The Physics of Spallation Processes Computer Modeling and Experiments

Frank Goldenbaum

- How are neutrons produced? Nuclear reactions: spallation, fission, fragmentation,multifragmentation,vaporization
- What is spallation? Definition, the process…
- Why are spallation reactions of interest? (applications, fund. physics)
- Computer models describing spallation reactions (INC and evap. model)
  - Limits and constraints
  - validation
- Experimental investigations (here: PISA & NESSI at COSY)
- Comparison between models and experiments
- Conclusion

The Physics of Spallation Processes
Computer Modeling and Experiments

MC computer simulation exercises (afternoon) LINUX GEANT4, INCL4.2, GEM

YOU !

- For «thin target setup»: getting familiar with intra-nuclear cascade and evaporation codes (INCL4.2+GEM)
  - calculation of particle (n, p, pion, He, IMF, FF, spallation products) production rates (double differential), multiplicities, energy spectra and angular distributions, study influence of
    1. incident energy
    2. target material
    3. physics parameters
- Alternatively: setting up simple, but realistic «thick target» 3-dim geometry (e.g. Pb cylinder) for GEANT4 and study particle fluxes, energies,…

Classification of nuclear reactions

A. Nucleon-Nucleus Reactions

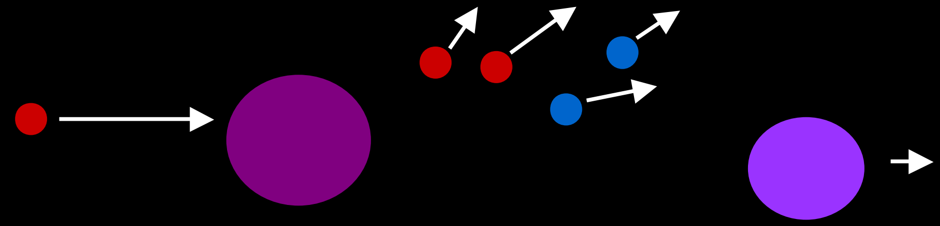
A.1 Spallation
A.2 Induced Fission

B. Nucleus-Nucleus Reactions

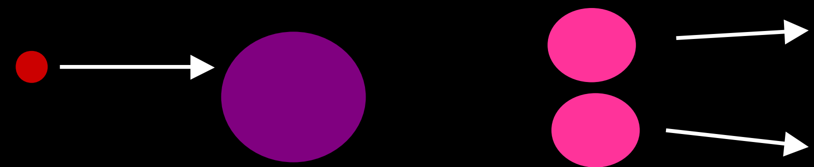
B.1 Fragmentation
B.2 Multifragmentation
B.3 Vaporization

Classification of nuclear reactions

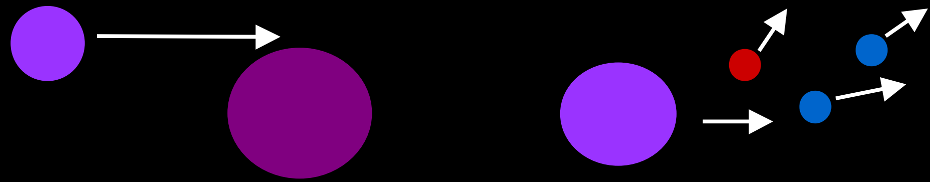
1. Spallation



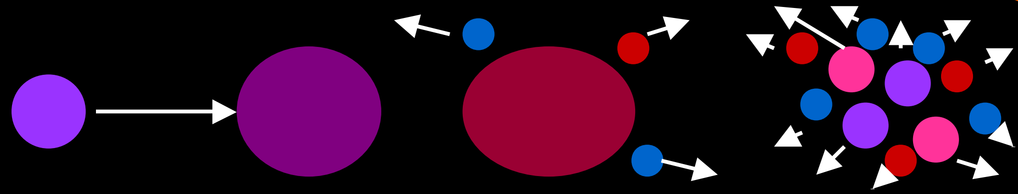
2. Induced Fission



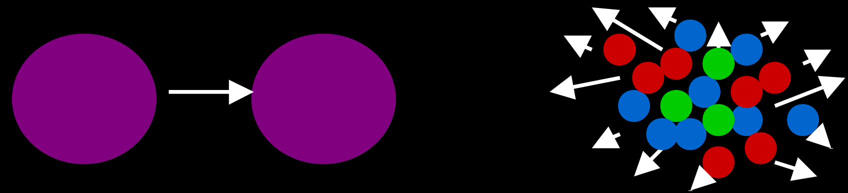
3. Fragmentation



4. Multifragmentation



5. Vaporization

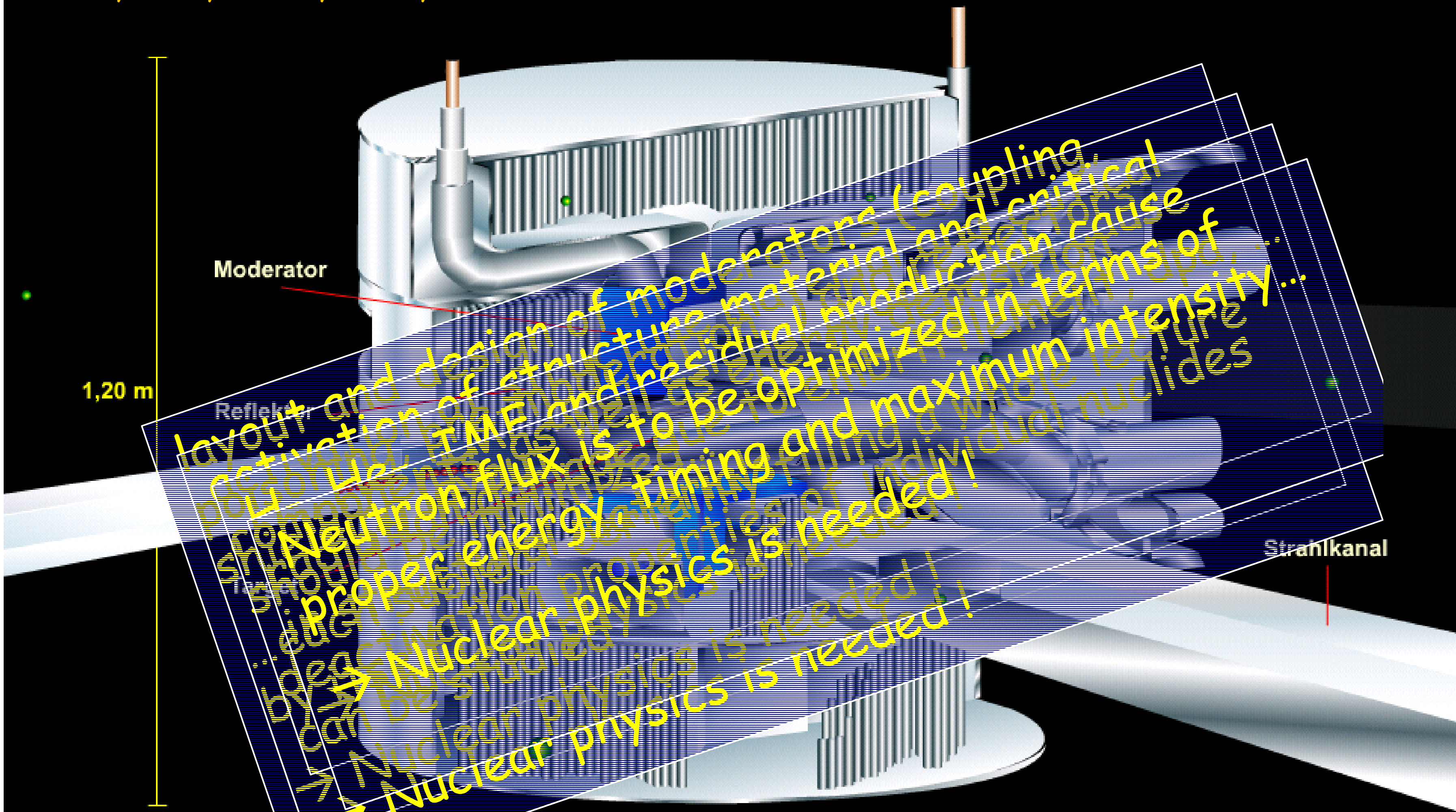


Why is particle physics needed in the context of spallation reactions?

important for many scientific and technological problems as e.g. there are:

The Target (ESS)

ESS, SNS, JSNS, ISIS,....



layout and design of moderators (coupling, ...

activation of structure material and critical ...

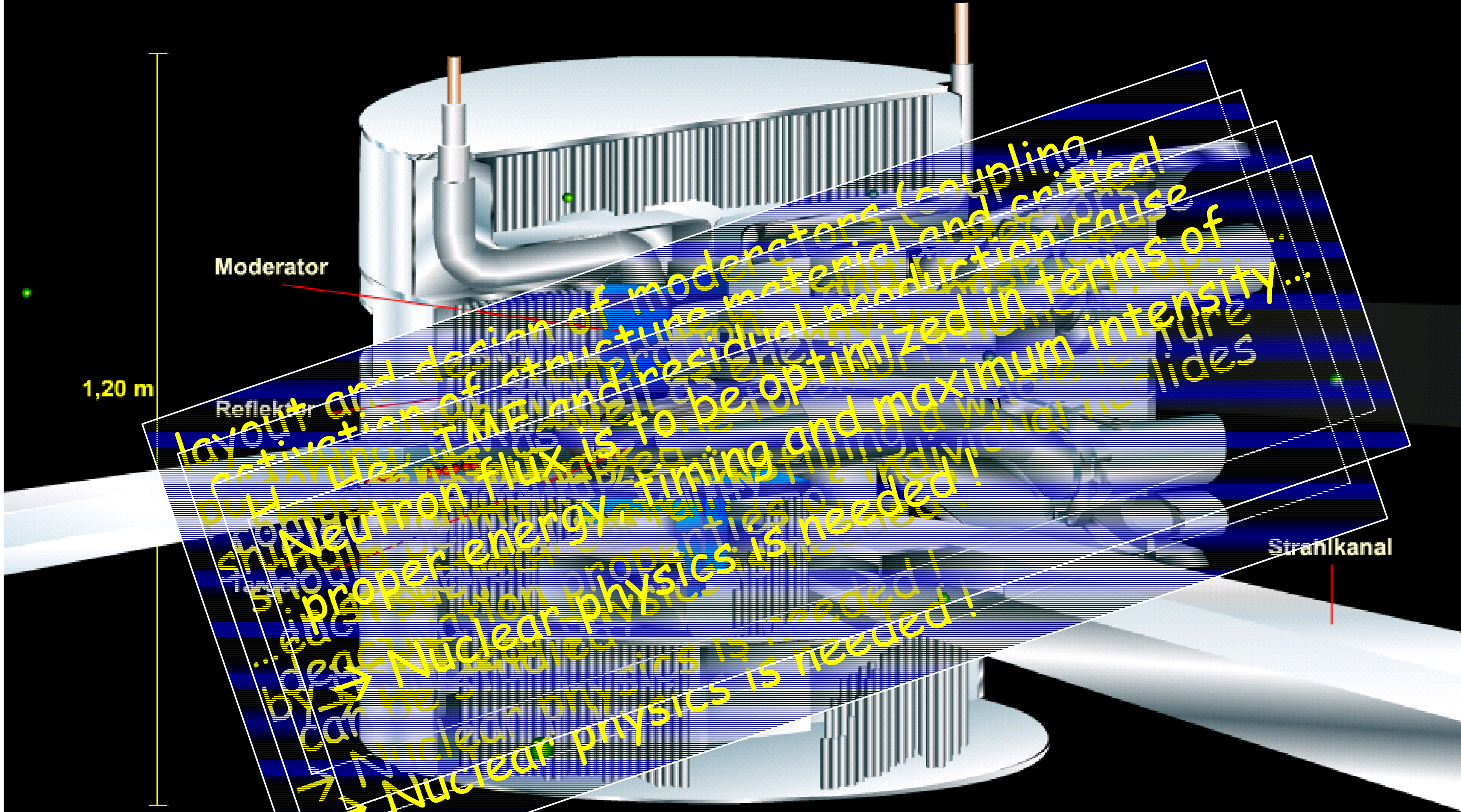
H, He, IMF and residual production cause ...

Neutron flux is to be optimized in terms of proper energy, timing and maximum intensity...

→ Nuclear physics is needed !

The Target (ESS)

ESS, SNS, JSNS, ISIS,….



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activation of structure material and critical

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Neutron flux is to be optimized in terms of proper energy, timing and maximum intensity…

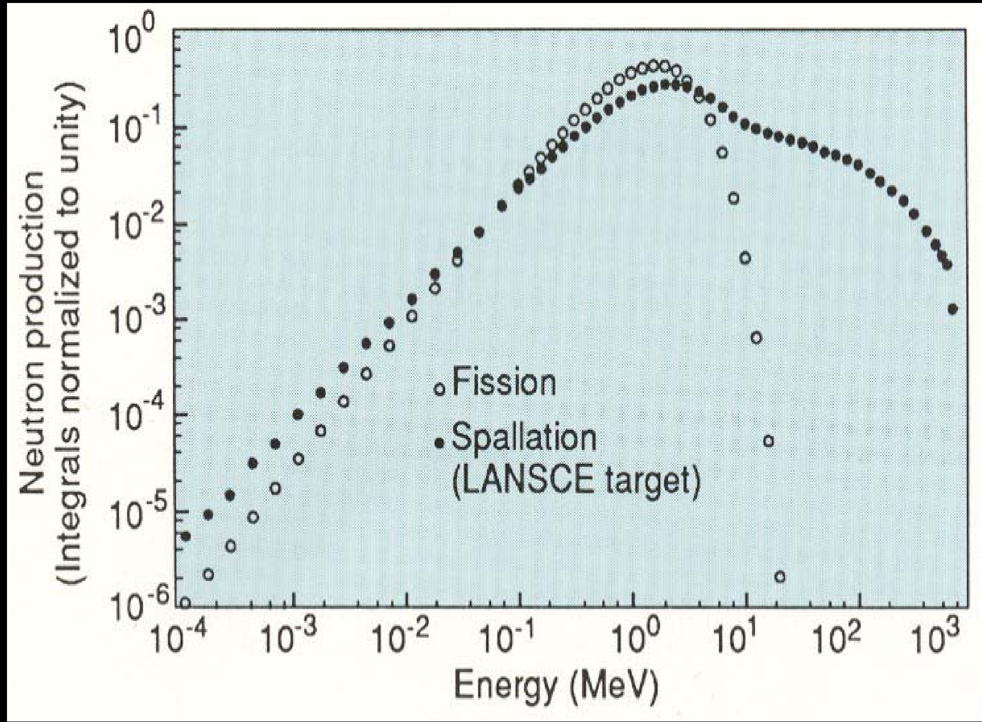
→ Nuclear physics is needed !

Spallation vs ...

Process	Example	Yield	Energy Deposition [MeV/n]
DT solid target	400keV deuterons on tritium in Titan	4.0×10^{-5} n/d	10 000
Deuteron stripping	35 MeV deuterons on liquid Lithium	2.5×10^{-3} n/d	10 000
electrons Bremsstrahlung (Photo-neutrons)	100MeV electrons on U-238	5.0×10^{-2} n/e	2000
Fission	U-235 (n,f)	1 n/fission	180
DT-fusion	laser or ion-beams imploding pellets	1 n/Fusion	3
spallation	1 GeV protons on Pb	30 n/p	20

spectra...

Shielding problem…



The integral neutron spectrum can be fitted with a Maxwellian distribution:

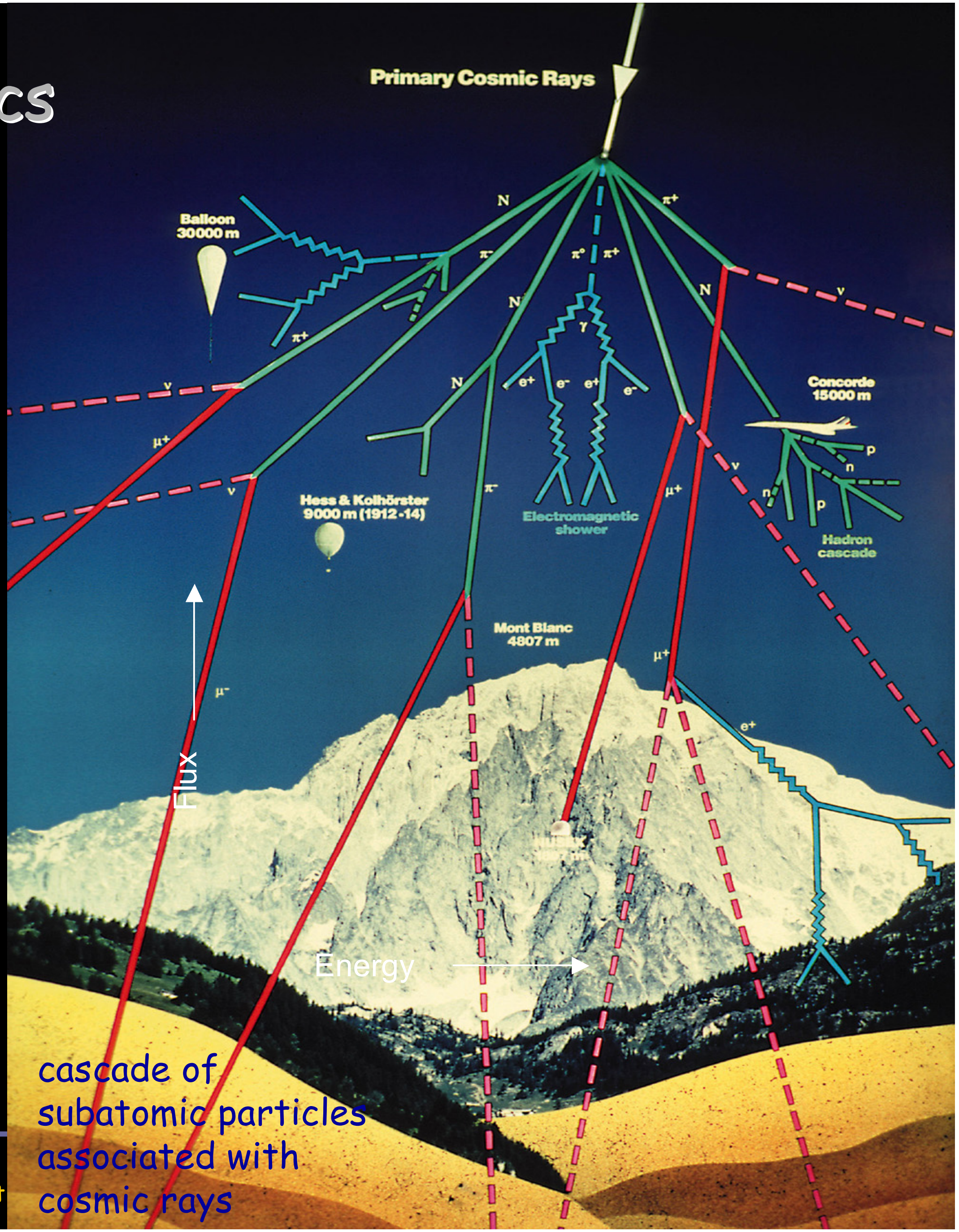
$$N_M(E) = \frac{2E^{1/2}}{\pi^{1/2} T_M^{3/2}} . \exp\left(-\frac{E}{T_M}\right)$$

With T_M the only parameter characterizing the distribution. The average neutron energy is given by $\langle E_n \rangle = 3/2\ T_M$.

^{235}U(n,f): T_M = 1.352 MeV
$\langle E_n \rangle$ = 2.028 MeV

Astro particle physics

- cosmic rays, interaction with ISM, cosmogenic nuclide formation
- highly energetic photons and other particles
- neutrinos (Supernovae, sun, ?)
- antimatter-nuclei, antigalaxies
- dark matter ?
- ...



cascade of subatomic particles associated with cosmic rays

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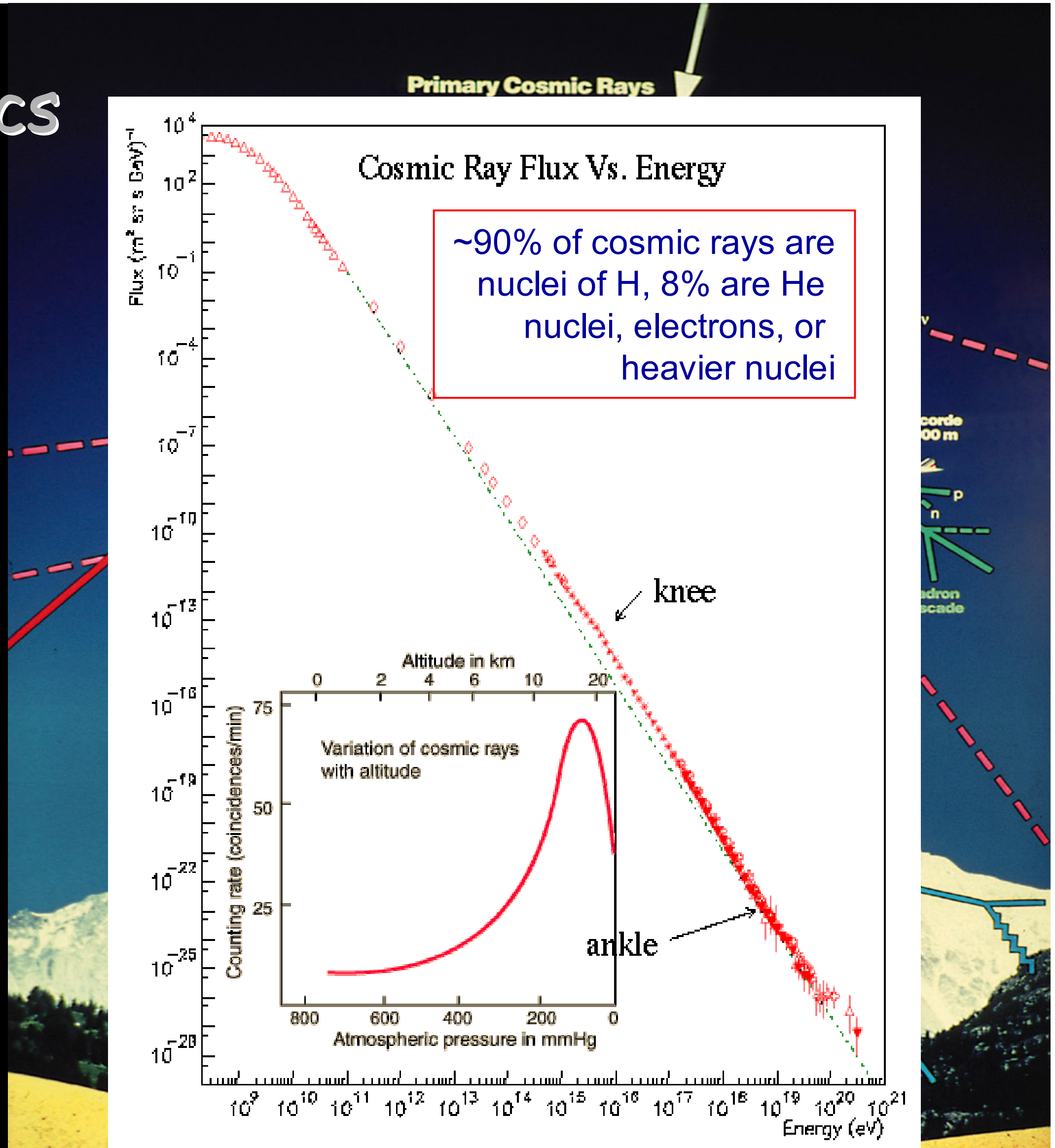

cascade of subatomic particles associated with cosmic rays

Astro particle physics

- c
wi
nu
- h
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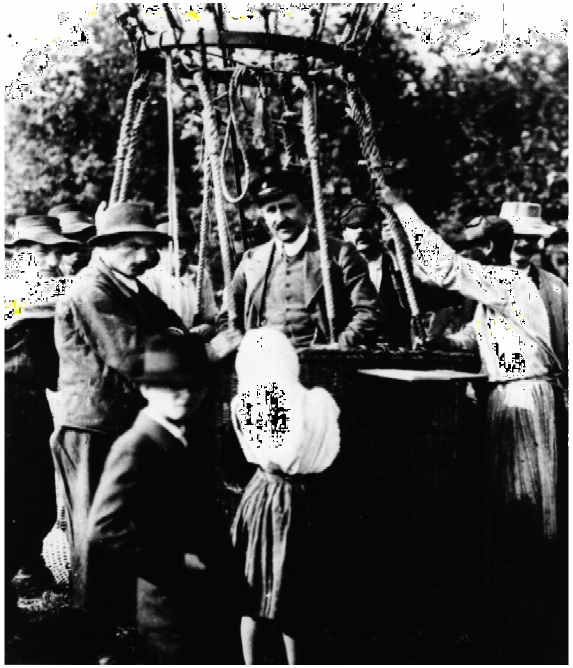
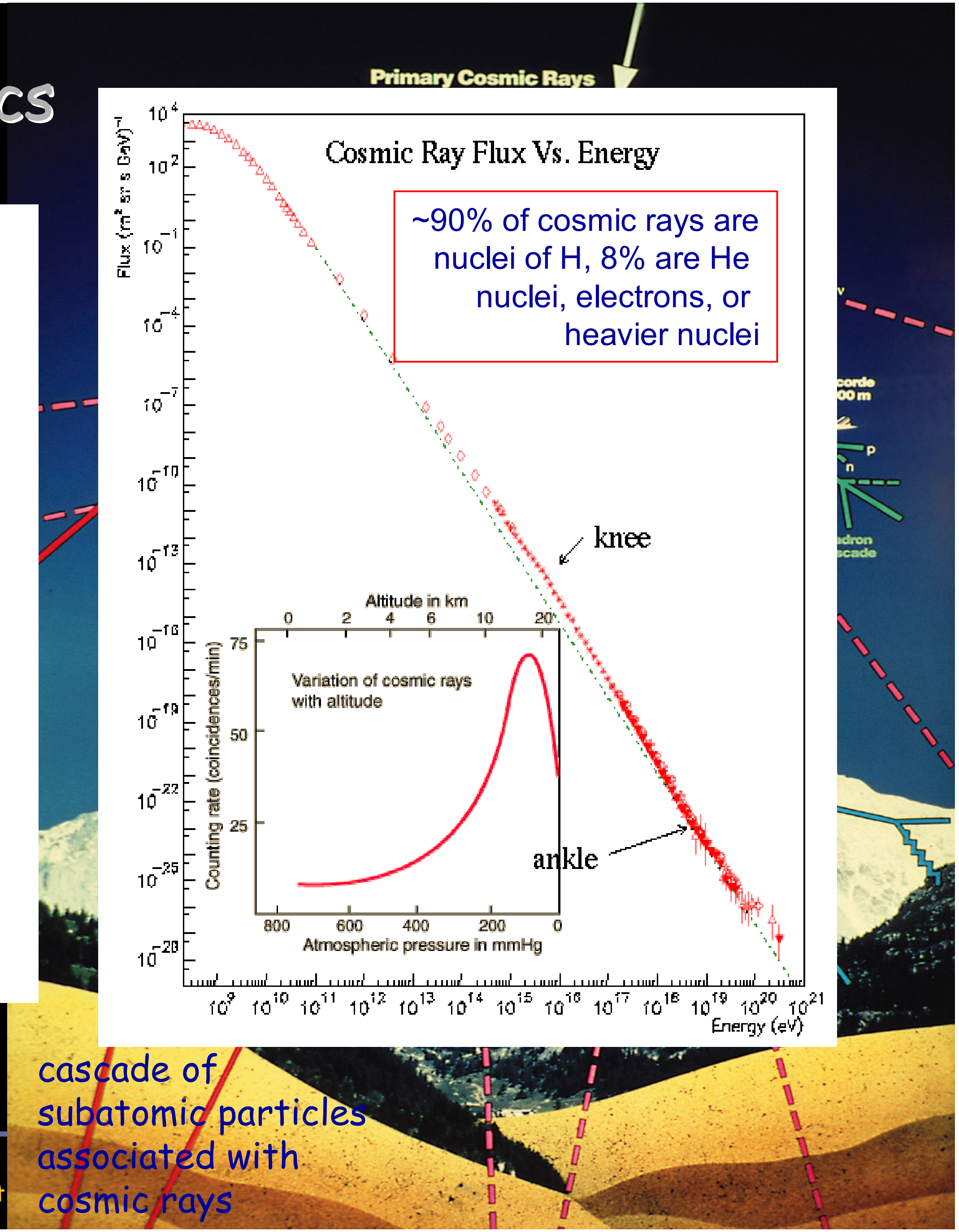
- c
an
- c
- …

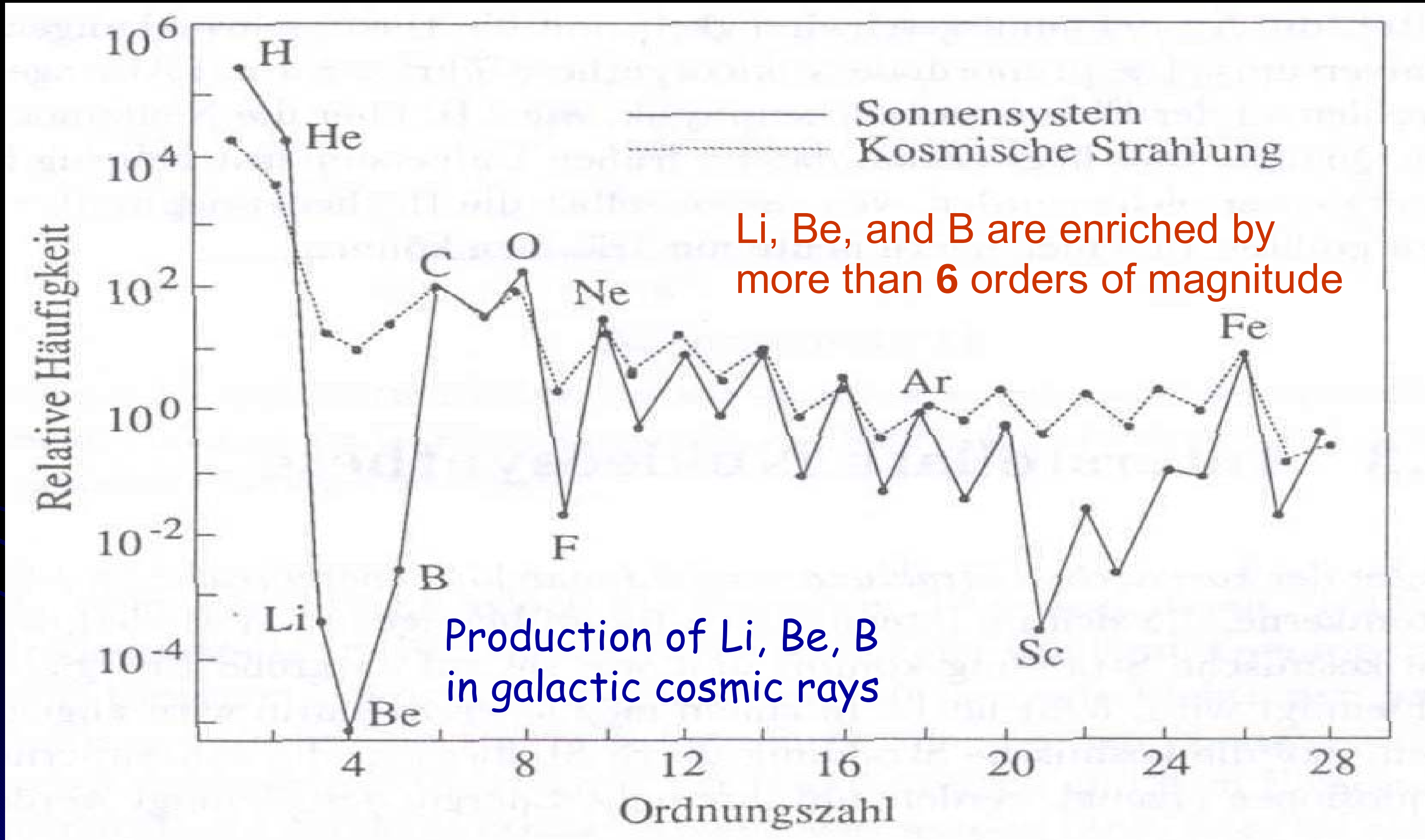
Victor Hess before his 1912 balloon flight in Austria, during which he discovered cosmic rays





cascade of subatomic particles associated with cosmic rays

Nucleosynthesis in stars: composition of cosmic rays at upper atmosphere compared to solar abundancies of atomic nuclei



Meyer, Ramalty and Weber, Phys.Today, 1974

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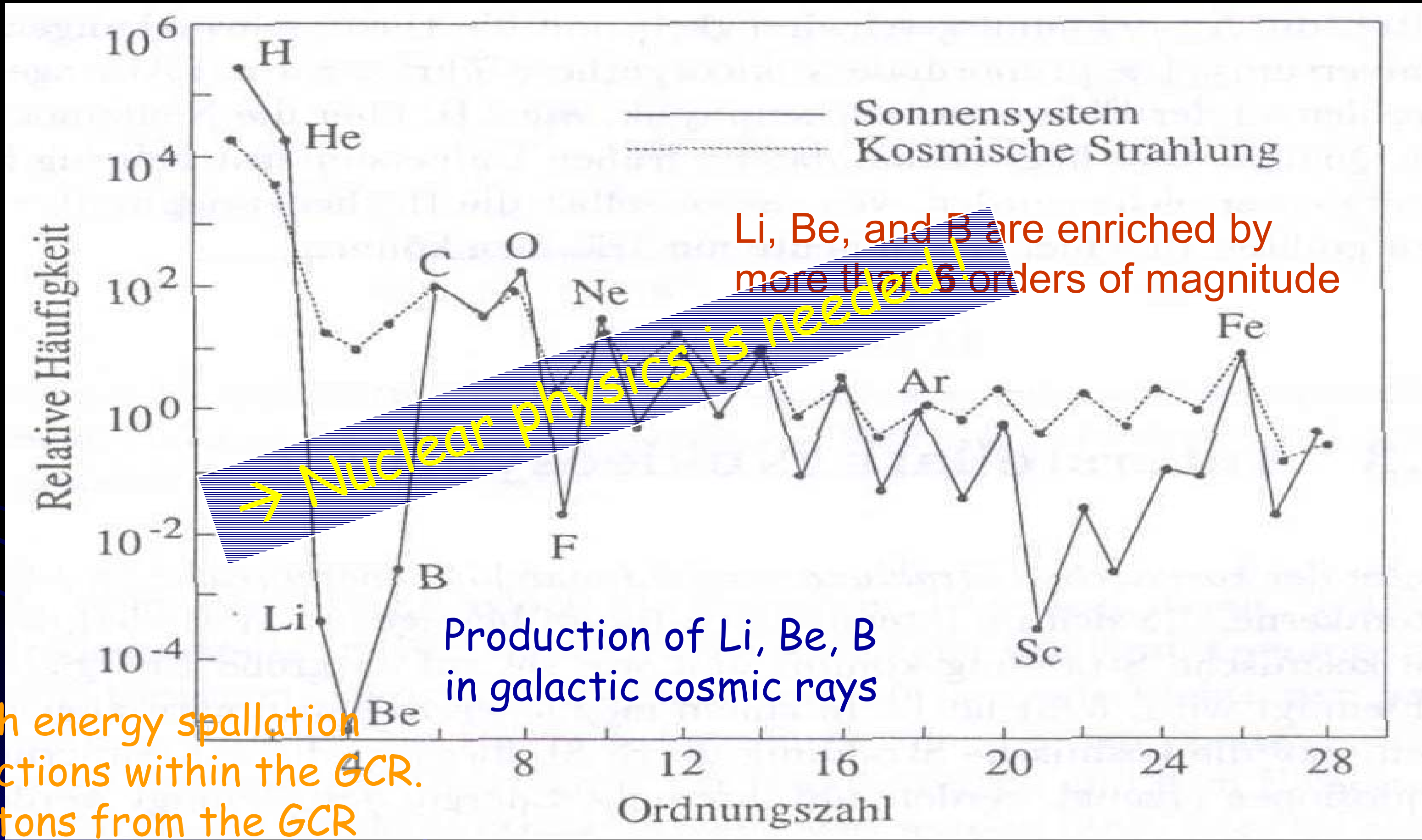


Meyer, Ramalty and Weber, Phys.Today, 1974

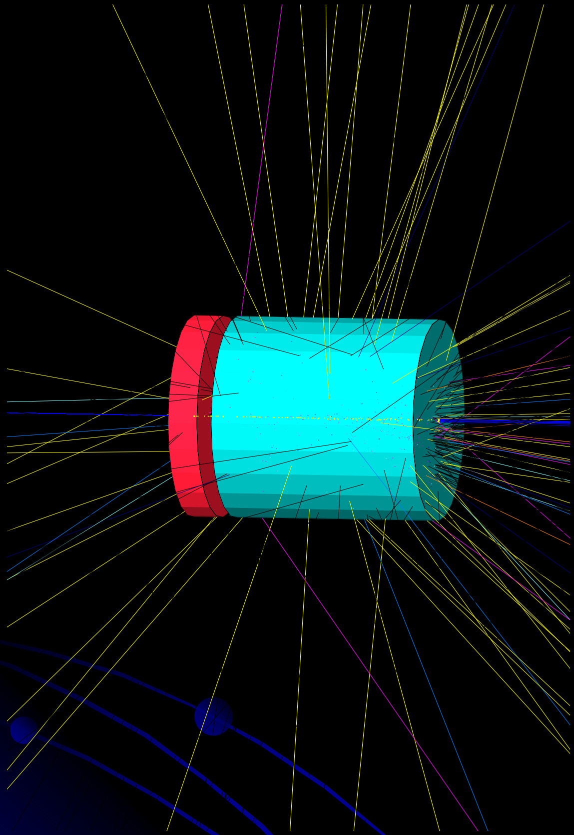
High energy spallation reactions within the GCR. Protons from the GCR produce Li, Be, and B in spallation reactions induced on C, N, O

Tasks – capabilities of models

- optimization:
  - maximum neutronen flux in proper energy- and time structure
  - limited material damage in critical components
  - small irradiation dose and energy-deposition
- simple variation of design-parameter (without experiments)
  - beam properties
  - geometry
  - Material
- evaluation of physics parameter
  - particle flux as function of space and time
  - energy deposition
  - activation of material
  - damage of material
  - irradiation dose

Illustration of complexity: Hadronic showers

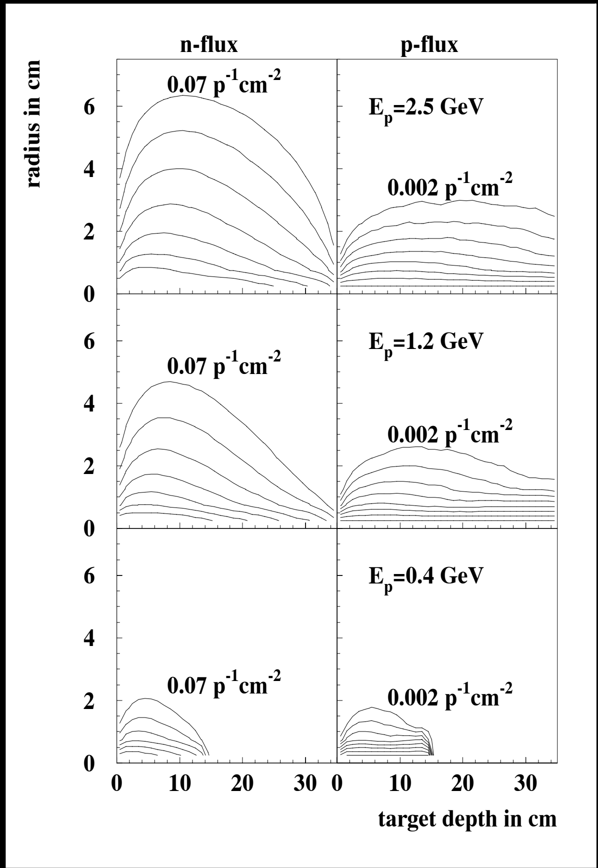
Transport of particles in thick targets



2.5 GeV p + Si/CsI (0.5/70mm)

GEANT4

Analytical approach difficult!



2.5 GeV p + Pb (15dia,35cm length), HERMES

Mainly secondary particle production→initial increase of particle intensity with depth and time

Track length flux of n and p reflects the radial and longitudinal propagation of particles involved in the INC

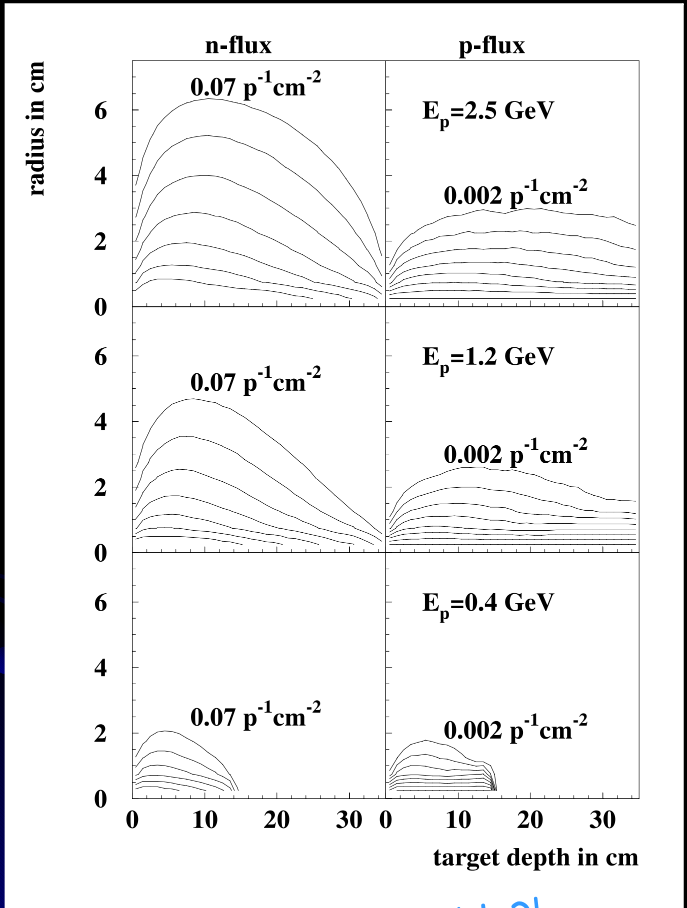
P develop along their trajectory in a more narrow cone (elec.stopping power)

At the end of internuclear cascade subsequent emission of low energy particles….

Complex record keeping of all particles in terms of energy location and direction

Spatial distribution of shower generation

p + Pb (15dia,35cm length), Hermes



Transport of particles in thick targets

Radial direction determined by intensity profile of incoming beam

Axially controlled by σ_{inel}=15.9πA$^{2/3}$ mb/A as consequence of σ_{inel} intensity of proton beam (power deposition, neutron release) decreases exponentially along axis of target

Parameterization of the axial distribution:

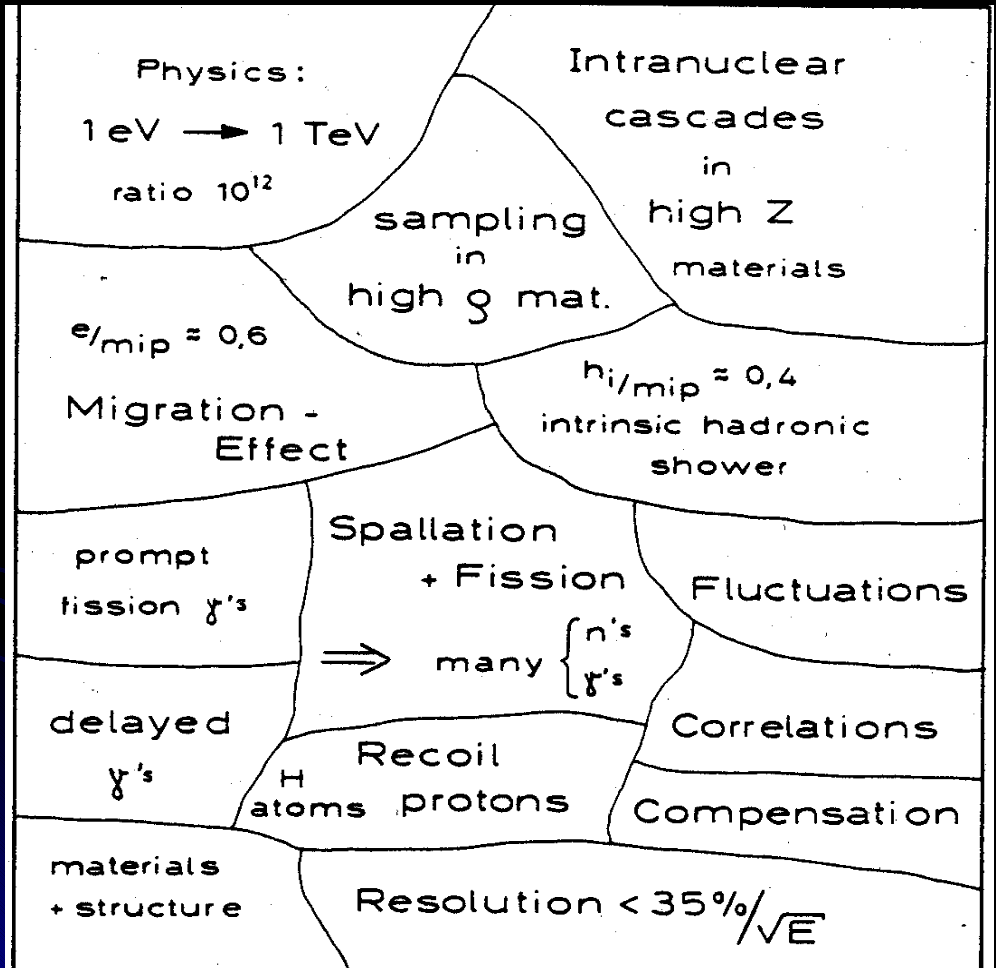
$$n(z) = N_0(1-\exp(\frac{-z-z_0}{\lambda_b}))\exp(-z/\lambda_a) \text{ with}$$

N,N$_0$ quantity to be described (neutron yield, power density, temperature, radial power integral,...), z_0 extrapolation length, λ_b buildup length, λ_a attenuation length (N_a/σ_{inel} where N_a is number of target nuclei per cm^3)

G.S.Bauer NIM A463 2001, 505

Analytical approach possible?!

The puzzle of physics



due to the many aspects involved in the physics description of these complex processes an analytic description is essentially impossible.

Sampling between GeV and meV !!!

therefore MC…

Why particle transport?

Due to significant increase of computing power Monte Carlo methods have turned out to be the first choice

→ „Monte Carlo is what nature does"

- in reactor-technique, fusion, spallation physics, spallation sources, transmutation, ADS design, shielding of particle beams, cosmic rays, therapy,…

- adresses to questions in material composition, geometry, particle- and beam parameters

- MC (nuclear physics implemented) important for many scientific and technological problems

General Boltzmann equation for particle transport and interaction with matter

$$\frac{1}{v_i}\left(\frac{\partial \Phi_i}{\partial t}\right) = -\vec{\Omega} \times grad\,\Phi_i + \Sigma_j [\int d\vec{\Omega}_i\, dE_B\, \sigma_{ij}\left(\vec{x}, E_B \rightarrow E, \vec{\Omega} \rightarrow \vec{\Omega}'\right) \times$$

$$\Phi_j\left(\vec{x}, E_B, \vec{\Omega}, t\right) - \int d\vec{\Omega}'\, dE_B \times \sigma_{ij}\left(\vec{x}, E \rightarrow E_B, \vec{\Omega} \rightarrow \vec{\Omega}'\right)\, \Phi_j\left(\vec{x}, E, \vec{\Omega}, t\right)] -$$

$$\sigma_i(\vec{x}, E)\;\; \Phi_i\left(\vec{x}, E, \vec{\Omega}, t\right) + (\partial/\partial E(\Phi_i S)) - \frac{1}{\lambda_i}\Phi_i + Y_i\left(\vec{x}, E, \vec{\Omega}, t\right)$$

Variable ϕ_i $(\vec{x}, E, \vec{\Omega}, t)$ ist der winkelabhängige Teilchenfluß

Non rel. integro-differential eqn. settled in 1872---continuity eqn in phase space consisting of 3 space coordinates, kin. energy and direction of motion

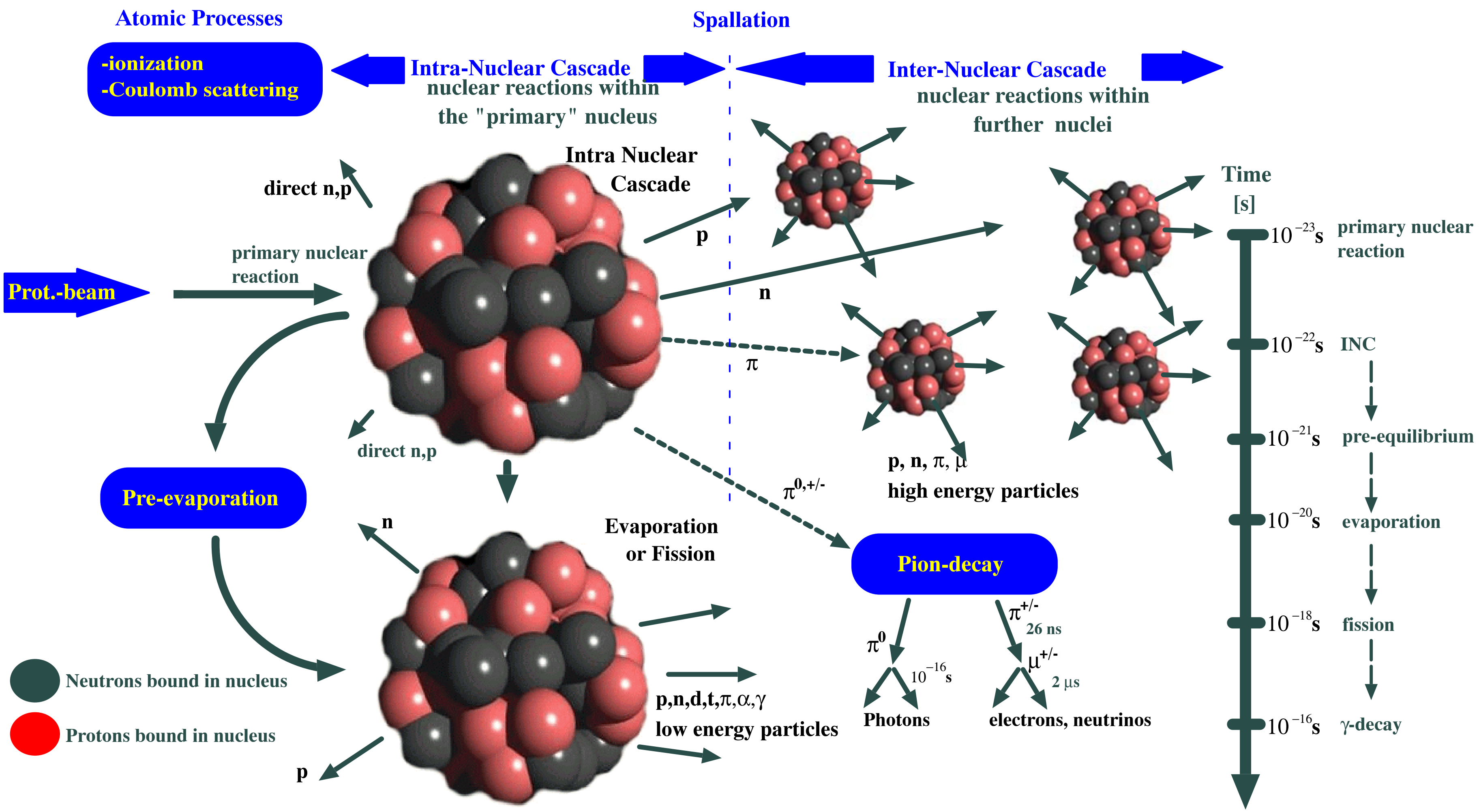
System of coupled transport eqn. difficult to solve in particular for hadronic cascades because of secondary particle production.

numerical procedures emerged i) deterministic methods: discrete ordinates…

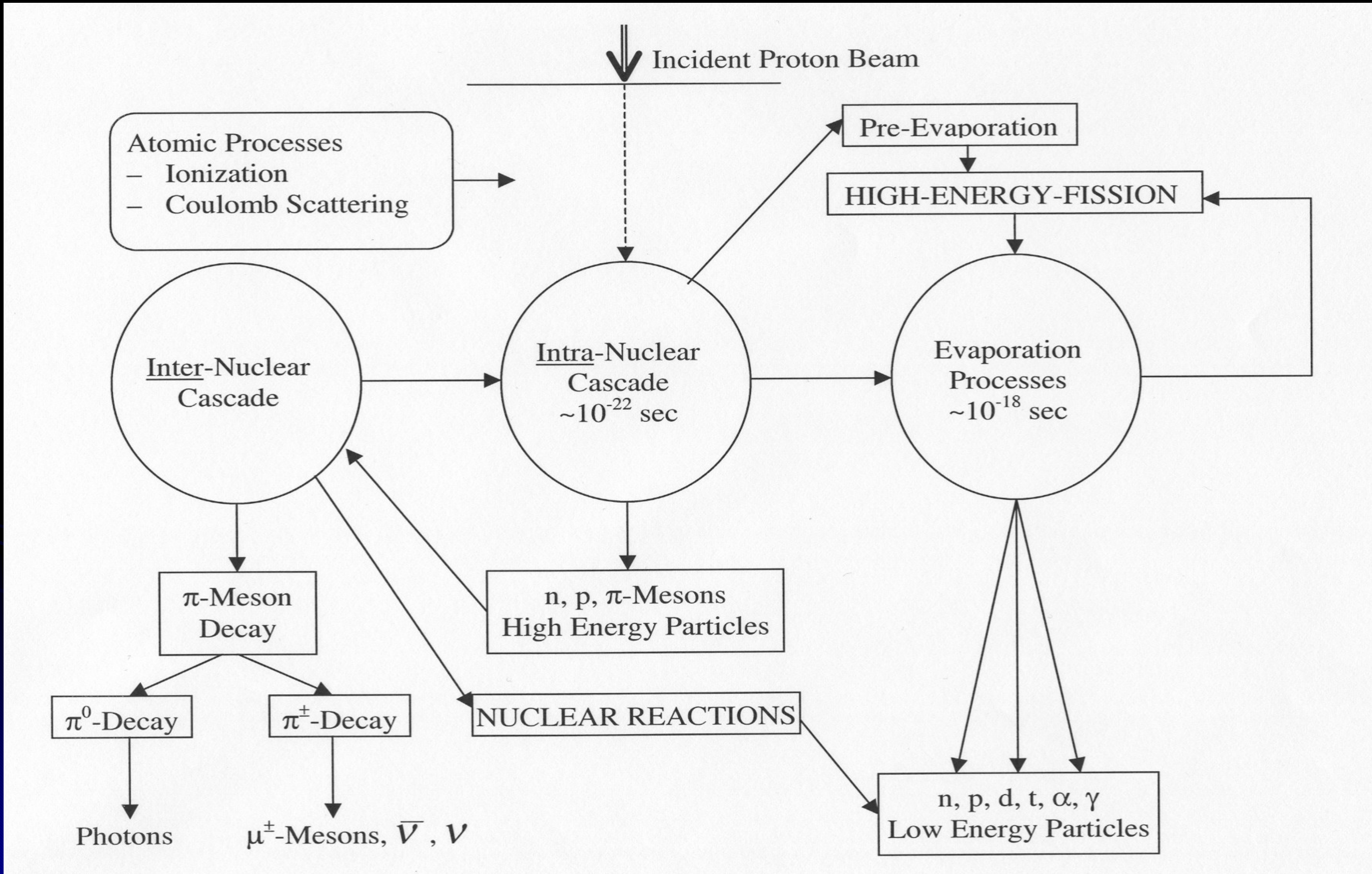
ii) MC: construct stochastical model in which the expected value of a random variable is equivalent to the physical quantity to be determined+ estimated by the average of many independent samples representing the random variable

Real phys. situation, no need for invoking transport eqn.; „only" complete math. description of probability relationships needed…

Modeling of transport processes



Modeling the two stages of the spallation process



INCE Event Generators
(standard use and recent new models)

Models	Main authors
Bertini INC Model	H. Bertini (ORNL) in HETC/LAHET
Dresner EVAP Model GEM_EVAP Model ABLA Model	L. Dresner (ORNL) in HETC/LAHET Furihata (Mitsubishi-Research) K.H.Schmidt (GSI)
ISABEL Model	Y. Yariv, Soreq, Israel
Cugnon INC Model	J. Cugnon, Univ. Liege
FLUKA Event Generators	A. Ferrari et al., Univ. Milano, CERN
GEMINI Evaporation Model	R. Charity, Washington Univ. St. Louis
CEM	S. Mashnik, LANL
MC4 Generators	G. Sterzenbach, FZ-Jülich
Moscow Generator	E. Golubeva et al., Troitsk
MICRES	D. Theis et al., Univ. Bonn
MARS	N. Mokhov, FNAL

Code systems

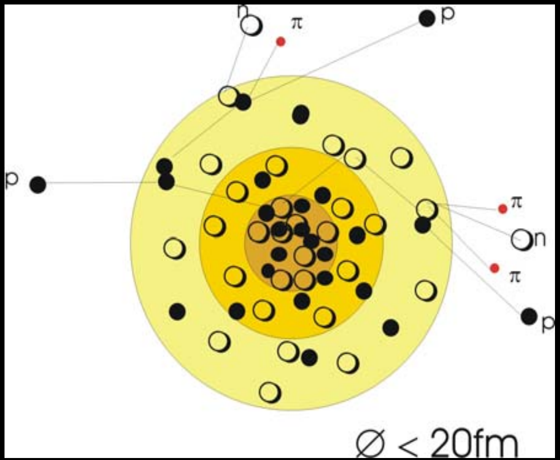
CALOR	T. Gabriel et al., ORNL	HETC based
HERMES	P. Cloth et al., FZ-Jülich	HETC based
LCS	R. Prael et al., LANL	HETC based
GEANT4	S.Agostinelli et al., CERN	HETC based
MCNPX	LANL (Test-Version) □ CEM, 150 MeV x-sec.	HETC based
TIERCE	O. Bersillon, CEA	HETC based
PSI-HETC/O5R	P. Atchison, PSI	HETC based
PHITS/NMTC/JAM	K.Niita et al., JAERI/KEK	HETC,JQMD
FLUKA	A. Fasso et al., CERN, Milano*	

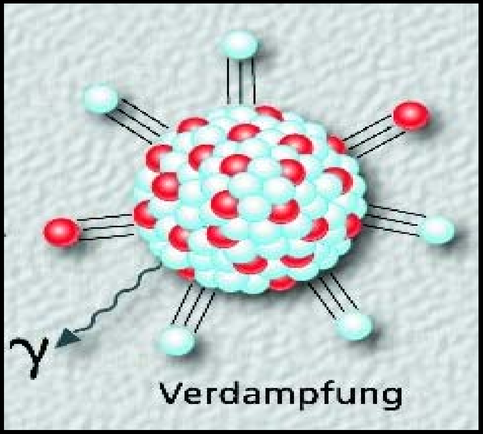
Cross Section Calculation and Evaluation

ALICE	M.Blann, LLNL
GNASH	P.G.Young, LANL, M.B.Chadwick, LLNL
NJOY	R.E.MacFarlane, LANL

Physical Processes and Models(1): codes applied

- spallation
  - intranuclear Cascade
    - INC+ISOBAR H.W.Bertini Phys.Rev.188(1969)1711
    - INCL J. Cugnon, Phys. Rev. C 22(1980)1885
    - ISABEL Y. Yariv and Z. Fraenkel, Phys. Rev. C 20(1979)2227
  - evaporation
    - EVAP (Dresner), GEM (Furihata), ABLA (Schmidt)
    - RAL (Atchinson)
    - Gemini (Charity)
  - optionally multistage preequilibrium exciton model
  - for ejectile energies <20 MeV neutron transport by MORSE and MCNP
  - Deexcitation by γ-Emission
    - NDEM (Database of nuclear Levels)
- Ionization
- Elastic Scattering (at high energies)
- Particle Decay (Pions)

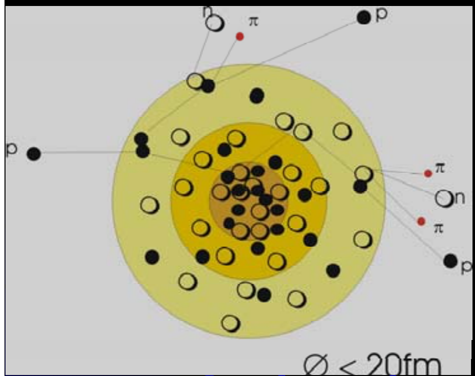




Physical Processes and Models(2): The INC

fundamental presumptions

- hadron-nucleus interaction is consequence of independent collisions of primary and secondary particles with nucleons of nucleus.
- trajectories of cascade particles treated "classical"---no interaction among each other.
- interaction based on elementary cross sections valid under vacuum. cross sections derived from empirical approximations of
  - $NN \to NN$ (elastic)
  - $\pi N \to \pi N$ (elastic)
  - $NN \to N^* N \to N\pi N$
  - $NN \to N^* N^* \to N\pi N \pi$
  - $\pi N \to \pi N^* \to \pi N\pi$
  - $N^* N \to NN$ (delta absorption)
  - $\pi N \to \pi N$ (charge exchange)



- Pauli blocking, Fermi motion of target and projectile nuclei, pion production, and effects of target mean field are included.
- nucleus considered as degenerated Fermi gas of n's and p's.

Physical Processes and Models(3): The INC

$\bar{p}p$ - interaction applied in INC models as a function of $\bar{p}$ momentum

for momenta $p_{\bar{p}} \leq 1\,\text{GeV/c}$
dominant channels for $\bar{p}p$ interactions:

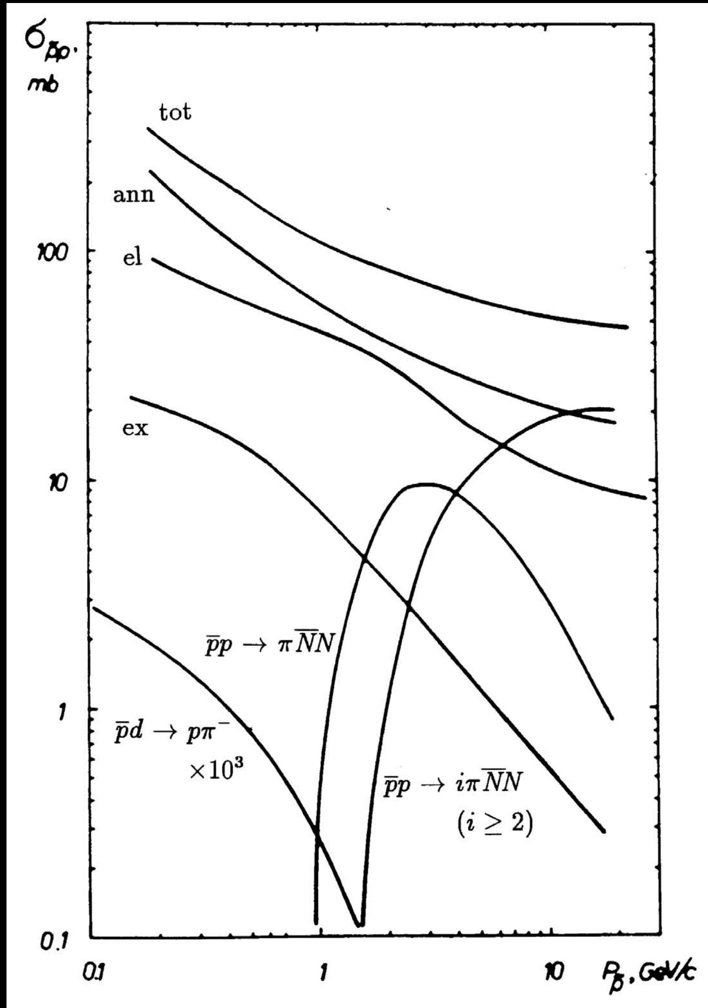
$\bar{p}p \rightarrow i\pi (i \geq 2) \Rightarrow$ annihilation
$\bar{p}p \rightarrow \bar{p}p \Rightarrow$ elastic scattering
$\bar{p}p \rightarrow \bar{n}n \Rightarrow$ charge exchange

for momenta $p_{\bar{p}} > 1\,\text{GeV/c}$ (multi-)pion production without annihilation accrue:

$\bar{p}p \rightarrow \pi \bar{N}N$
$\bar{p}p \rightarrow i\pi \bar{N}N (i \geq 2)$

most INC models also consider the absorption on two nucleons[Cug84]:

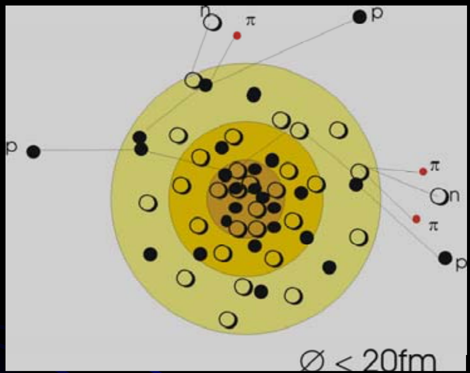
$\bar{N} + NN \rightarrow N + \pi$



Adopted from Ye.Golubeva, Nucl.Phys A483,1988

Physical Processes and Models(4): The INC

Assumptions for which fundamental presumptions (within the INC) are valid:



$\lambda = h/(2mE)^{1/2}$

λ=0.7 fm ↔ 1000 MeV

λ=2.7 fm ↔ 100 MeV

λ=9 fm ↔ 10 MeV

- De-Broglie-wavelength λ of cascade particles smaller than average distance of nucleons in nucleus ($\delta \approx 1.3$fm) and mean free path length L in nuclear matter: $\lambda \ll \delta$, $\lambda \ll L$
- duration of elementary impact $\tau_{int} \sim r_{int}/v$ smaller than time between two collisions, i.e. radius of strong interaction smaller than mean free path length: $r_{int} \ll L$
- number of participating cascade particles N_c should be considerably smaller than number of target nucleons A_t: $N_c \ll A_t$

Physical Processes and Models(4): The INC

production of pions

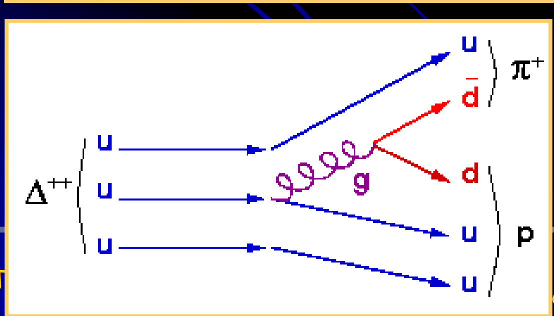
pions are decay products of Δ resonances. (mesons--exchange particles of the strong interaction between nucleons). Δ resonances and pions are coming from inelastic NN reactions at beam energies above few 100 MeV (M_π ~ 140 MeV).

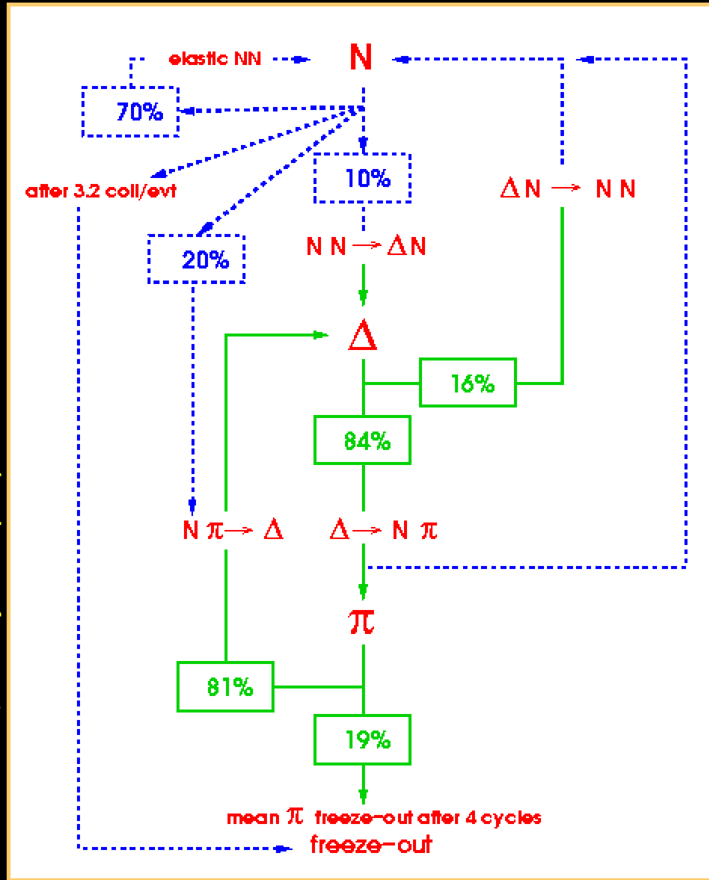
Pion cycle ($\Delta \rightarrow N\pi \rightarrow \Delta$)

• $NN \rightarrow \Delta N$	**hard Δ production**
• $\Delta \rightarrow N\pi$	**Δ decay**
• $\Delta N \rightarrow NN$	**Δ absorption**
• $N\pi \rightarrow \Delta$	**soft Δ production**

4 sorts of Δ's

$\Delta^{++} \rightarrow 1\ (p+\pi^+)$
$\Delta^{+} \rightarrow 2/3\ (p+\pi^0) + 1/3\ (n+\pi^+)$
$\Delta^{0} \rightarrow 2/3\ (n+\pi^0) + 1/3\ (p+\pi^-)$
$\Delta^{-} \rightarrow 1\ (n+\pi^-)$

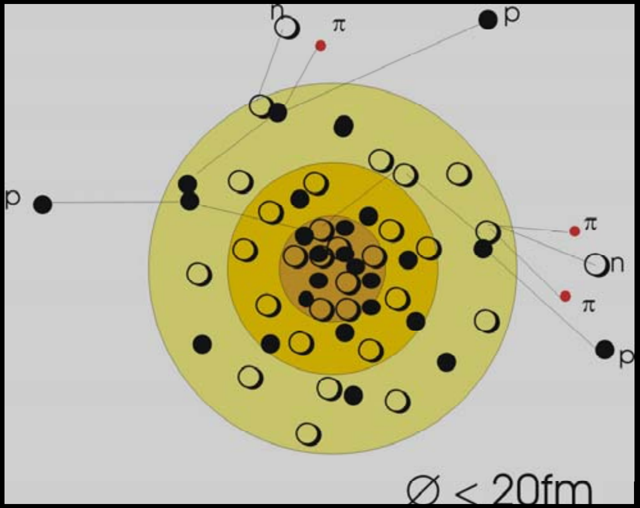




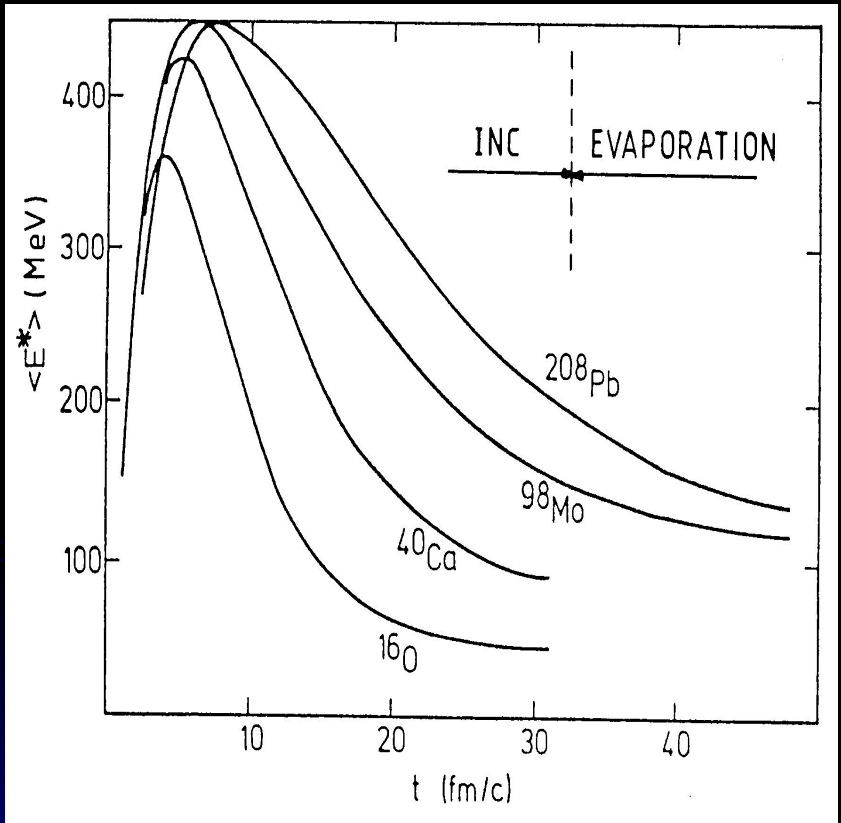
C. Hartnack et al., Nucl. Phys. A 495(1989)303

Physical Processes and Models(5): The INC

- Reactions / cross sections
  - NN → NN (elastic)
  - NN → N* N → Nπ N
  - NN → N* N* → Nπ N π
  - πN → πN (elastic)
  - πN → πN* → π Nπ
  - πN → πN (charge exchange)
  - Further channnels ?
  - Further particle species ?
- nucleon density distribution, Pauli principle (time dependent ?) (~ 10^{-22} s)
- scattering on nucl. potential ?
- cut off criteria: energy / time
- collective interactions ?
- coalescence (cluster) .... !!



Hot nuclei / time scale



J.Cugnon, Nucl.Phys.B8, 255 (1989)

Dynamical picture of the energy dissipation

- E* increases during the first πN collisions
- during this very fast stage of the INC, pre-equilibrium processes cool down nucleus
- statistical equilibrium after ~30 fm/c
- final stage: evaporation from a thermalized nucleus

(reaction shown here: pbar annihilation at rest)

Physical Processes and Models(6): Evaporation

These models are used to simulate the second step of the reaction, i.e. the decay of the excited residue.

Main features:

- life-time of the excited residue much longer than its formation time
  T(residue) = several hundreds of fm/c
  T(formation) ~ 30 fm/c
- individual properties of quantum states have negligible effect at high excitation energy, due to the small distance between the energy levels, in particular in heavy nuclei.

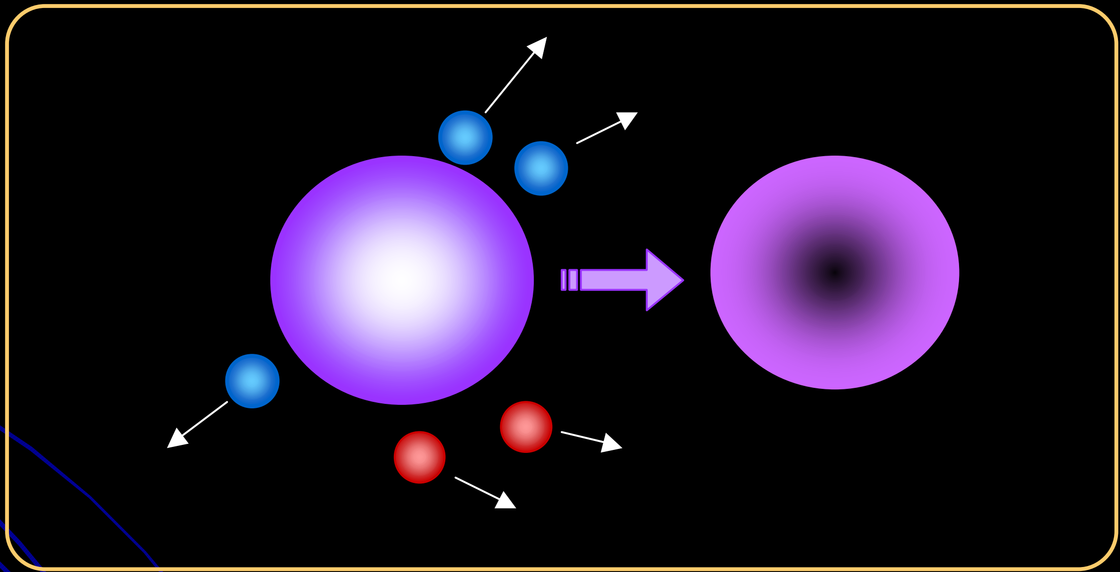
All the states are equiprobable so the deexcitation of the nucleus may be treated in a statistical way.

In other words, a statistical model considers the probabilities of the different deexcitation possibilities with comparable weights, which correspond to individual processes of similar time scales.

Physical Processes and Models(7): Evaporation

Most of the current evaporation code describe the residue deexcitation according to the Weisskopf theory which is based on the energy conservation and the assumption of the micro-reversibility of the process.

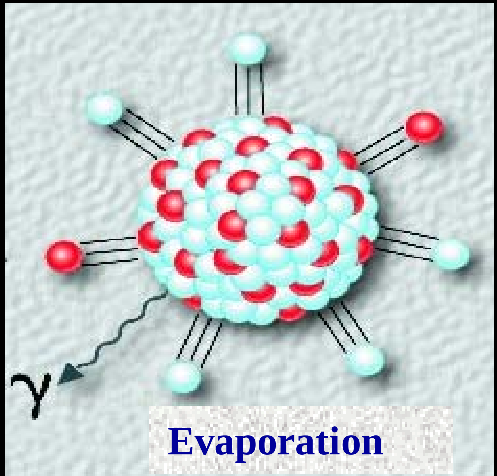
This assumption is verified for the light particle emissions (n, p, d, t, ^{3}He, ^{4}He), but not for the emission of heavier nuclei or for fission.



Note: the average total neutron multiplicity is about 4 times the multiplicity of the neutrons coming from the cascade stage.

Physical Processes and Models(8): Evaporation SM

$$\Gamma_i = (2S_i + 1) m_i \int_{k_i V_i}^{U - Q_i - \delta} \varepsilon \sigma_{i,capt}(\varepsilon) \omega (U - Q_i - \delta - \varepsilon) d\varepsilon$$



$$\sigma_{capture,i}(\varepsilon) = (1 + C_i)(1 - \frac{k_i V_i}{\varepsilon}) \pi R^2$$

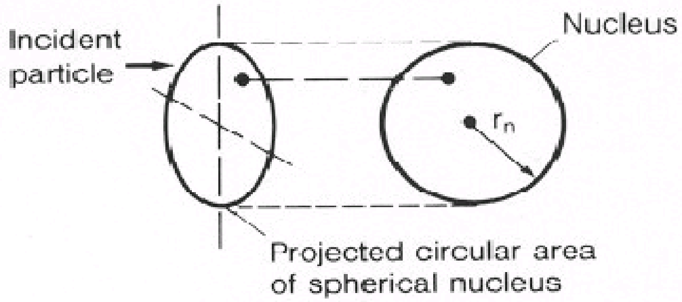
$$\omega(E') = \omega_0 e^{2\sqrt{a(E' - \delta)}}$$

$$a = \frac{A'}{B_0}(1 + Y_0 \frac{(A' - 2Z')^2}{A'^2})$$

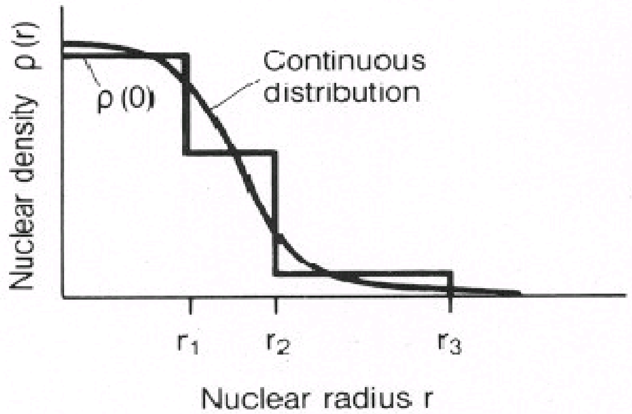
- Extension of SM to high E*
- Validity of the SM at high E*
  - small lifetime of hot nucleus
  - system equilibrated?

- Which particles should be considered?
- Is there a dependency of V from U ?
- How precise accounted for tunneling?
- σ and V depend on nucleus radius $R_0 A^{1/3}$, therefore R_0 is a critical parameter!
- B_0 critical parameter for level density ω!

1. Entry into nucleus:
   - select uniformly over projected area

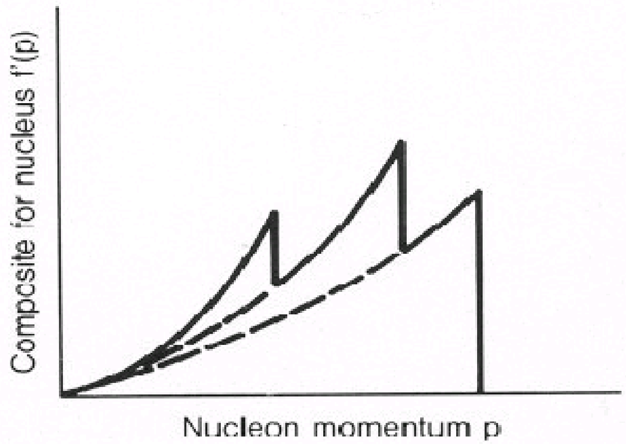


2. Nucleon Density Inside Nucleus:
   - 3-Region Approximation.
   - $[n/p]_{\text{each region}} = [(A-Z)/Z]_{\text{whole nucleus}}$



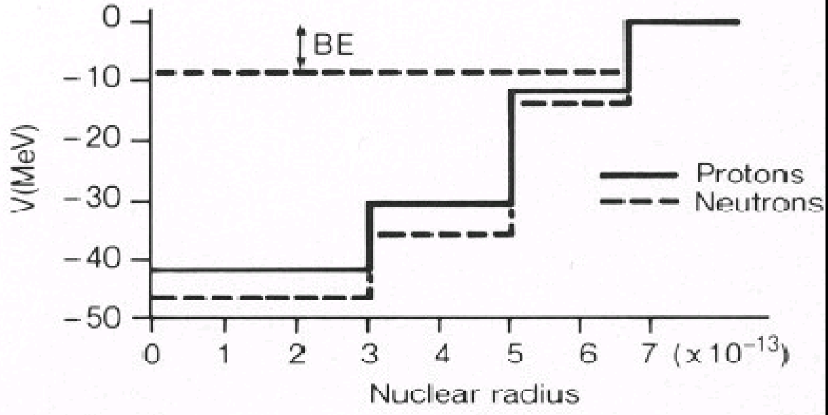
3. Nucleon Momenta:
   - Assume Fermi distribution, $f(p) = cp^2$
   - Normalization,

$$\int_0^{p_f} f(p)dp = \begin{Bmatrix} n_i \\ p_i \end{Bmatrix} \text{ in each region}$$



4. Nucleon Potential Energies:
- $-V = E_f + BE$

  $BE = 7$ MeV



5. Cross Section Needed:
- nucleon-nucleon
- pion-nucleon

6. Exclusion Principle:

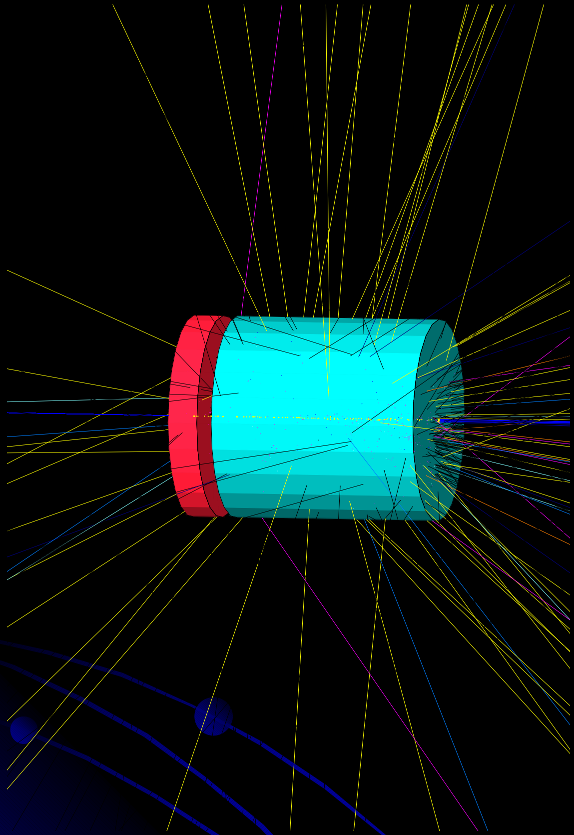
   – reject outcome if state filled

7. Pion Production by the Isobar Model (Lindenbaum / Sternheimer)

8. Evaporation Code EVAP (Dresner) with updates, e.g. with high energy fission model

9. Outcome of INCE
   - E, Ω of emitted particles: n, p, π^+, π^-, π^0, d, t, ^{3}He, α
   - residual E^*
   - residual A, Z of nucleus

Illustration of complexity: Hadronic showers

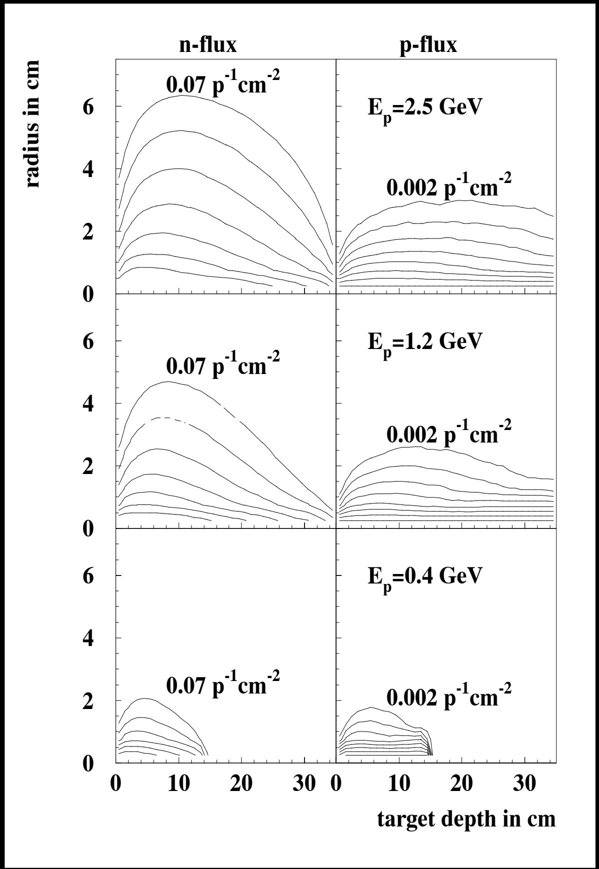


2.5 GeV p + Si/CsI (0.5/70mm)

GEANT4

Analytical approach difficult!

Transport of particles in thick targets



2.5 GeV p + Pb (15dia,35cm length), HERMES

Mainly secondary particle production→initial increase of particle intensity with depth and time

Track length flux of n and p reflects the radial and longitudinal propagation of particles involved in the INC

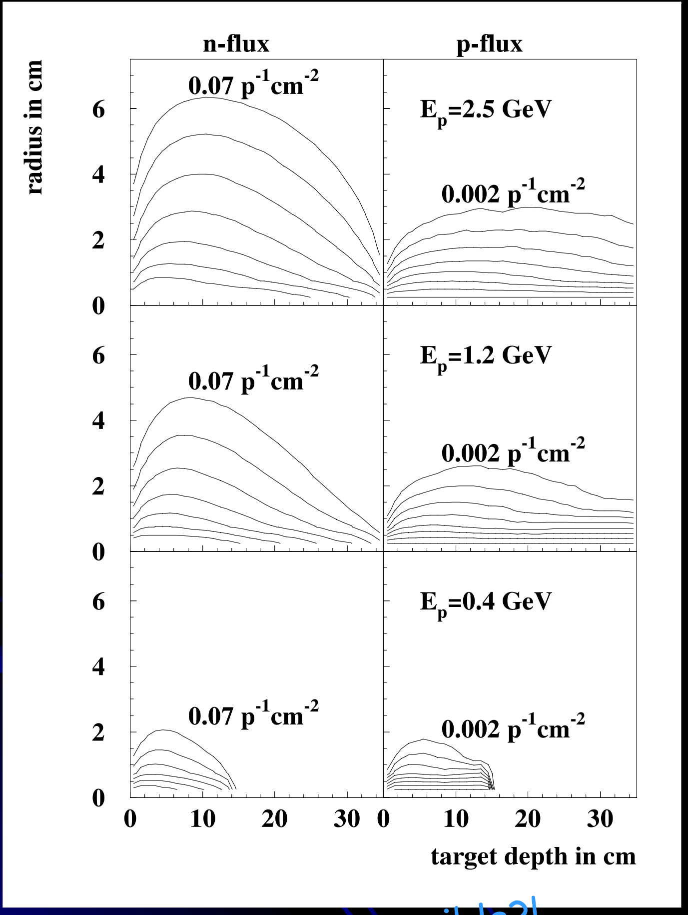
P develop along their trajectory in a more narrow cone (elec.stopping power)

At the end of internuclear cascade subsequent emission of low energy particles….

Complex record keeping of all particles in terms of energy location and direction

Spatial distribution of shower generation

p + Pb (15dia,35cm length), Hermes



Analytical approach possible?!

Transport of particles in thick targets

Radial direction determined by intensity profile of incoming beam

Axially controlled by $\sigma_{inel}=15.9\pi A^{2/3}$ mb/A as consequence of σ_{inel}intensity of proton beam (power deposition, neutron release) decreases exponentially along axis of target

Parameterization of the axial distribution:

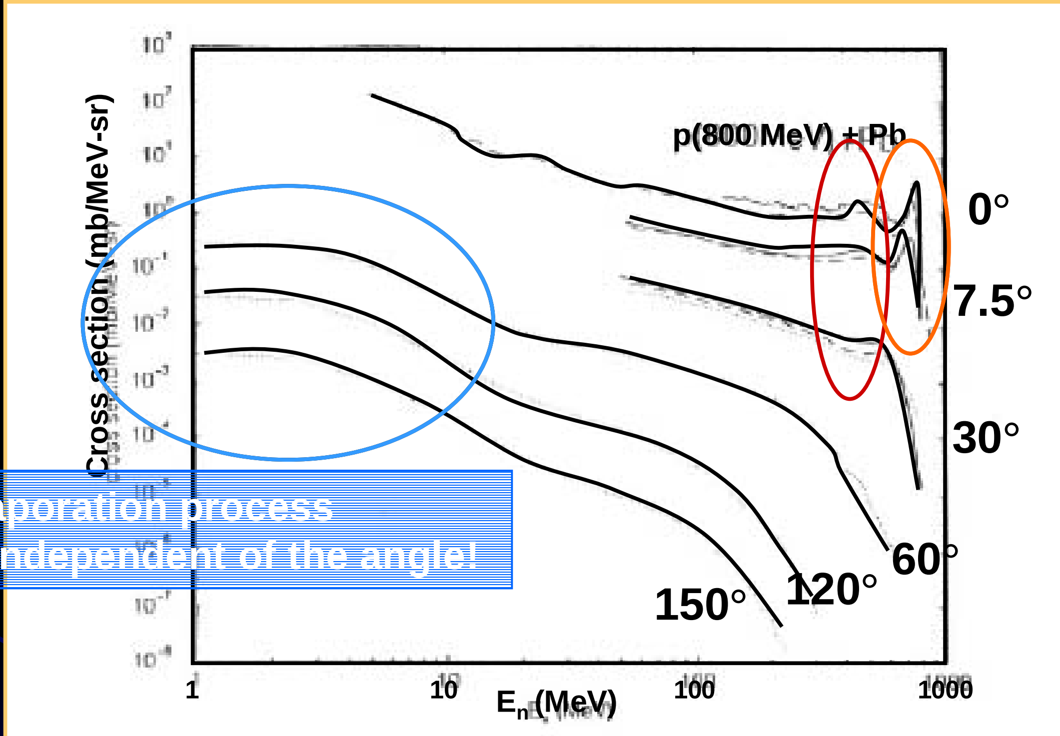
$$n(z) = N_0(1-\exp(\frac{-z-z_0}{\lambda_b}))\exp(-z/\lambda_a) \text{ with}$$

N,N_0 quantity to be described (neutron yield, power density, temperature, radial power integral,...), z_0 extrapolation length, λ_b buildup length, λ_a attenuation length (N_a/σ_{inel} where N_a is number of target nuclei per cm^3)

G.S.Bauer NIM A463 2001, 505

Light particle emission

Neutron spectra



evaporation process
↳ independent of the angle!

due to quasi-elastic scattering
↳ peripheral collisions

due to quasi-inelastic scattering
↳ neutron ejected by the proton which is excited to a Δ^+ resonance

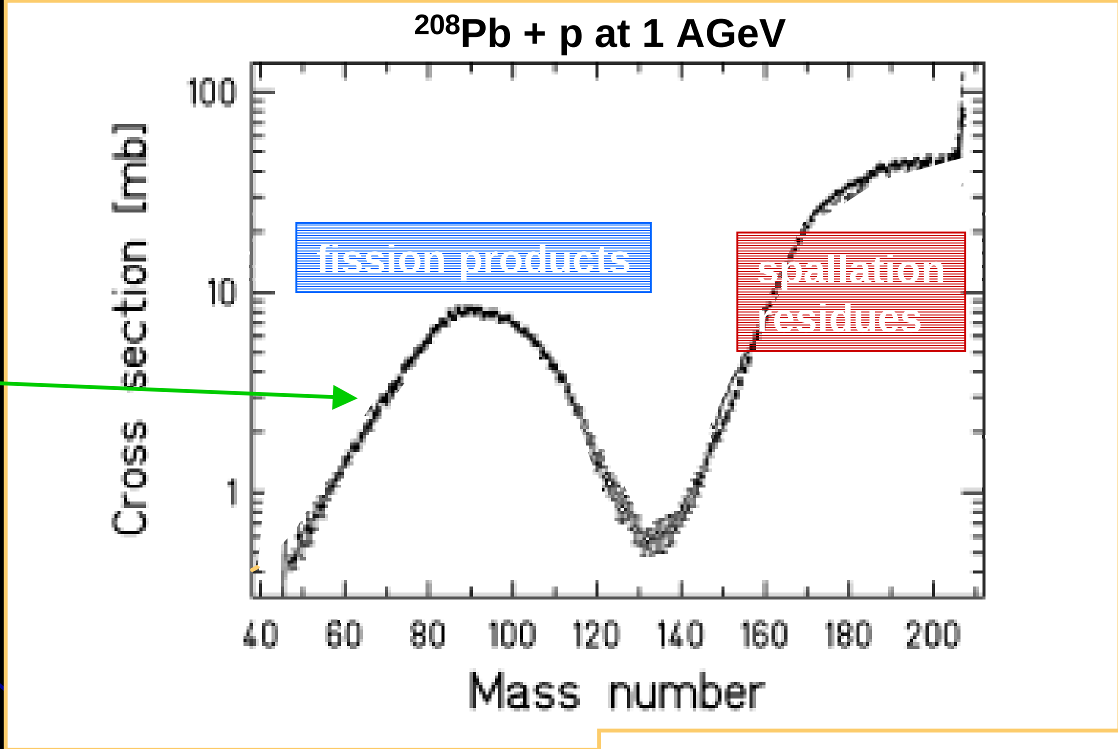
Conclusion: the spallation reaction is a TWO STEP process!

Proton spectra similar shapes as the neutron spectra

Residues

They are observed in the very late stage of the process: after the cascade, the evaporation, and the possible β-decay of very-short-lived emitters.

Intermediate Mass Fragments (IMF)



T. Enqvist et al. / Nuclear Physics A 686 (2001) 481–524

very light fragments: produced by fast ejection (cascade) + evaporation of the remnant

Residues

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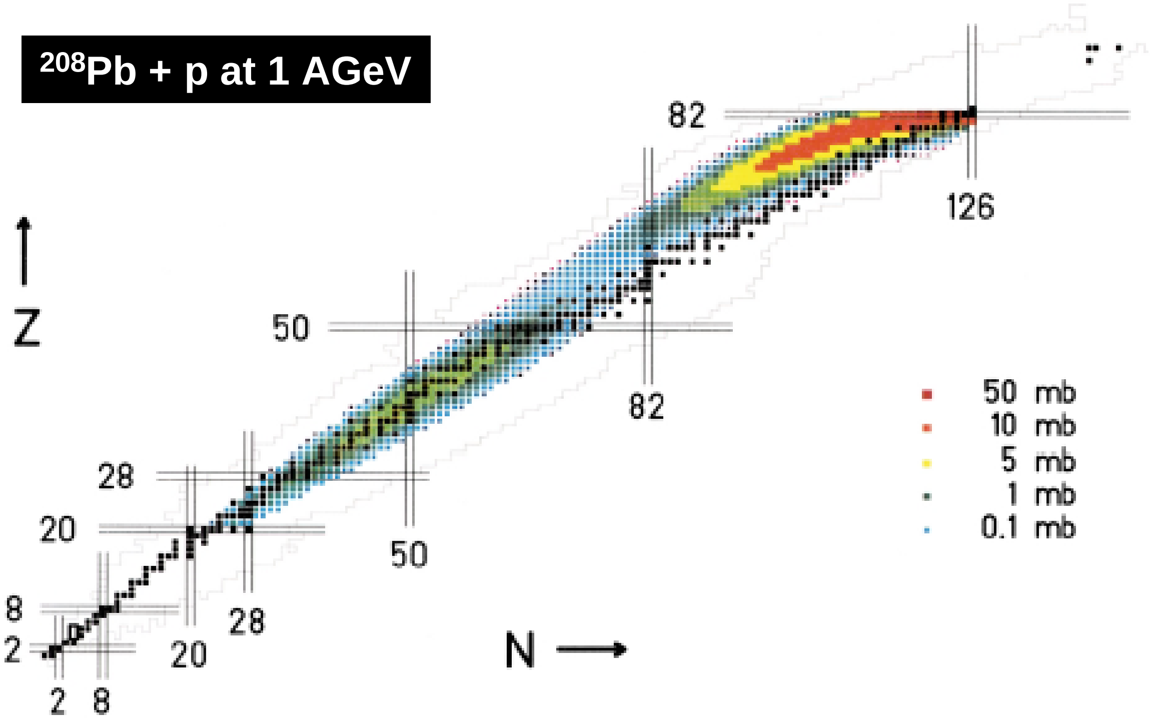

Fig. 19. Two-dimensional cluster plot of the isotopic production cross sections obtained in the present work shown as chart of the nuclides. Full black squares correspond to the stable isotopes. Spallation and fission are separated by a minimum of cross sections at $Z = (58 \pm 3)$.

Comparison with experimental results

J. Cugnon et al. / Nuclear Physics A 620 (1997) 475–509 503

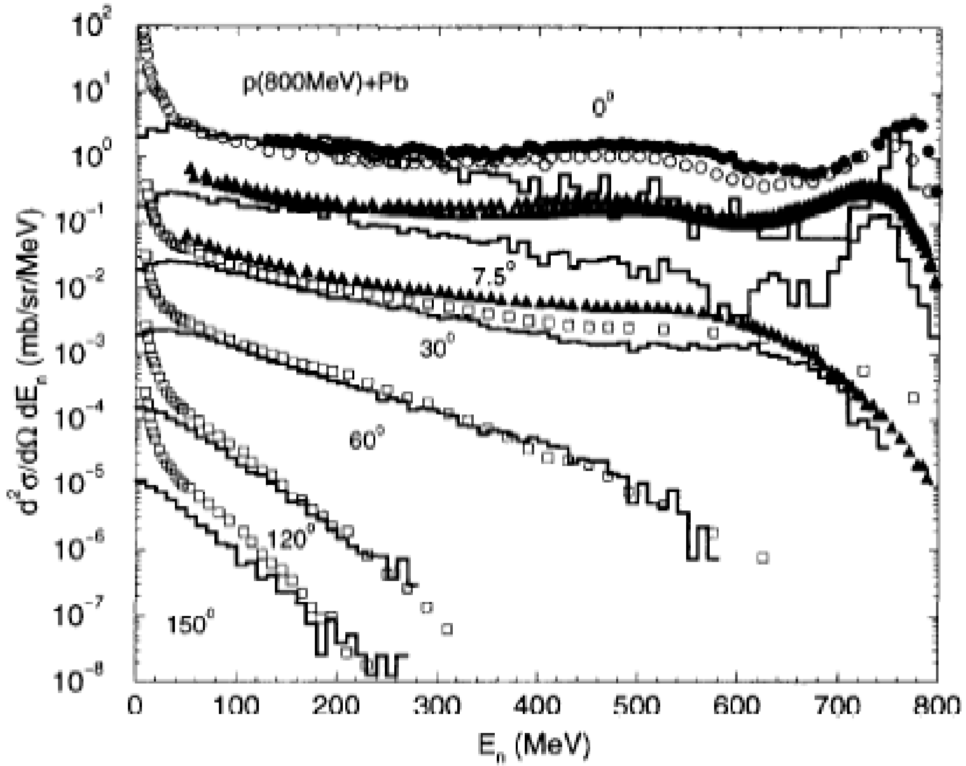

Fig. 21. Neutron double differential cross-sections in p(800 MeV)+Pb reactions. Comparison between experiment (symbols) and the results of the INC+percolation model (histograms) described in Section 5. Same convention as in Fig. 2.

Comparison with experimental results

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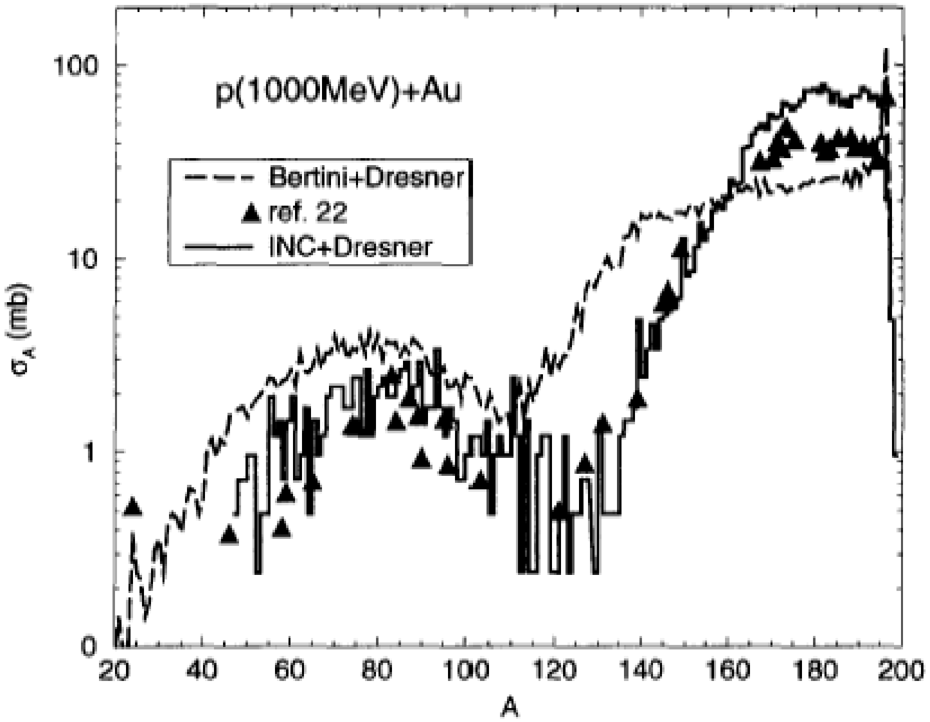
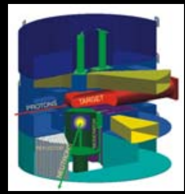


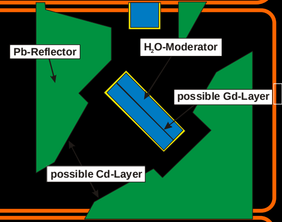
Fig. 7. Residue mass spectrum after p(1 GeV)+^{197}Au reactions. Data (symbols) are taken from Ref. [22]. Theoretical results (histograms) are obtained in a INC+evaporation model, summing over ~10^5 events; full lines correspond to the standard Liège cascade and dashed lines, to the Bertini model. In both cases, the evaporation model of Ref. [21] is used.

Some related subjects...

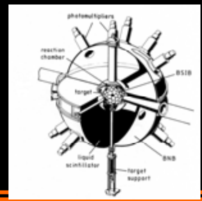
1. Residual nuclei prod., radioact., afterheat, energy depo.



2. Moderators



3. Experiment NESSI



4. Experiment PISA

5. Experiment JESSICA