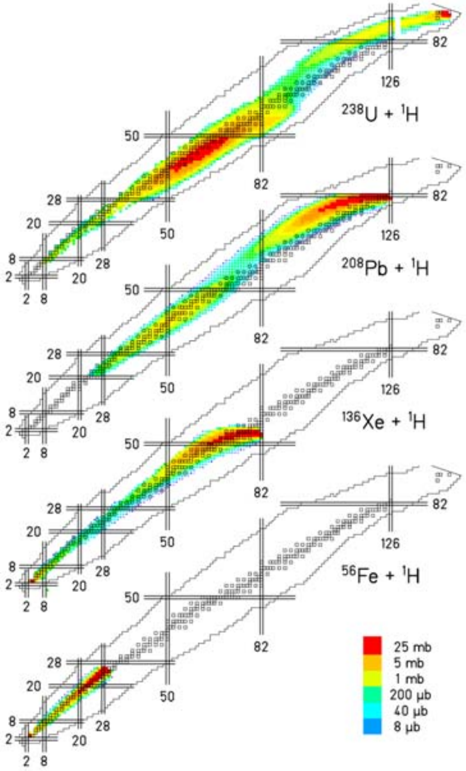
- In the evaporation:
  - Can be treated on the same formalism as nucleons (state density, inverse cross section)

Residues production

- New data obtained with reverse kinematics methods led to a considerable progress in reaction modeling
- Models:
  - Heavy evaporation residues: generally good very close to the target nucleus
  - Fission fragments: quite good, enough for activity calculations
  - Light evaporation residues: most models generally bad
  - Intermediate mass fragments: all models are wrong by orders of magnitude

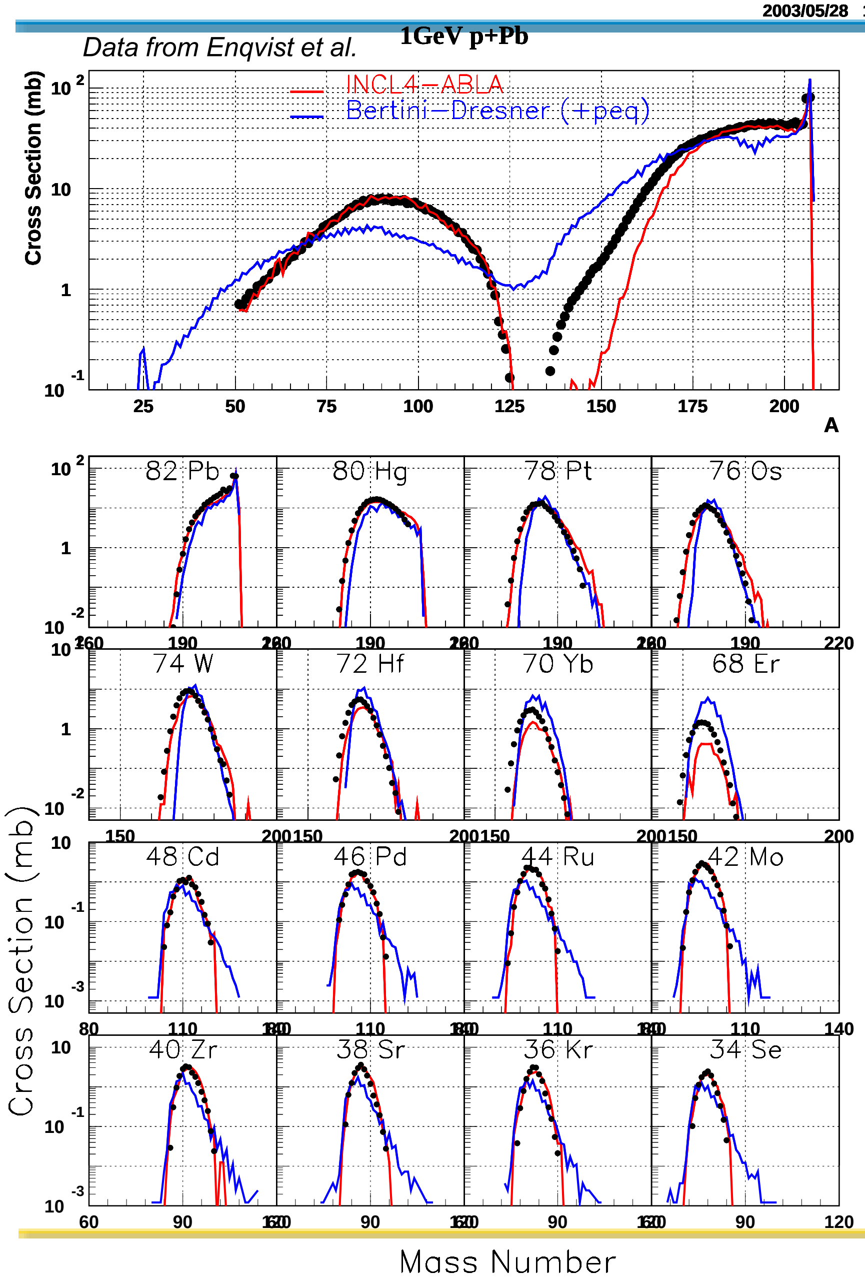
FRS experiments at GSI
(coll. GSI, Santiago Univ., CEA/DSM, IN2P3)



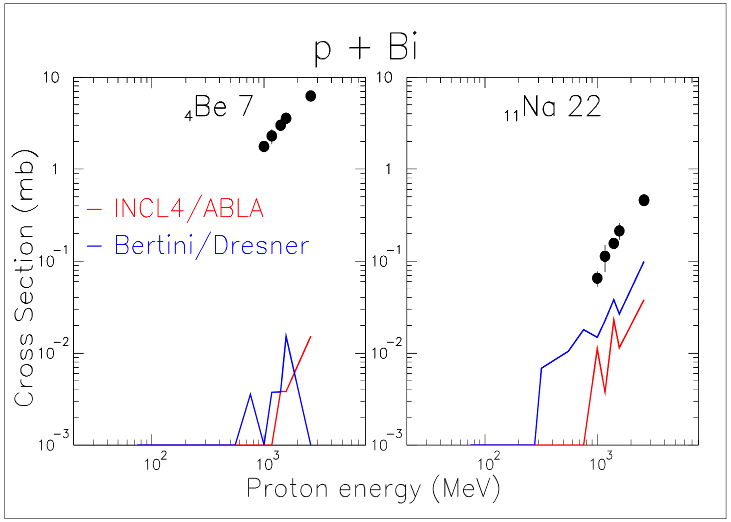


Residues production: heavy systems

Data from Enqvist et al.



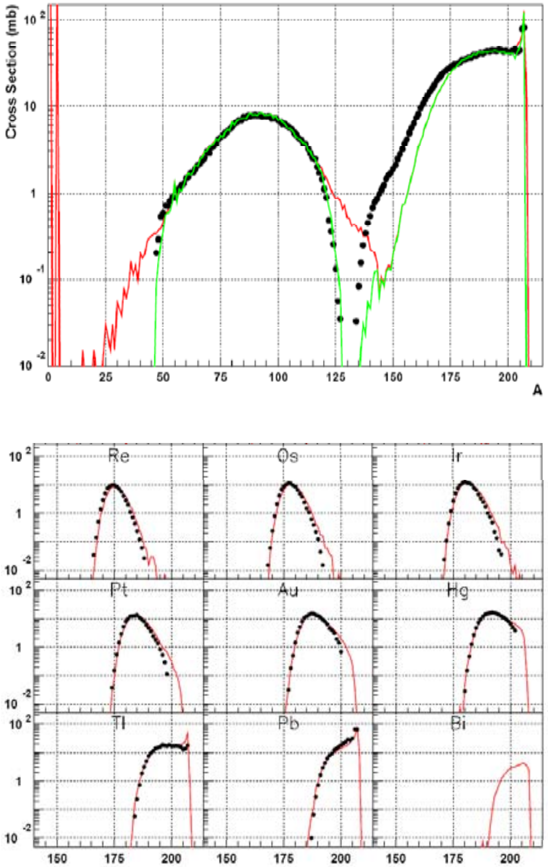
Data from Michel et al.



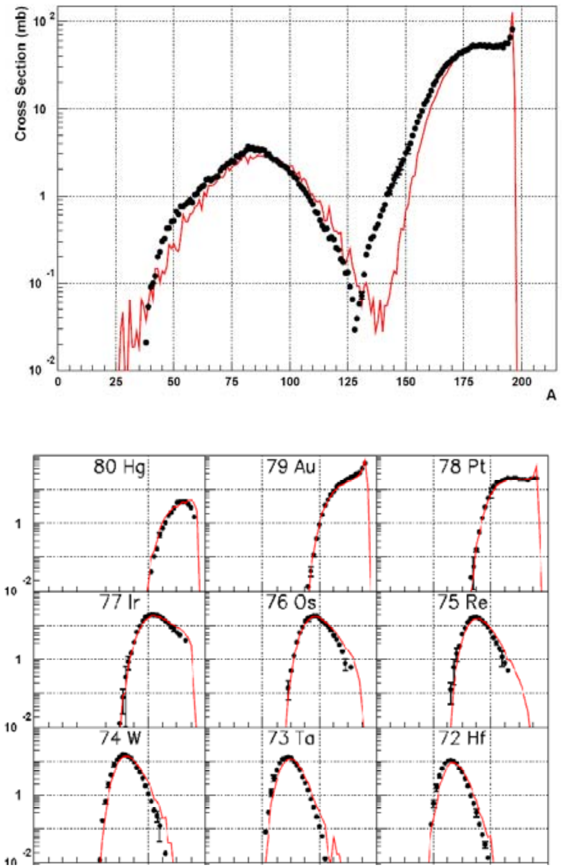
- INCL4/ABLA agrees much better with GSI data than Bertini/Dresner for fission fragments, very heavy residues and isotopic distribution shape
- Both fail for light evaporation residues and intermediate mass fragments

Residues production: heavy systems

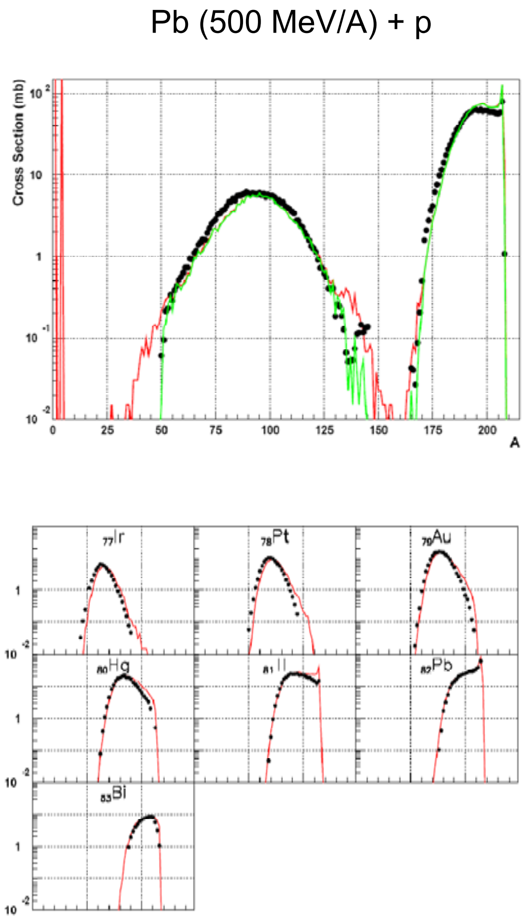
Pb (1 GeV/A) + p



Au (800 MeV/A) + p



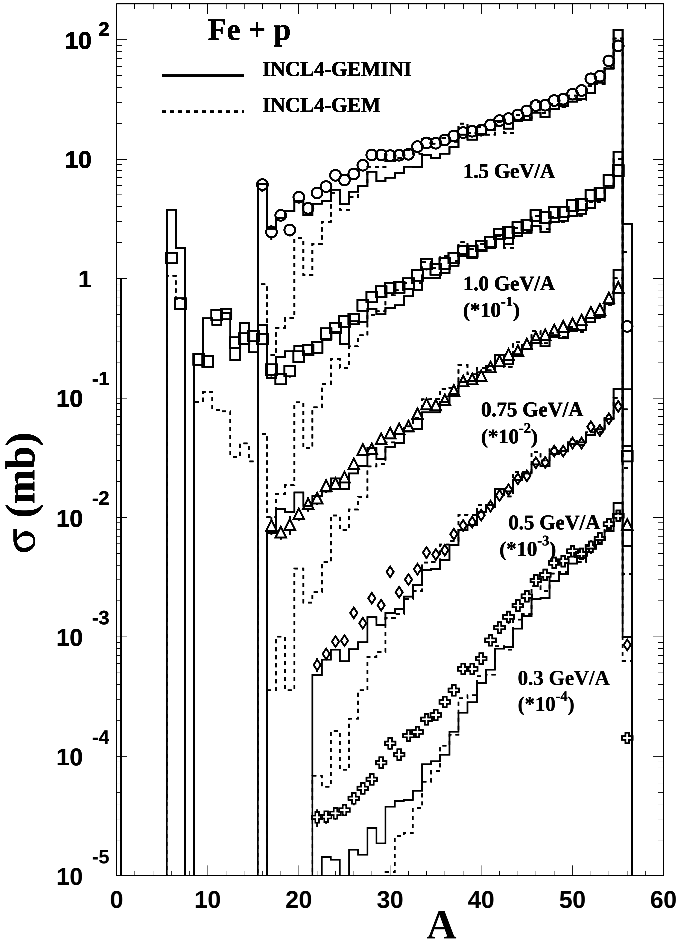
Pb (500 MeV/A) + p



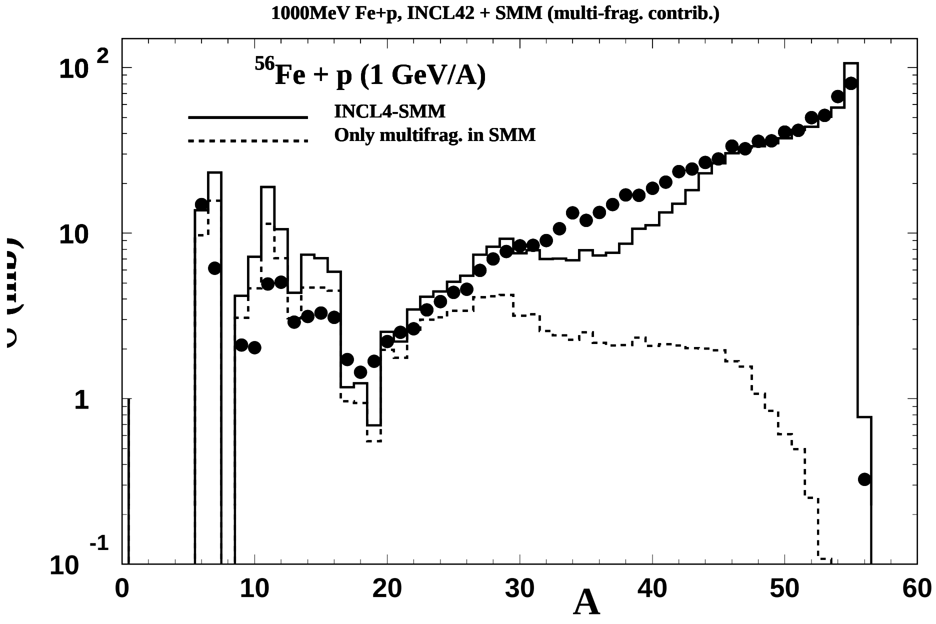
The only evaporation is not enough to explain the distributions at high excitation energy

Residues production: light systems

P Napolitani et al, C70 (2004) 054607



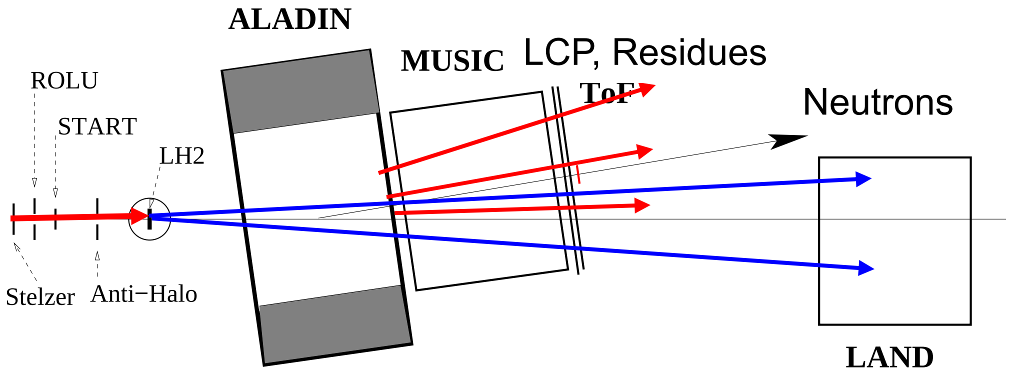
NOTE: same beam energy, therefore higher excitation energy (per nucleon) on a lighter nucleus (nucleus diameter/volume)



Transition state model
(Gemini)

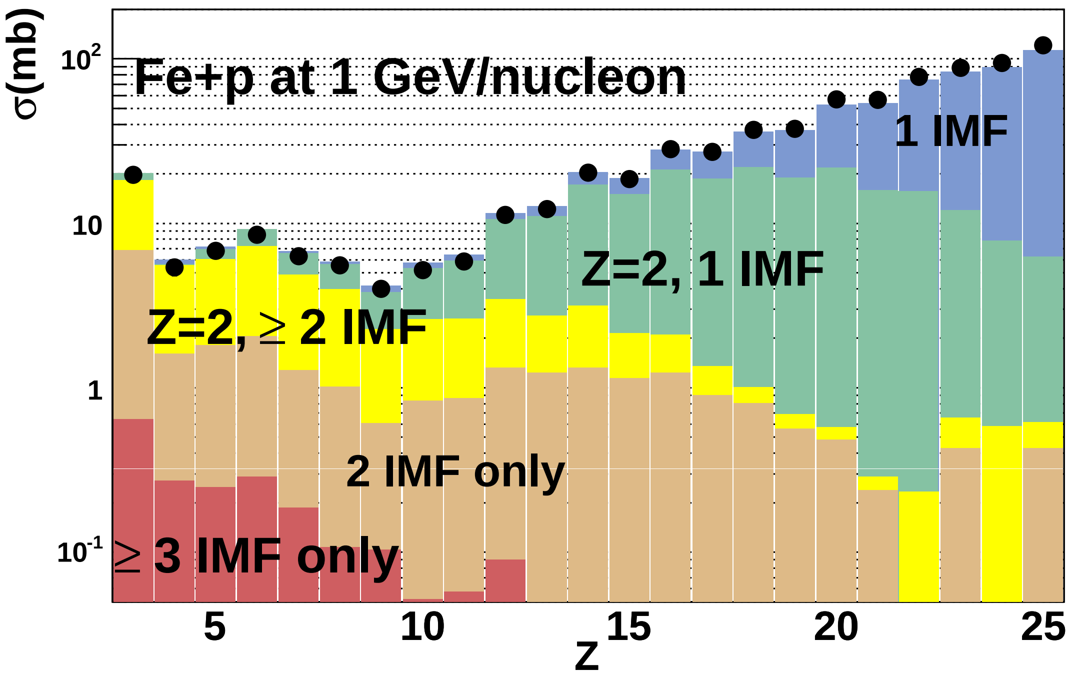
…or multifragmentation ?
(SMM)

Study of the mechanism: coincidence technique

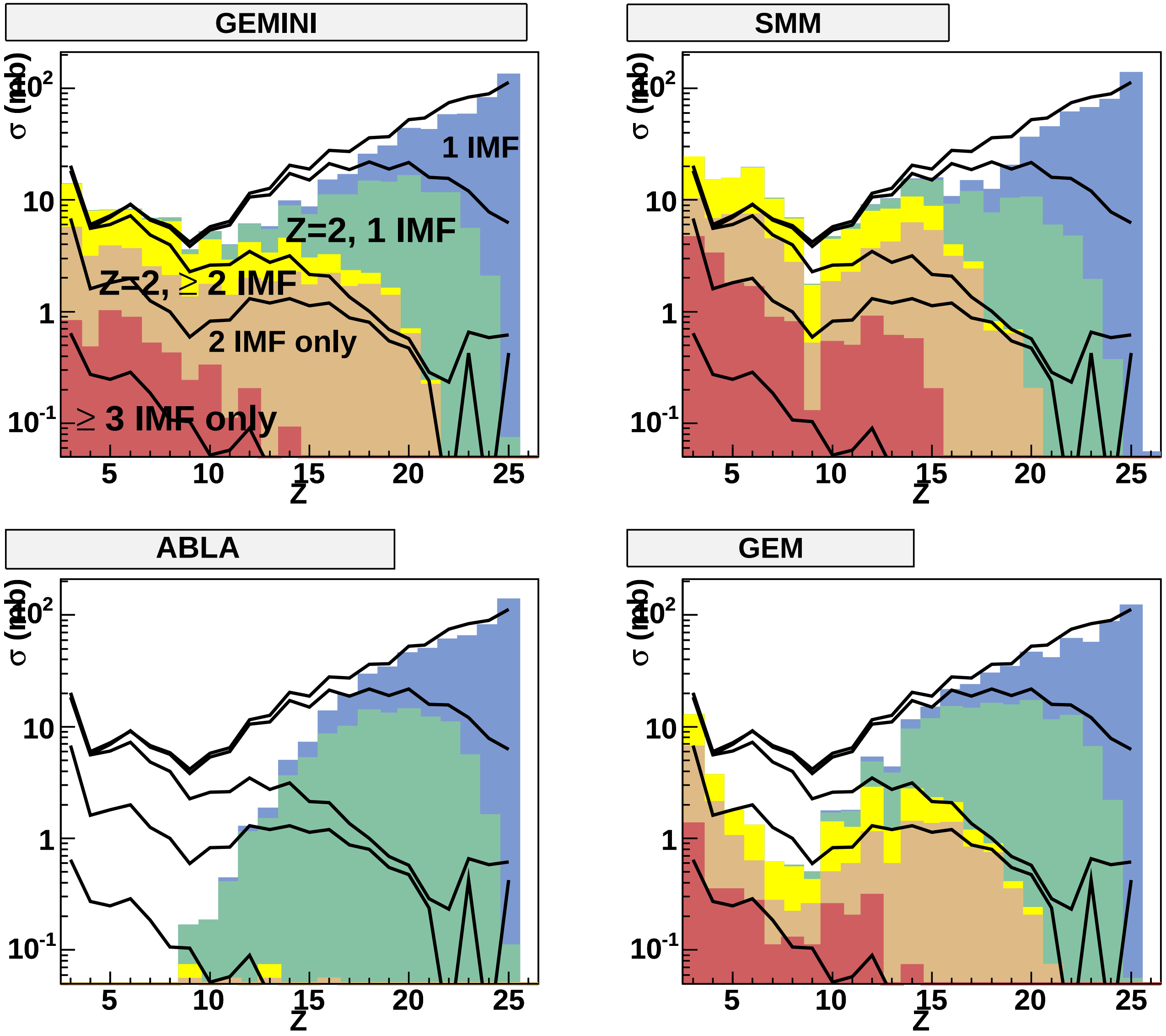


Contributions to the cross sections

E. Legentil (PhD thesis): Spaladin experiment (GSI)



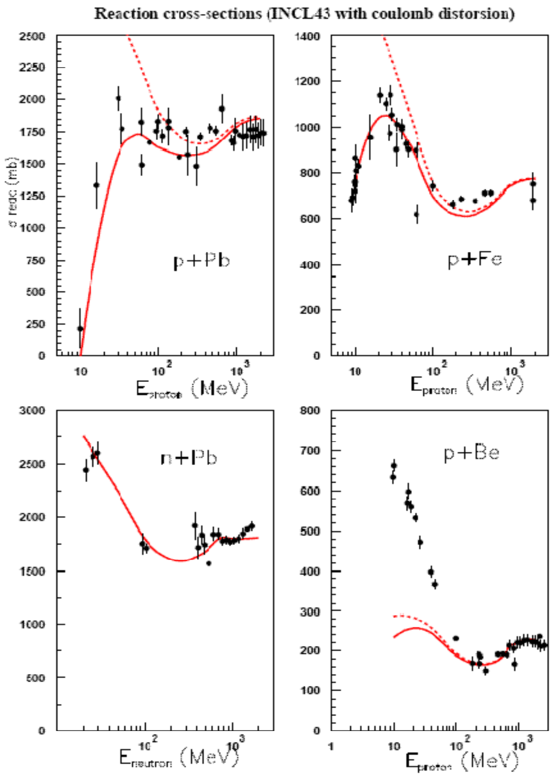
Study of the mechanism: models/data



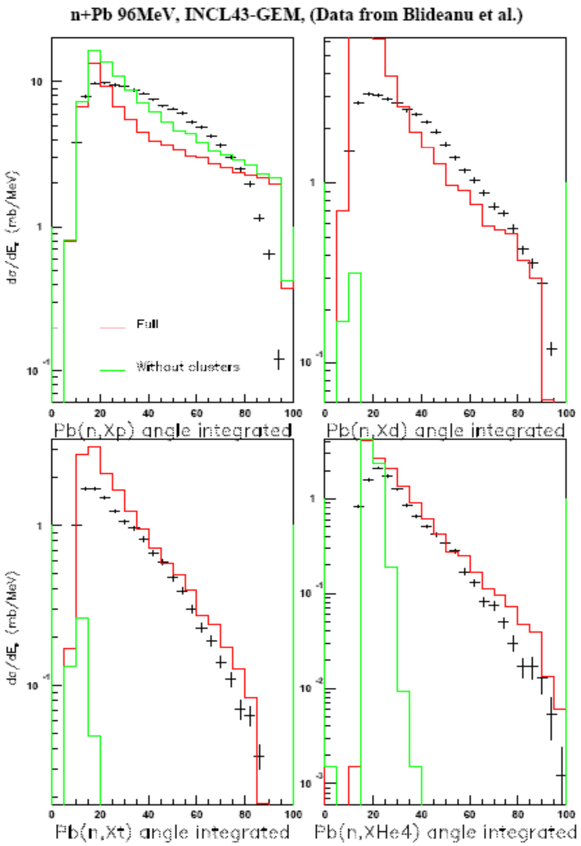
Black: data
Histos: model

Best agreement: Gemini Hausser-Feshbach Z<5, Transition State Model above.

Validity at lower energy



Reaction σ is correct:
Absolute normalization
in the calculation



LCP production
(but to p detriment)

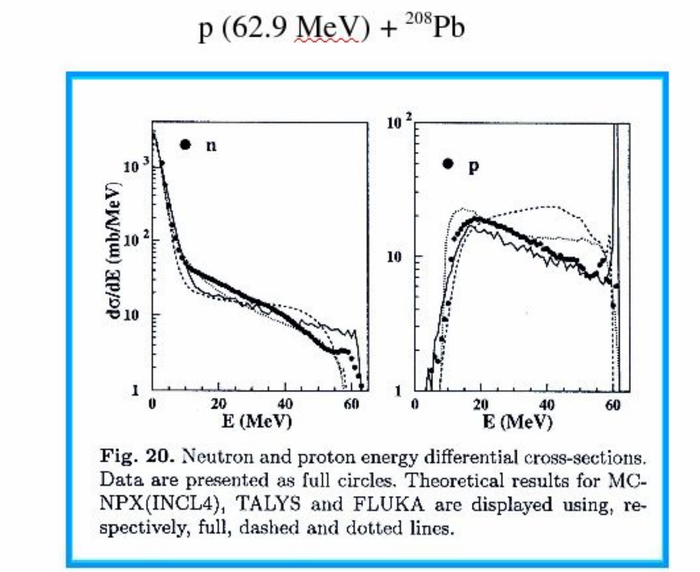


Fig. 20. Neutron and proton energy differential cross-sections. Data are presented as full circles. Theoretical results for MC-NPX(INCL4), TALYS and FLUKA are displayed using, respectively, full, dashed and dotted lines.

A. Guertin et al, EPJ A23(2005)49

Solid: INCL4+ABLA
Dashed: TALYS
Dotted: FLUKA

INCL at low energy under development
Good hope of model continuity...

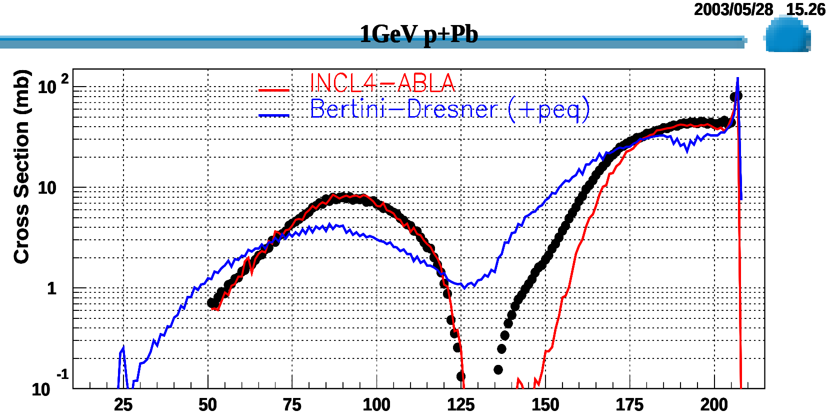
Pay attention to Bertini-Dresner-Atchison!

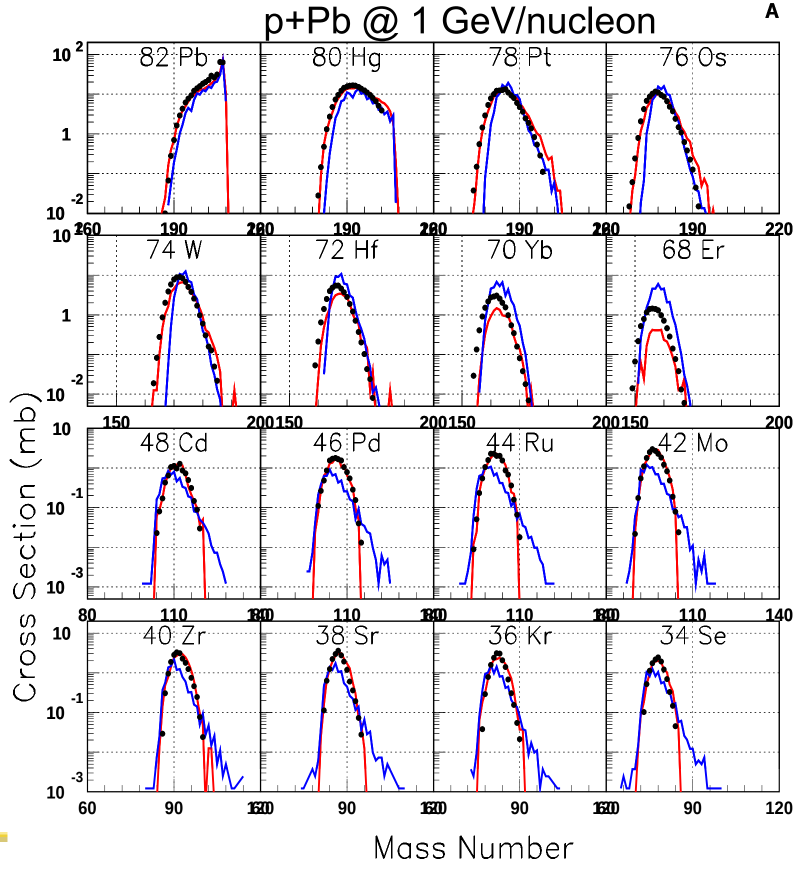
Mais:

- Default option in LAHET
- Calculation is fast
- Global order of magnitude is correct (i.e. on neutron production)

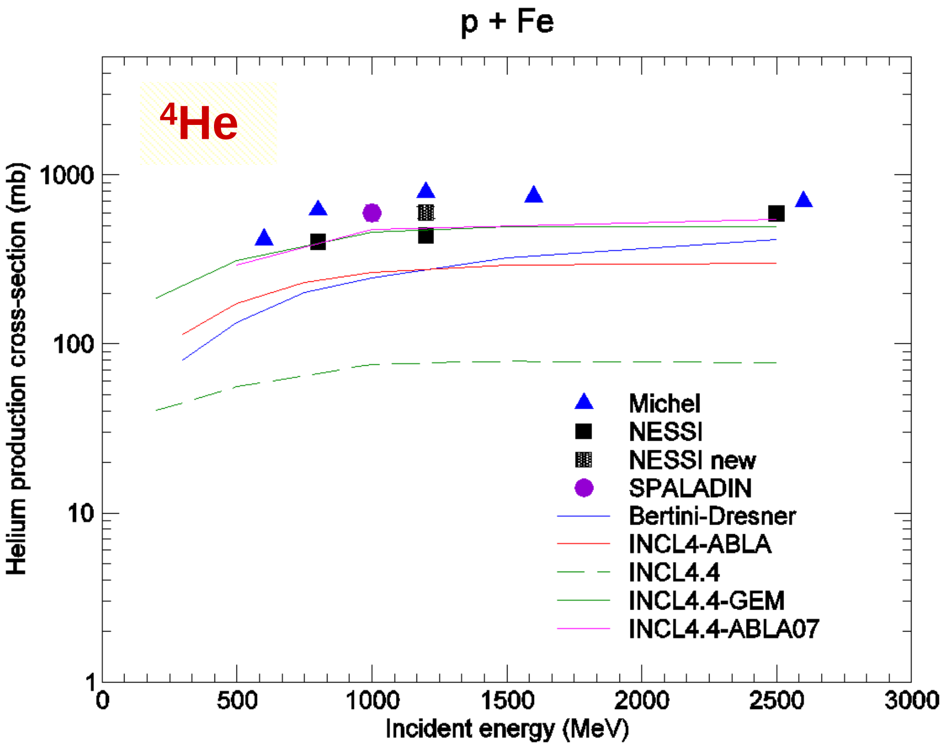
BUT

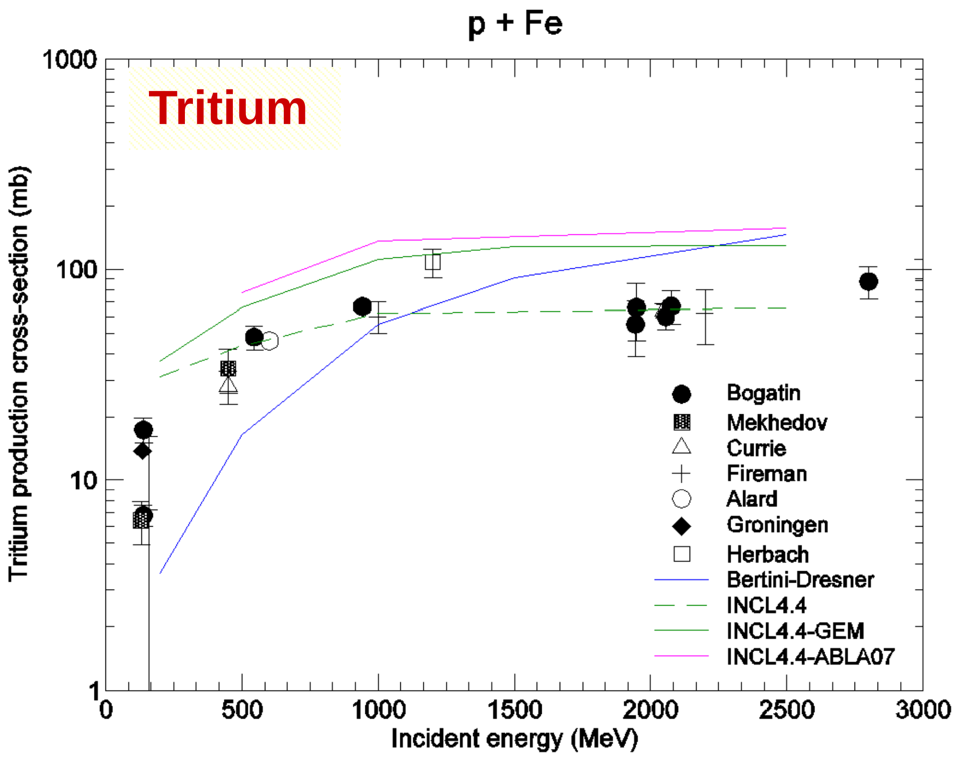
- E* too much high
- Fission/evaporation badly balanced
- Isotopic yields doubtful





Gas production in Fe

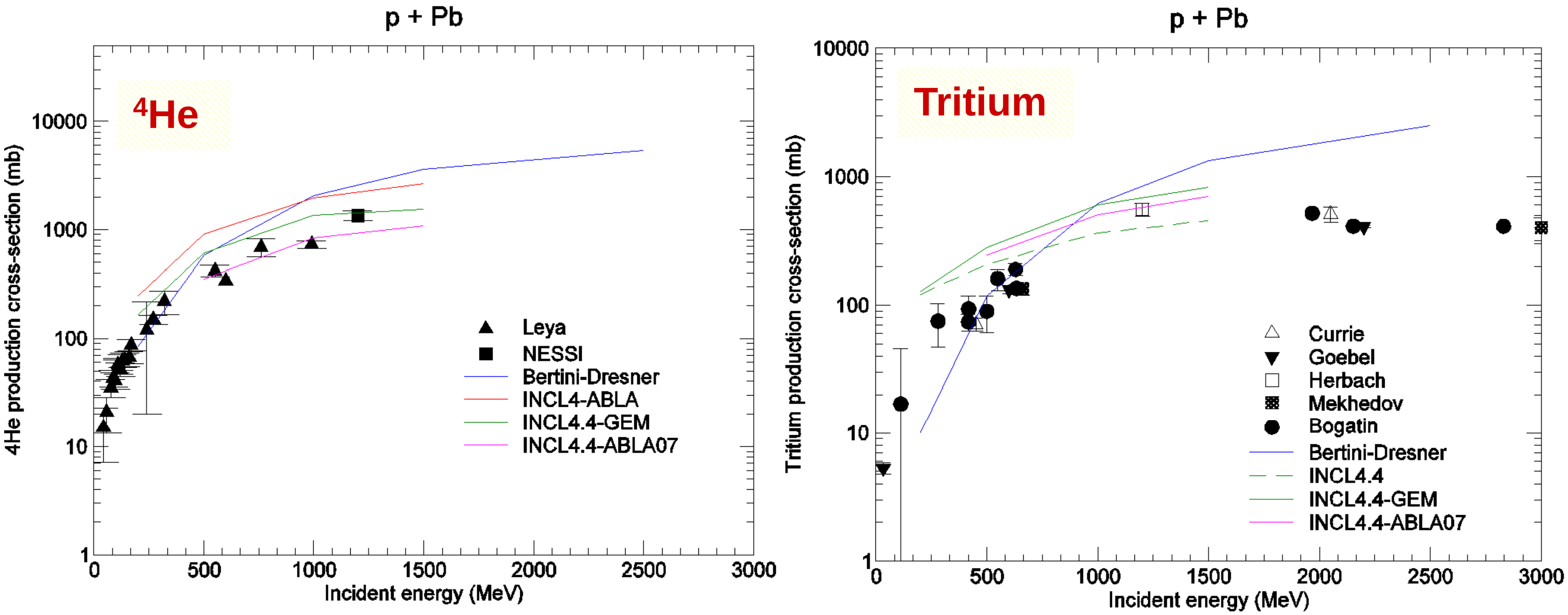




- **INCL4.4-ABLA07 now produces tritium**

- **Situation improved compared to models presently in MCNPX**

Gas production in Pb

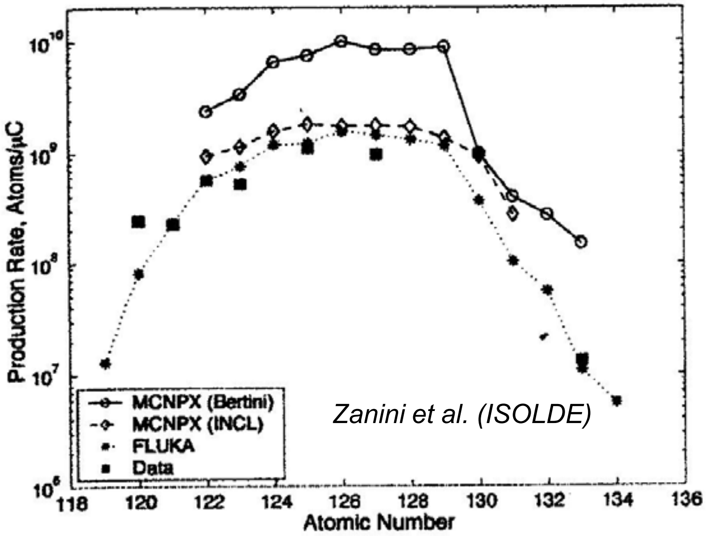


- **INCL4.4-ABLA07 now produces tritium**
- **Situation improved compared to models presently in MCNPX**

Xe production on thick target

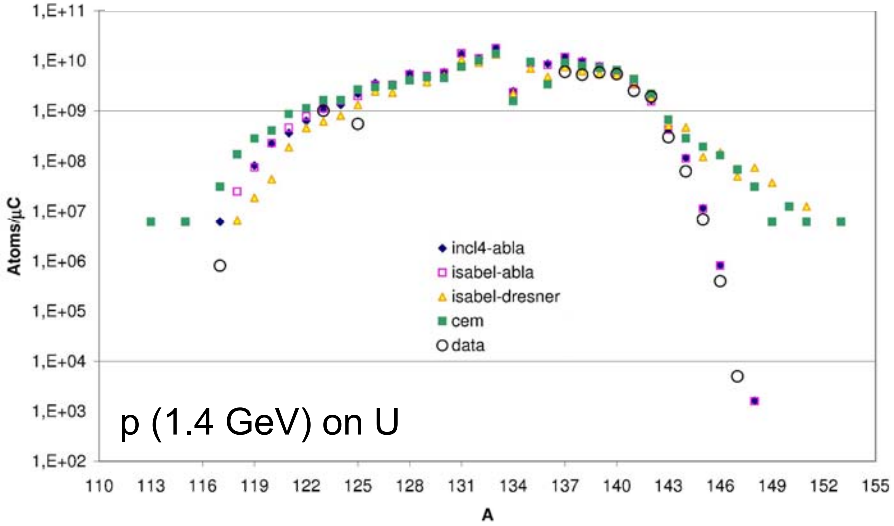
Influence from the:
- cascade (production level)
- evaporation (isotopic yield)

p (1.4 GeV) on Pb-Bi



Zanini et al. (ISOLDE)

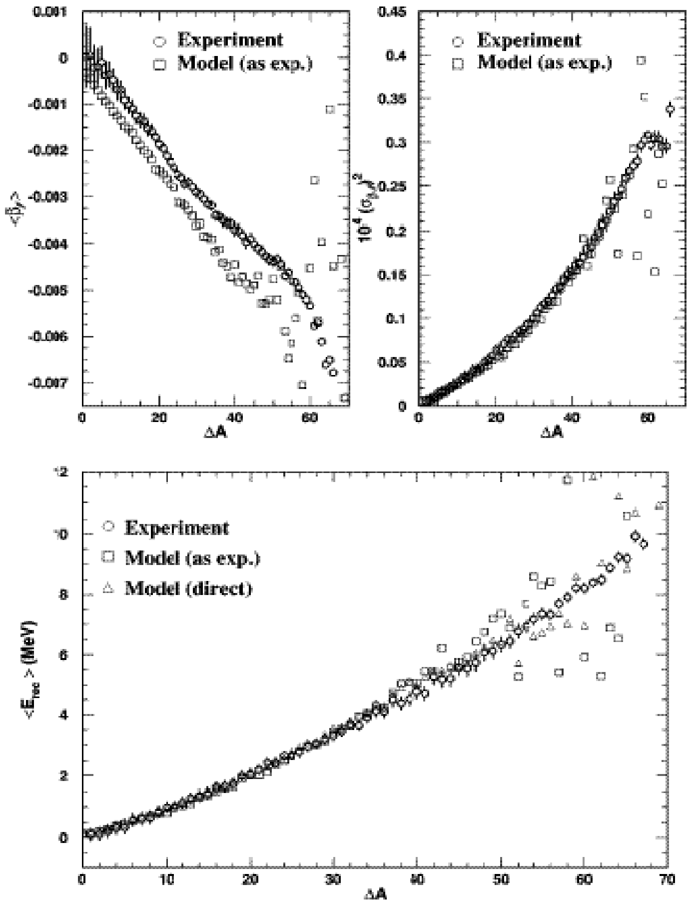
FIGURE 3. Same as Fig. 2 but for Xe isotopes.

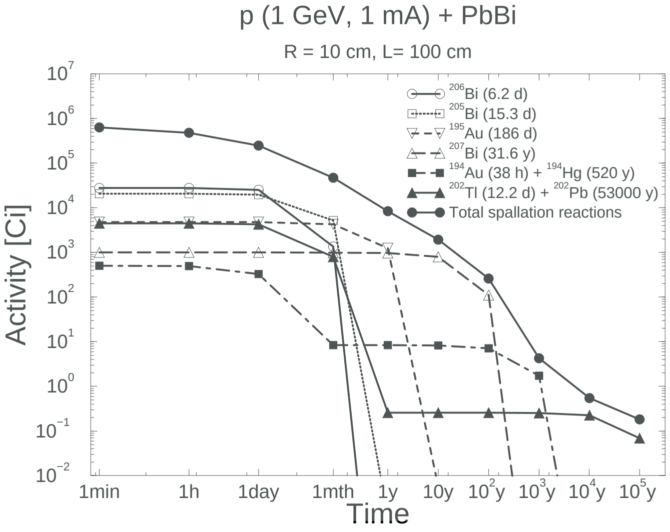


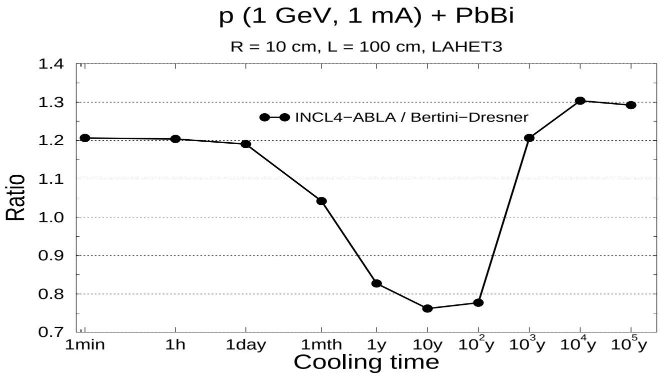
p (1.4 GeV) on U

Velocity and recoil energy

Pb (1 GeV/A) + p (GSI)







GSI: Measurement of recoil velocity distributions
And mean energy
INCL4+ABLA seems correct
DPA calculations are meaningful

Activity calculations:
Multiple contributions (mostly heavy nuclei)
INCL4-ABLA and Bertini-Dresner equivalent

Conclusions

- **Large set of available high-energy data allowing the testing of nuclear models**
- **INC models**
  - **The widely used Bertini model ruled out (lead to too high excitation energies)**
  - **Isabel and INCL models seem to agree quite well with the data**
  - **Encouraging behaviour of the INCL4 version**
- **De-excitation models**
  - **Dresner-Atchison unable to reproduce isotopic distributions, fission, LCP emission**
  - **GSI model better for residues but deficiencies for LCP emission**
- **Perspectives**
  - **Improvements still needed to have a model reproducing all the bulk of data**
  - **Coincidence experiments will allow a deeper insight into the reactions mechanisms**