Detectors in Nuclear Physics: Monte Carlo Methods

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Lectures I-II

INTRODUCTION

What is Monte Carlo ?

(a mathematical method using random sampling)

- The originators : Von Neumann and Ulam 1949
- The method : Random sampling from pdf's to construct solutions to problems.

John Von Neumann

(1903-1957)

Stanislow M. Ulam

(1909-1984)

Why call it Monte Carlo?

After the city in the Monaco principality ...

Sampling from a probability distribution

Sampling from a generic distribution

- Using one random number
- Integrate the distribution function, analytically or numerically, and normalize to 1 to obtain the normalized cumulative distribution:

$$F(\xi) = \frac{\int_{x_{min}}^{\xi} f(x)\,\mathrm{d}x}{\int_{x_{min}}^{x_{max}} f(x)\,\mathrm{d}x}$$

- Sample a uniform pseudo-random number ξ
- Get the desired result by finding the inverse value $X = F^{-1}(\xi)$, analytically or most often by interpolation (table look-up)

Since ξ is uniformly random, we have

$$P(a < x < b) = P(F(a) < \xi < F(b)) = F(b) - F(a) = \int_a^b f(x)dx$$

Sampling from a probability distribution

Example

take $f(x) = e^{-\frac{x}{\lambda}}$, $x \in [0, \infty]$

Cumulative distribution:

$$F(t) = \int_0^t e^{-\frac{x}{\lambda}}\,dx = \lambda \times (1 - e^{-\frac{t}{\lambda}})$$

Normalized:

$$F'(t) = \int_0^t \frac{e^{-\frac{x}{\lambda}}}{\lambda}\,dx = 1 - e^{-\frac{t}{\lambda}}$$

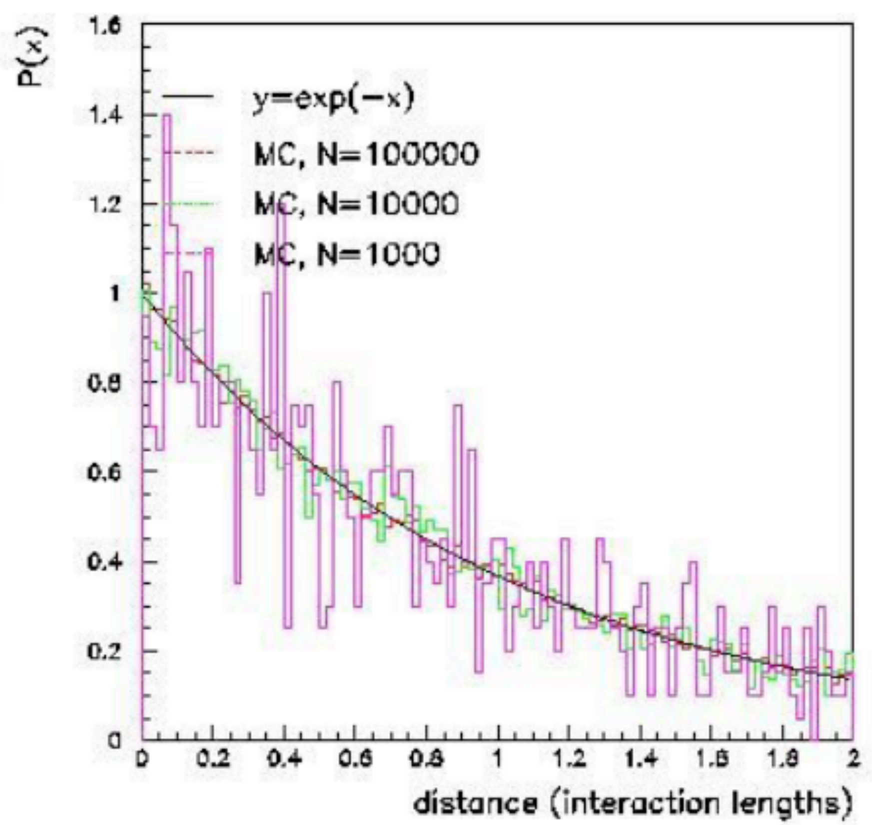
Sample a uniform $\xi \in [0, 1]$

$$1 - e^{-\frac{t}{\lambda}} = \xi$$

sample t by inverting

$$t = -\ln(\xi - 1) \times \lambda$$

repeat N times



Practical rule: a distribution can be sampled directly if and only if its pdf can be integrated and the integral inverted

Sampling from a distribution

- Using two random numbers (rejection technique)
- Choose a constant value $C > f(x)$ for any x
- Sample two random numbers ξ_1 and ξ_2
- If $\xi_2 < f(\xi_1)/C$, $\boxed{X = \xi_1}$,

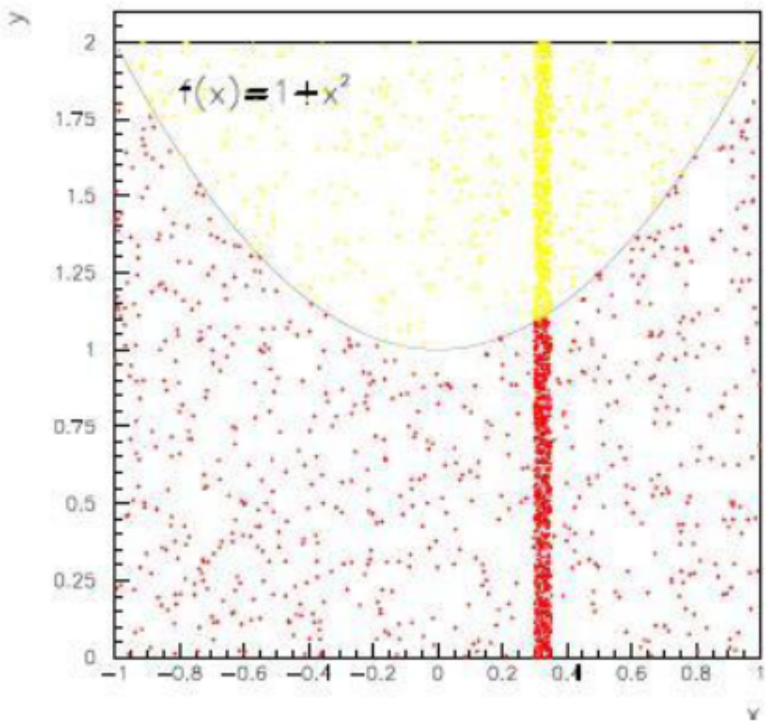
  otherwise re-sample ξ_1, ξ_2

The probability that a ξ_1 value is accepted is $f(\xi_1)/C$ for any ξ_1:

$$P(x)\,dx = P(\xi_1 = x)\,dx \cdot f(\xi_1 = x)/C$$

Since $P(\xi_1)\,dx = const$,

$$P(x)\,dx = const \cdot f(x)$$



The problem of radiation transport

- Each particle is represented by a point in phase space **P**=(**r**, E, **Ω**, *t*)
- Transport calculations are attempts to solve the Boltzmann Equation, i.e., a balance equation accounting for all "produced" (e.g., sources, "in-scattering") and "destroyed" (e.g., absorption, "out-scattering") particles at each point of the phase space
- The MC method can be formulated as an integral form of the Boltzmann equation, e.g., the "emergent particle density equation"

Density of emerging (from source or collision) particles of given position, energy, direction at a given time

$$\chi_{E\Omega}(\mathbf{r}, E, \mathbf{\Omega}, t) =$$

Collision integral operator

$$s_{E\Omega}(\mathbf{r}, E, \mathbf{\Omega}, t) + \hat{C}(\mathbf{r}, E' \rightarrow E, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \cdot \hat{T}(\mathbf{r}' \rightarrow \mathbf{r}, E', \mathbf{\Omega}') \, \chi_{E\Omega}(\mathbf{r}', E', \mathbf{\Omega}', t)$$

Density of particles generated by external source

Transport integral operator

What is the Monte Carlo method?

"The Monte Carlo technique for the simulation of the transport of electrons and photons through bulk media consists of using knowledge of the probability distributions governing the individual interactions of electrons and photons in materials to simulate the random trajectories of individual particles. One keeps track of physical quantities of interest for a large number of histories to provide the required information about the average quantities" *

In principle, very straightforward application of radiation physics. Much easier to understand than convolution / superposition

Virtually no approximations of consequence.

*TG105 quotes Rogers&Bielajew, 1990, in Dosimetry of Ionizing Radiation V3 http://www.physics.carleton.ca/~drogers/pubs/papers/RB90.pdf

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Analog versus condensed history MC

Analog (event-by-event) MC simulation

1. Select the distance to the next interaction
(random sampling e.g. based on probability p(r)dr that photon interacts in an interval dr at a distance r from initial position:

$$p(r)dr = e^{-\mu r}\mu dr \qquad r = -\frac{\ln(1-\xi)}{\mu}$$

2. Transport the particle to the interaction site taking into account geometry constraints

3. Select the interaction type *(random sampling based on interaction cross section)*

$$1 \text{ if } \xi \le \frac{\sigma_1}{\sum_i \sigma_i};\ 2 \text{ if } \xi \le \frac{\sigma_1+\sigma_2}{\sum_i \sigma_i} \ldots; n \text{ if } \mathrm{i}\xi \le \frac{\sigma_1+\sigma_2+\ldots\sigma_n}{\sum_i \sigma_i}$$

4. Simulate the selected interaction

…and repeat steps 1-4 until the original particle and all secondary particles leave the geometry or are locally absorbed (E < threshold)

- ***Suited for neutral particles***
- ***Not practicable for charged particles (large number of interactions)***

Analog versus condensed history MC

Condensed history MC simulation

- Many "small-effect" (*"soft"*) interactions can be grouped into few condensed history "steps"
- Sample of the cumulative effect from proper distributions of grouped single interactions (multiple scattering, stopping power,…)
- *"Hard"* collisions (e.g., δ-ray production) can be explicitly simulated in an analog matter

Example of e⁻ track

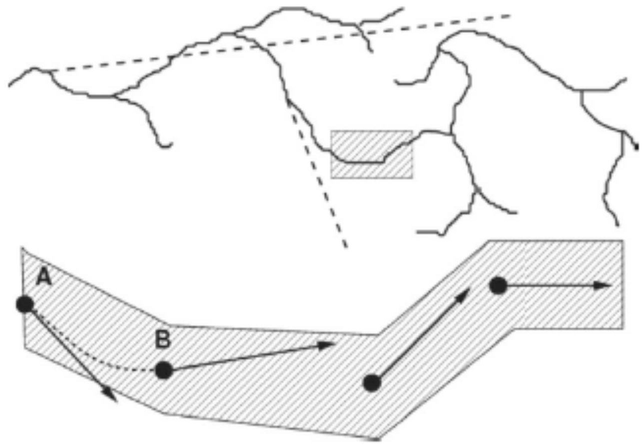

FIG. 1. Illustration of a class II condensed history scheme for electron transport. The upper portion shows a complete electron track including secondary electrons and photons (shown with dashed lines and not including their interactions) with energies above the hard collision thresholds. The lower portion is a magnified view of the shaded box.

I Chetty et al, Report of the AAPM Task Group 105, Med Phys 34, 2007

Approach followed in all general purpose MC codes

MC methods for radiation transport

Accuracy and reliability of MC results depends on

- Physical processes accounted for
- Models or data on which pdfs are based
- Randomness of pseudo-random event generators for sampling
- Selection of energy cuts and step sizes in particle transport
- Number of "histories" N (statistics)

Computational time and Efficiency

- Typical computational times of analog / condensed history transport can be still very expensive (hours to days depending on N) for photon and ion therapy, though reduced via parallelization of runs on high performance computer clusters
- Efficiency $\varepsilon=(s^2T)^{-1}$ is rather independent of N, being s^2 (variance of the quantity of interest) $\propto$ 1/N, T (computing time) $\propto$ N

Efficiency enhancing methods in MC

Efficiency enhancing methods

- Variance reduction techniques (aiming to reduce the variance s^2 while not biasing the result)

  - Sampling from artificial distributions, particle weights to account for bias
  - Cannot reproduce physical correlations/fluctuations
  - Enable faster convergence (ONLY for privileged observables)

- examples
  - splitting (brem splitting: UBS, DBS; in-phantom)
  - Russian roulette
  - interaction forcing
  - track repetition
  - STOPS (simultaneous transport of particle sets)
  - -enhanced cross sections (brem: BCSE)

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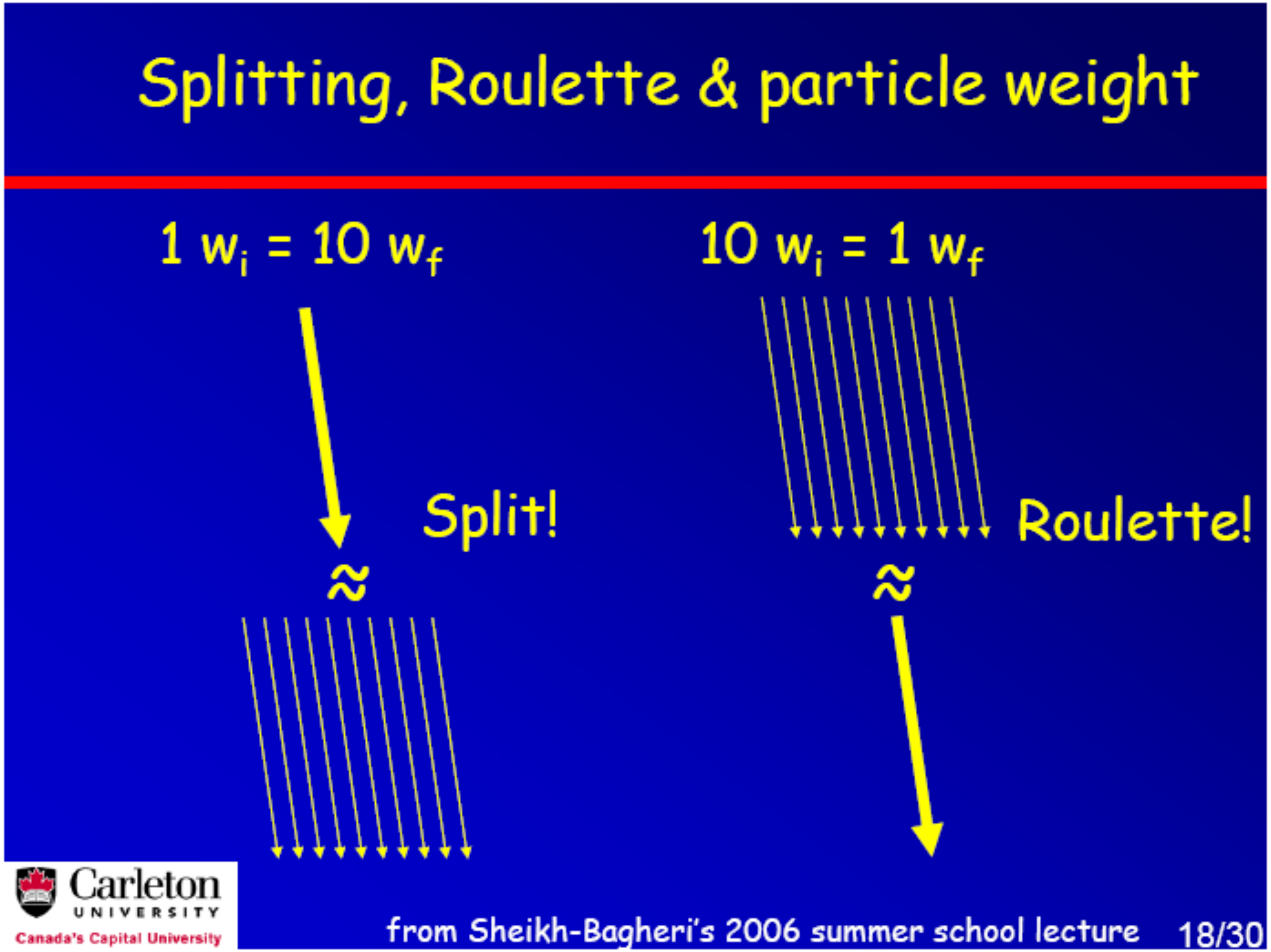
- for a recent review, see Sheikh-Bagheri et al's 2006 AAPM summer school chapter

  http://www.physics.carleton.ca/~drogers/pubs/papers/SB06.pdf

Efficiency enhancing methods in MC



Efficiency enhancing methods in MC

Efficiency enhancing methods

- Variance reduction techniques (aiming to reduce the variance s^2)

  - Sampling from artificial distributions, particle weights to account for bias

  - Cannot reproduce physical correlations/fluctuations

  - Enable faster convergence (ONLY for privileged observables)

- Setting of energy thresholds and step sizes (reduce time per history)

- Re-use of particle tracks (particle track-repeating algorithms)

Rapidly spreading for clinical MC in conventional therapy (photons and electrons) and under investigation for ions

To be used with care!

The commonly recognized merits of MC

MC are powerful computational tools for:

- Realistic description of particle interactions, especially in complex geometries and inhomogeneous media where analytical approaches are at their limits of validity

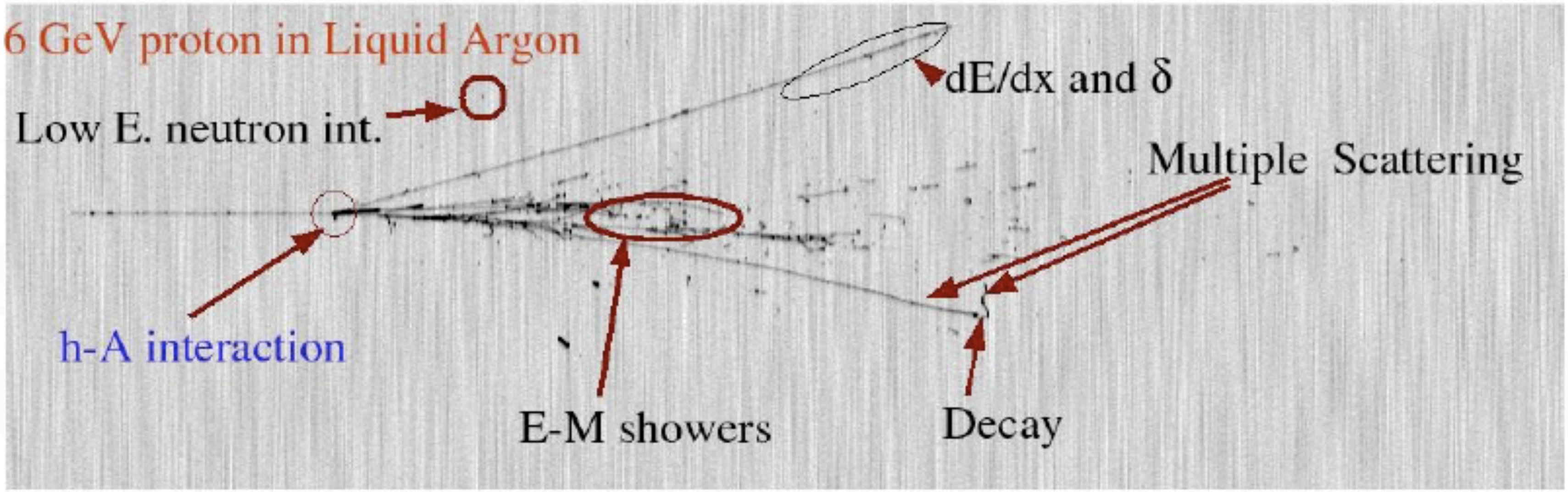
- Possibility to investigate separate contributions to quantities of interest which may be impossible to be experimentally assessed and/or discriminated

FLUKA

FLUKA

Main authors: A. Fassò, A. Ferrari, J. Ranft, P.R. Sala

Contributing authors: G.Battistoni, F.Cerutti, T.Empl, M.V.Garzelli, M.Lantz, A. Mairani, V.Patera, S.Roesler, G. Smirnov, F.Sommerer, V.Vlachoudis



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>3000 users **http://www.fluka.org**

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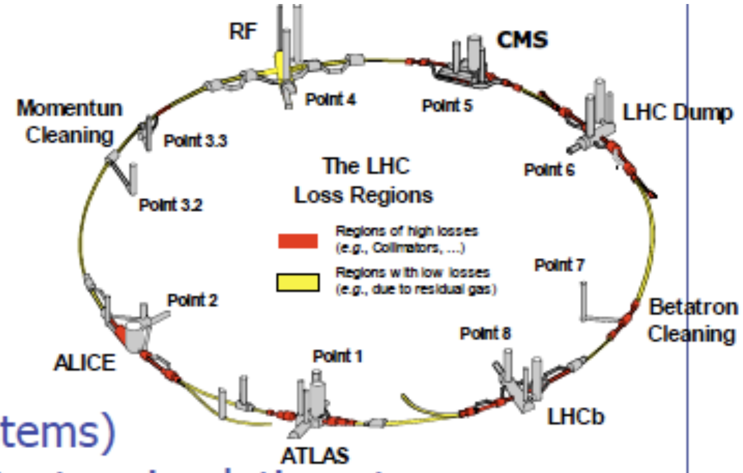
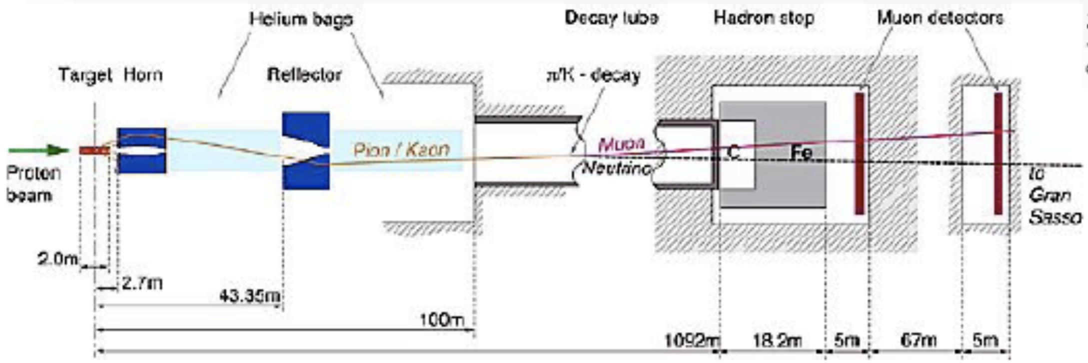
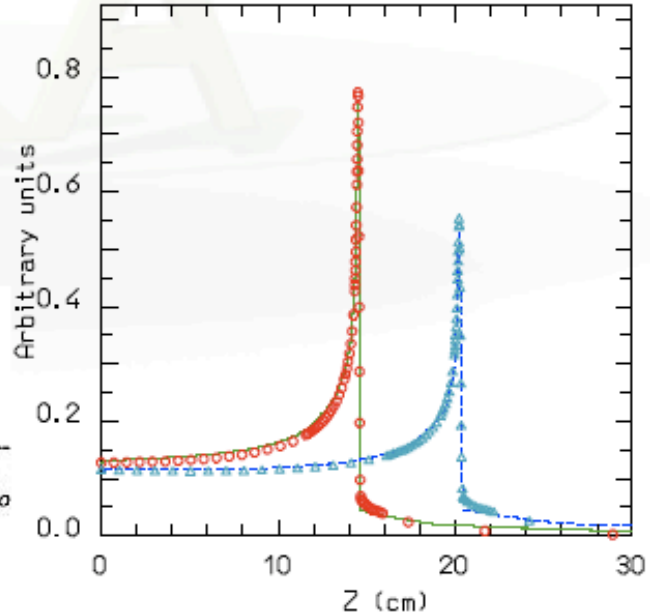
FLUKA Applications



- Cosmic ray physics
- Neutrino physics
- Accelerator design (→ n_ToF, CNGS, LHC systems)
- Particle physics: calorimetry, tracking and detector simulation etc. (→ ALICE, ICARUS, ...)
- ADS systems, waste transmutation, (→"Energy amplifier", FEAT, TARC,...)
- Shielding design
- Dosimetry and radioprotection
- Space radiation
- Hadrontherapy
- Neutronics





The History

The early days

The beginning: 1962: Johannes Ranft (Leipzig) and Hans Geibel (CERN): Monte Carlo for high-energy proton beams

The name: 1970: study of event-by-event fluctuations in a NaI calorimeter (FLUktuierende KAskade)

Early 70's to ≈1987: J. Ranft and coworkers (Leipzig University) with contributions from Helsinki University of Technology (J. Routti, P. Aarnio) and CERN (G.R. Stevenson, A. Fassò)

Link with EGS4 in 1986, later abandoned

The modern code: some dates

Since 1989: mostly INFN Milan (A. Ferrari, P.R. Sala): little or no remnants of older versions. Link with the past: J. Ranft and A. Fassò

1990: LAHET / MCNPX: high-energy hadronic FLUKA generator *No further update*

1993: G-FLUKA (the FLUKA hadronic package in GEANT3). *No further update*

1998: FLUGG, interface to GEANT4 geometry

2000: grant from NASA to develop heavy ion interactions and transport

2001: the INFN FLUKA Project

2003: official CERN-INFN collaboration to develop, maintain and distribute FLUKA

The FLUKA Code design - 1

- Sound and updated physics models
  - Based, as far as possible, on original and well-tested microscopic models
  - Optimized by comparing with experimental data at single interaction level: ***"theory driven, benchmarked with data"***
  - Final predictions obtained with minimal free parameters fixed for all energies, targets and projectiles
  - Basic conservation laws fulfilled "a priori"

→ ***Results in complex cases, as well as properties and scaling laws***, arise naturally from the underlying physical models

→ ***Predictivity where no experimental data are directly available***

It is a "condensed history" MC code, with the possibility use of single instead of multiple scattering

The FLUKA Code design - 2

- Self-consistency
  - Full cross-talk between all components: hadronic, electromagnetic, neutrons, muons, heavy ions
  - Effort to achieve the same level of accuracy:
    - for each component
    - for all energies
  - → Correlations preserved fully within interactions and among shower components
  - → ***FLUKA is NOT a toolkit! Its physical models are fully integrated***

The Physics Content of FLUKA

- Nucleus-nucleus interactions 100 MeV/n – 10000 TeV/n

  New model (BME, under development): from Coulomb Barrier
- Electromagnetic and μ interactions 1 keV – 10000 TeV
- Hadron-hadron and hadron-nucleus interactions 0–10000 TeV
- Neutrino interactions NEW! (new DIS and RES generator!)
- Charged particle transport including all relevant processes
- Transport in magnetic field
- Neutron multigroup transport and interactions 0 – 20 MeV

  NEW! new library with 260 groups
- Analog calculations, or with variance reduction

Code complexity

- Inelastic h-N: ~***72000 lines***
- Cross sections (h-N and h-A), and elastic (h-N and h-A): ***~32000 lines***
- (G)INC and preequilibrium (PEANUT): ***~114000 lines***
- Evap./Fragm./Fission/Deexc.: ***~27000 lines***
- ν-N interactions: ***~35000 lines***
- A-A interactions:
  - ✓ FLUKA native (including BME): ***~8000 lines***
  - ✓ DPMJET-3: ***~130000 lines***
  - ✓ (modified) rQMD-2.4: ***~42000 lines***
- **FLUKA** in total (including transport, EM, geometry, scoring): ***~680000 lines***
- ... + ***~20000 lines*** of ancillary off-line codes used for data pre-generation
- ... and ***~30000 lines*** of post-processing codes

EM INTERACTION

Topics

- General settings
- Interactions of leptons/photons
  - Photon interactions
    - Photoelectric
    - Compton
    - Rayleigh
    - Pair production
    - Photonuclear
    - Photomuon production
  - Electron/positron interactions
    - Bremsstrahlung
    - Scattering on electrons
  - Muon interactions
    - Bremsstrahlung
    - Pair production
    - Nuclear interactions

- Ionization energy losses
  - Continuous
  - Delta-ray production
- Transport
  - Multiple scattering
  - Single scattering

These are common to all charged particles, although traditionally associated with EM

- Transport in Magnetic field

Ionization energy losses

- Charged hadrons
- Muons
- Electrons/positrons

All share the same approach

- Heavy Ions

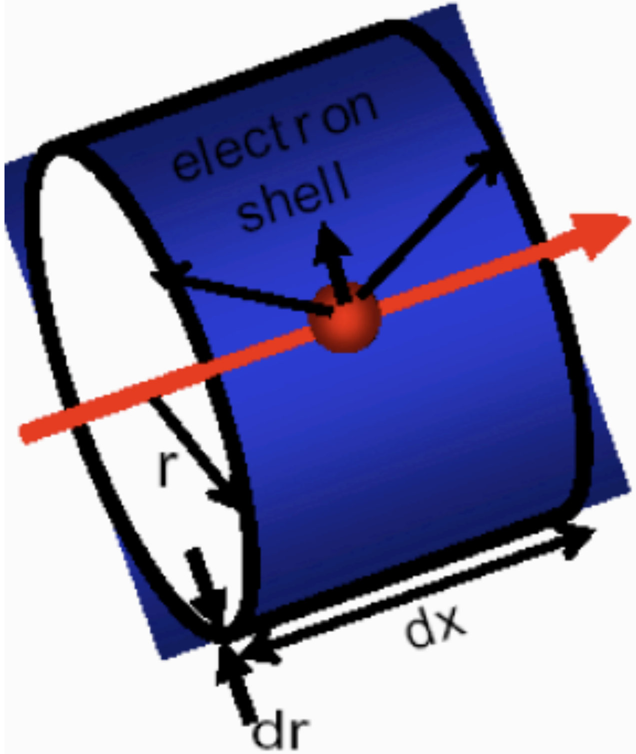
They need some extra features

Phenomenological Model Of Energy Loss in Matter

Integrate over radial coordinate:

$$\frac{dE(x)}{dx} = \int_{r_{min}}^{r_{max}} dr \frac{dE(r,x)}{dr\,dx}$$

$$-\frac{dE(x)}{dx} \sim \left[\frac{4\pi e^4 Z_p^2}{m_e v^2} N_e\right] \cdot \ln\left(\frac{r_{max}}{r_{min}}\right)$$



r_{min} corresponds to maximum kinetic energy T_{max} gained by e-

It corresponds to head-on-collision:

$$v = \frac{2M}{m+M} v_0 \xrightarrow{M>>M} v = 2v_0 \longrightarrow T_{max} = \frac{1}{2} m(2v)^2 = 2mv^2$$

$$T_{max} = \frac{(\Delta p_{max})}{2m_e} = \frac{2Z_p^2 e^4}{m_e v^2 r_{min}^2} = 2m_e v^2$$

$$r_{min}^2 = \frac{Z_p^2 e^4}{m_e v^4}$$

r_{max} corresponds to minimum kinetic energy T_{min} gained by e-

$$T_{min} = IE = ionization\ en \begin{cases} (12 \cdot Z_T + 7)\, eV & for\ Z_T < 13 \\ (9.76 \cdot Z_T + 58.8 \cdot Z_T^{-0.19})\, eV & for\ Z_T \geq 13 \end{cases} \sim 10\,Z\ \text{eV}$$

$$T_{min} = IE = \frac{2Z_p^2 e^4}{m_e v^2 r_{max}^2}$$

$$r_{max}^2 = \frac{2Z_p^2 e^4}{(IE) m_e v^2}$$

Estimate of Radial Limits:

$$-\frac{dE(x)}{dx} \sim \left[\frac{4\pi e^4 Z_p^2}{m_e v^2} N_e\right] \cdot \ln\left(\frac{r_{max}}{r_{min}}\right) \approx \frac{4\pi Z_p^2 e^4}{m_e v^2} N_e \frac{1}{2} \ln\left[\frac{2 m_e v^2}{IE}\right]$$

Insert: ρ = atomic density, Z_T = atomic number of target

$N_e = Z_T \cdot \rho$

$$-\frac{1}{\rho}\frac{dE}{dx} \approx \frac{4\pi Z_p^2 e^4}{m_e v^2} Z_T \frac{1}{2} \ln\left[\frac{2 m_e v^2}{IE}\right]$$

Phenomenological model

Bethe-Bloch Quantum Mechanical Equation

(for heavy particles $M \gg m_e$)

Average energy loss

$$-\frac{1}{\rho}\frac{dE}{dx} \approx 0.1535 \frac{Z_p^2}{\beta^2}\frac{Z_T}{A_T}\left[\ln\left(\frac{2 m_e c^2}{IE(1-\beta^2)}\right)^2 - 2\beta^2\right] \frac{MeV}{g/cm^2}$$

ρ = atomic density

Z_T = atomic number of target

A_T = mass number of target

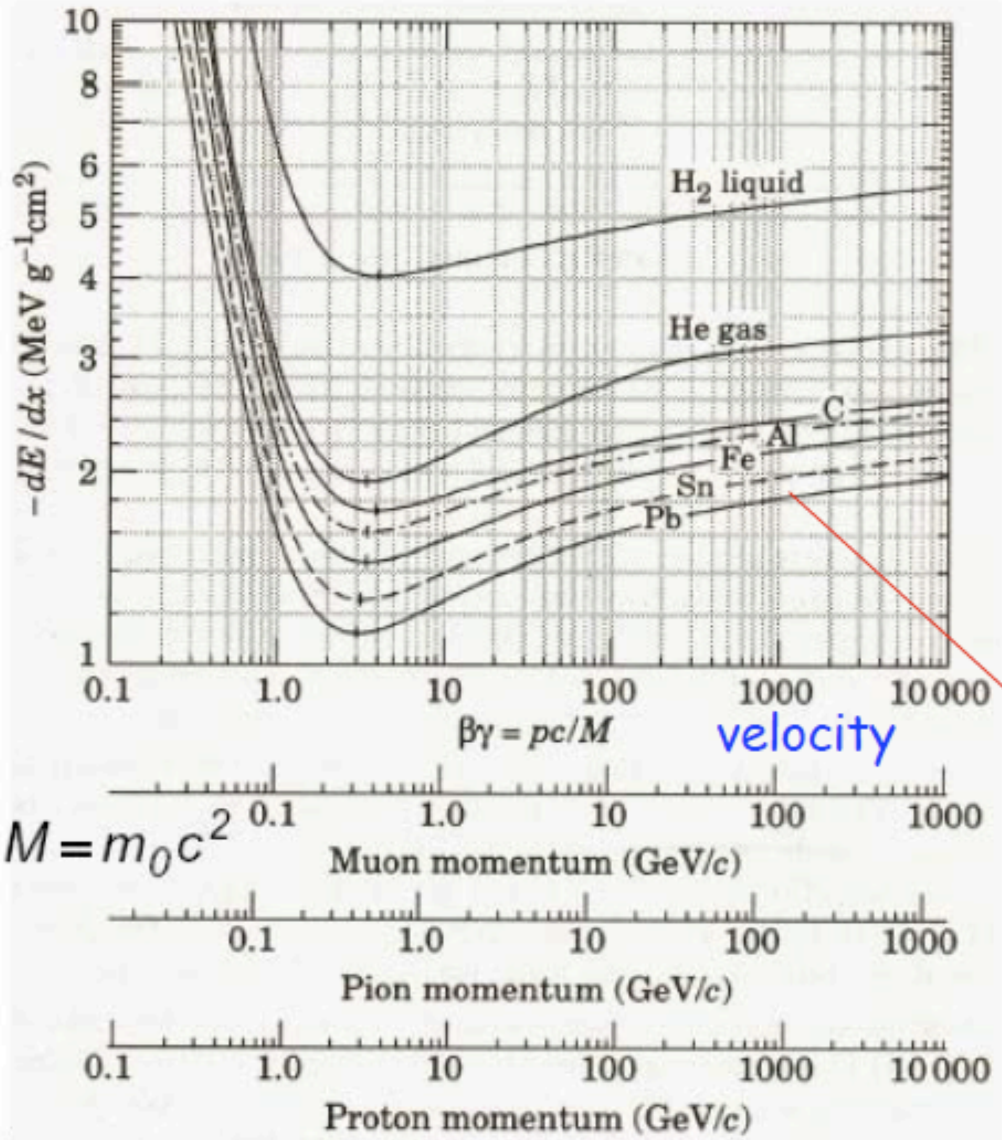
$$IE = h(\nu_e) \approx \begin{cases} (12 \cdot Z_T + 7)\,eV & \text{for } Z_T < 13 \\ (9.76 \cdot Z_T + 58.8 \cdot Z_T^{-0.19})\,eV & \text{for } Z_T \geq 13 \end{cases}$$

$$-\frac{dE}{dx}$$

- $\approx \rho Z_T \rightarrow$ *Large in dense material*
- $\approx Z_p^2 \rightarrow$ *Large for heavy ions*
- $\approx 1/v^2 \rightarrow$ *Large for slow particles*

Stopping Power of Relativistic Particles

Review of Particle Properties, Phys. Rev. D50, 1173 (1994)



$M = m_0 c^2$

$$E^2 = (pc)^2 + \left(m_0 c^2\right)^2$$

m_0 = particle rest mass

v = particle velocity

$c = 2.9979 \cdot 10^8\, ms^{-1}$

$\beta = v/c$

$$\gamma = \left(\sqrt{1-\beta^2}\right)^{-1}$$

$$pc = (\gamma m_0) vc = \gamma\beta m_0 c^2$$

Relativistic rise: *part of the energy is subtracted by light (Cerenkov radiation)*

Note: here ρdE/dx → dE/dx

Delta Ray Contribution, an example I: ^{12}C ion therapy

For an incident particle with mass M and momentum $M\beta\gamma c$, the maximum kinetic energy T_{MAX} which can be imparted to a free electron with mass m_e in a single collision, is given by the following expression **[Ref. 3.2]**:

$$T_{MAX} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2m_e\gamma/M + (m_e/M)^2} \qquad (3.1).$$

When $2m_e\gamma/M << 1$, such in the case of Carbon ions, the above relation can be further simplified and the following "low energy" approximation is used:

$$T_{MAX} = 2m_e c^2 \beta^2 \gamma^2 \qquad (3.2).$$

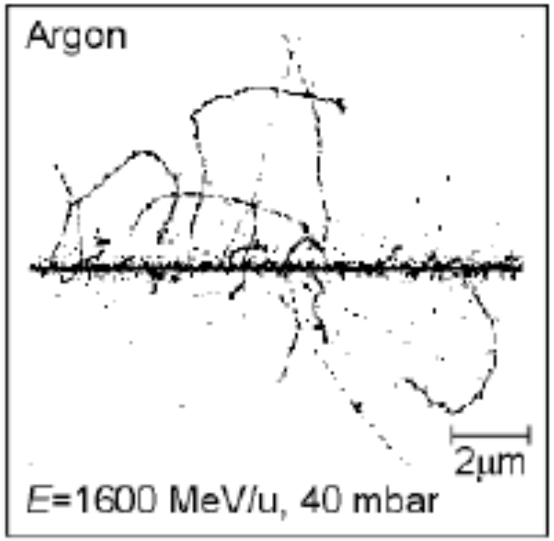
Using this relation the δ-rays maximum kinetic energy has then been determined for an incident ^{12}C ion beam with kinetic energy varying between 80 MeV/n and 430 MeV/n corresponding to a range in tissue between 20 mm and 330 mm respectively: resulting values are included in the interval ranging from 180 keV to 1.16 MeV.

In order to estimate the number of δ-ray electrons ejected by an incident carbon ion per unit length of ion path the following formula **[Ref. 3.2]**, representing the distribution of secondary electrons with kinetic energies $T >> I$ (I = mean excitation energy = 75 eV in water), can be used:

$$\frac{d^2N}{dTdx} = \frac{1}{2}Kz^2\frac{Z}{A}\frac{1}{\beta^2}\frac{F(T)}{T^2} \qquad (3.3).$$

Here β and z are the velocity and the charge of the primary particle while the spin dependent factor $F(T)$ is given by:

$$F(T) = 1 - \beta^2\, T/T_{MAX}$$



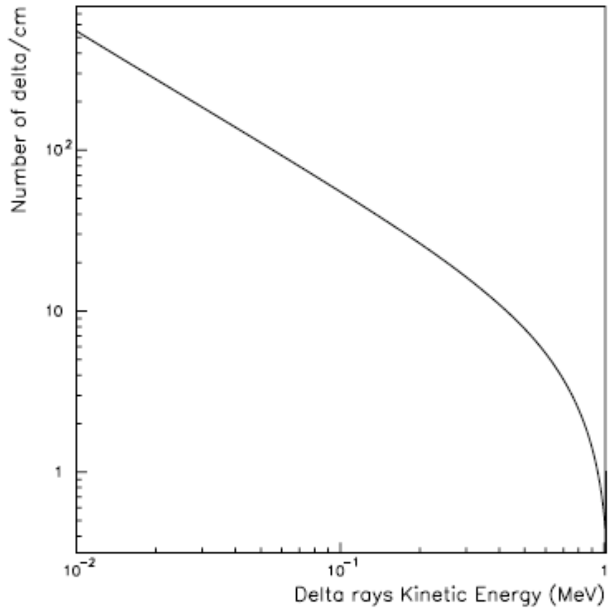


Fig. 3.1: Secondary electron spectrum from incident ^{12}C ion beam with initial kinetic energy E = 430 MeV/n in water.

Continuous energy losses

Below the δ-ray threshold, energy losses are treated as "continuous", with some special features:

- Fluctuations of energy loss are simulated with a FLUKA-specific algorithm
- The energy dependence of cross sections and dE/dx is taken into account exactly (see later)
- Latest recommended values of ionization potential and density effect parameters implemented for elements (Sternheimer, Berger & Seltzer), but can be overridden by the user with (set yourself for compounds!)

Ionization fluctuations -I

The Landau distribution is limited in several respects:

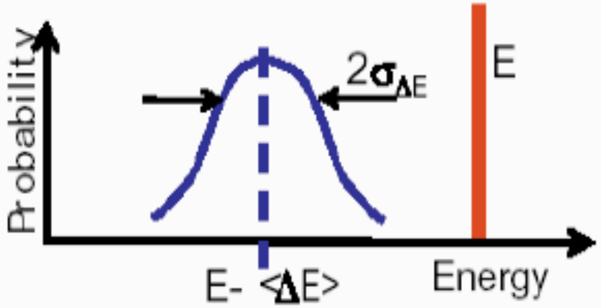
- Max. energy of δ rays assumed to be ∞ $\Longrightarrow$ cannot be applied for long steps or low velocities
- cross section for close collisions assumed equal for all particles
- fluctuations connected with distant collisions neglected $\Longrightarrow$ cannot be applied for short steps
- incompatible with explicit δ-ray production

The Vavilov distribution overcomes some of the Landau limitations, but is difficult to compute if step length or energy are not known *a priori*.

Energy Loss Distributions

Absorber of thickness x; (ρ,Z_T,A_T), many statistical scattering events

→ Central Limit Theorem: Gaussian distribution in energy loss ΔE



$$\Gamma_{FWHM} = 2.35 \cdot \sigma$$

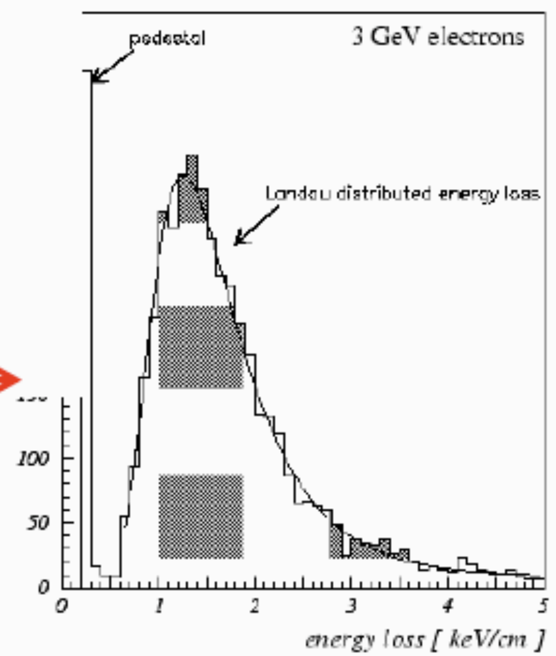
The distribution is Gaussian only if Δx is large enough

$$P(\Delta E) \propto \exp\left\{-\frac{\left(\Delta E - \langle \Delta E \rangle\right)^2}{2\sigma_{\Delta E}}\right\}$$

$$\sigma_{\Delta E} = 4\pi N_A r_e^2 m_e^2 c^4 \rho \frac{Z_T}{A_T} x = 0.1569 \rho \frac{Z_T}{A_T} x \text{ MeV}^2$$

Thin absorber: Asymmetric tail towards higher ΔE

*Landau has shown that the **asymmetric tail** is due to **great energy losses** in **close collisions***

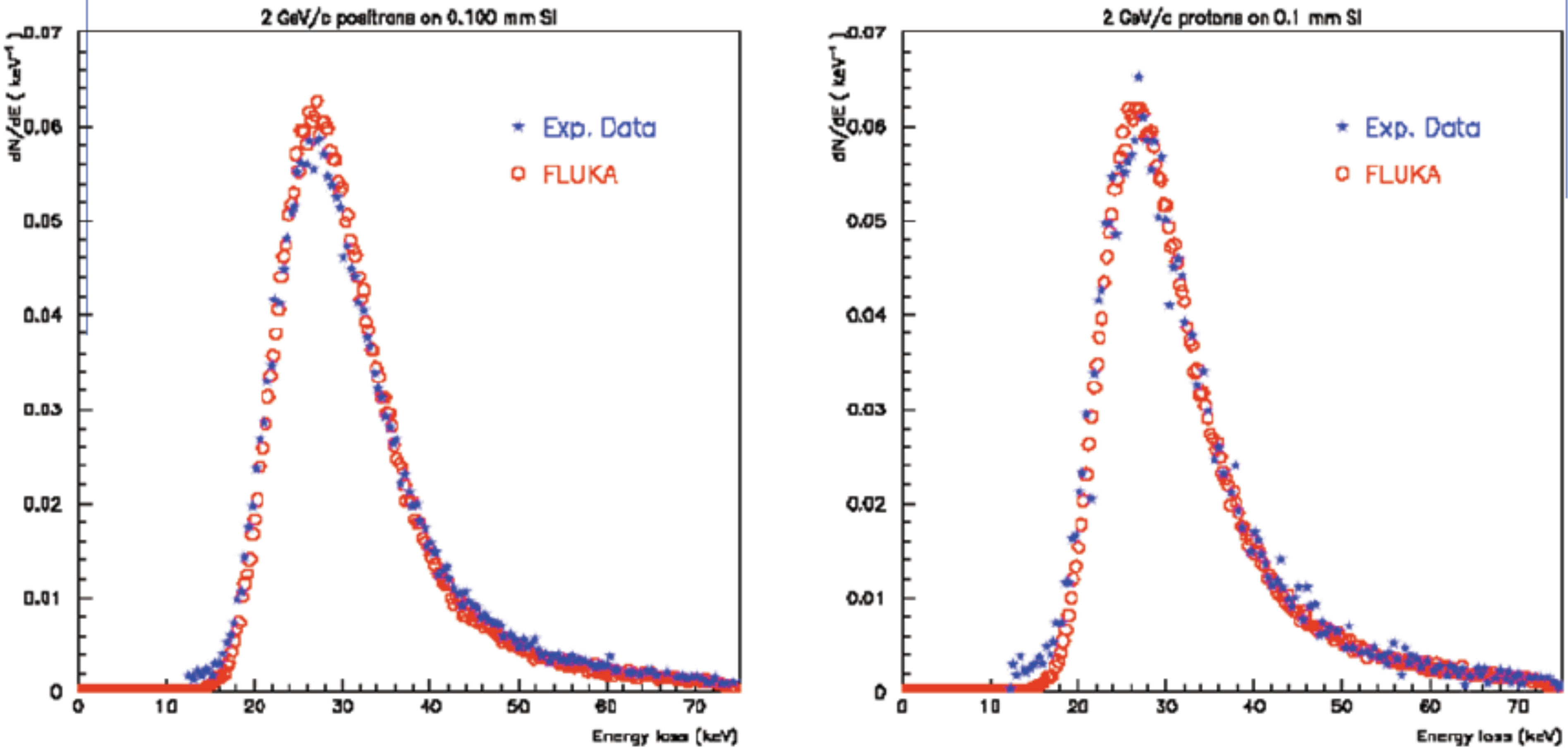


Ionization fluctuations -II

The FLUKA approach:

- based on general statistical properties of the cumulants of a distribution (in this case a Poisson distribution convoluted with $\mathbf{d}\boldsymbol{\sigma}/\mathbf{d}\boldsymbol{E}$)
- integrals can be calculated analytically and exactly *a priori* $\Longrightarrow$ minimal CPU time
- applicable to any kind of charged particle, taking into account the proper (spin-dependent) cross section for δ ray production
- the first 6 moments of the energy loss distribution are reproduced ($k_n =< (x- < x >)^n >$)

Ionization fluctuations -III



Experimental [1] and calculated energy loss distributions for 2 GeV/c positrons (left) and protons (right) traversing 100μm of Si

J.Bak et al. NPB288, 681 (1987)

Energy dependent quantities I

- Most charged particle transport programs sample the next collision point evaluating the cross section at the beginning of the step, neglecting its energy dependence and the particle energy loss
- The cross section for δ ray production at low energies is roughly inversely proportional to the particle energy
  $\Longrightarrow$ a typical 20% fractional energy loss per step would correspond to a similar variation in the cross section
- Some codes use a rejection technique based on the ratio between the cross section values at the two step endpoints, but this approach is valid only for a monotonically decreasing cross section

Energy dependent quantities II

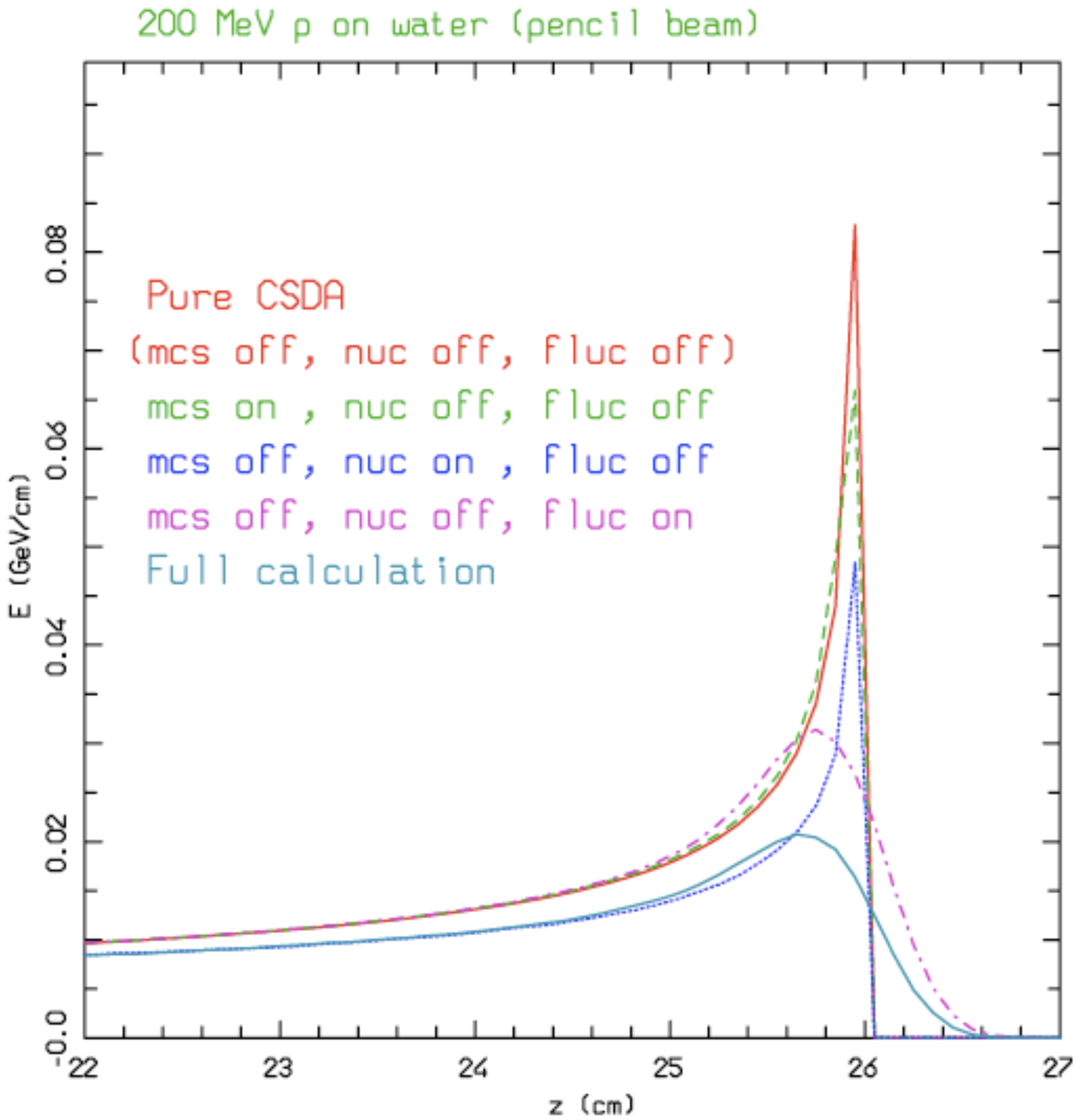
FLUKA takes into account exactly the continuous energy dependence of

- discrete event cross-section
- stopping power

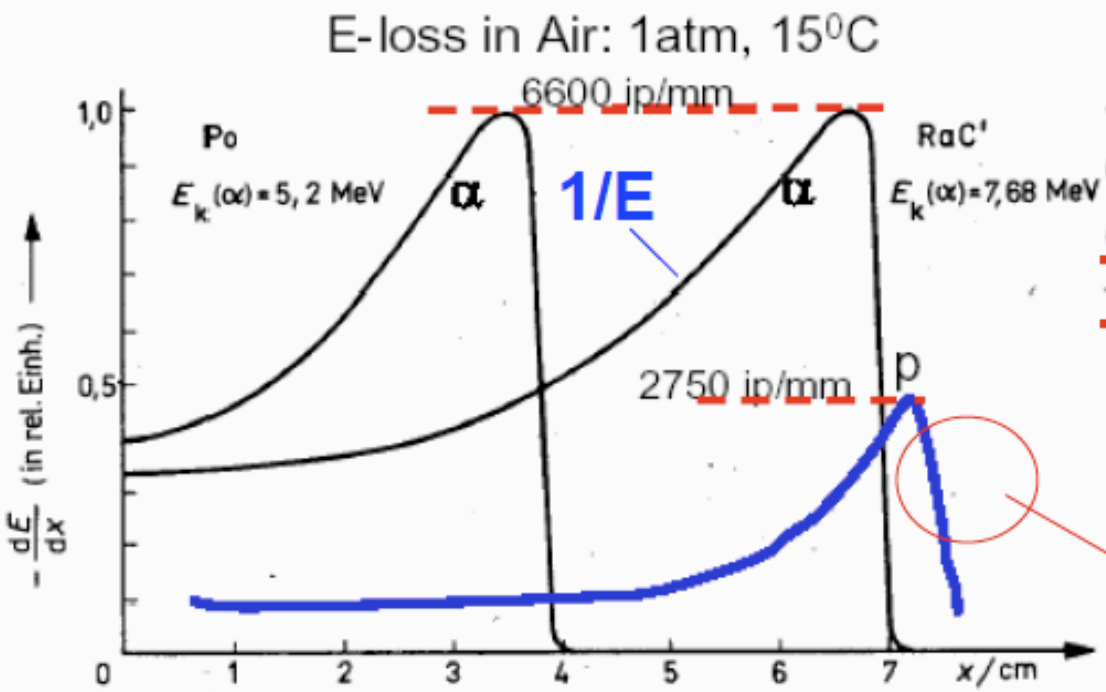
basing the rejection technique on the ratio between the cross section value at the second endpoint and its maximum value between the two endpoint energies.

Playing with a proton beam

Dose vs depth energy deposition in water for a 200 MeV p beam with various approximations for the physical processes taken into account



Range and Specific Ionization



Stopping power dE/dx (specific energy loss) depends on energy E and therefore on x

➔ **Bragg Curve**

Highest E loss close to end of path ➔ Bragg maximum

Charge is reduced due to electrons pick up

$$\frac{dE}{dx} \triangleq \frac{\#\left(e^{-} - ion\ pairs\right)}{unit\ \ length}$$

Main E-loss mechanism: ionization, production of $\boldsymbol{\delta}$ **electrons**, electron-ion pairs

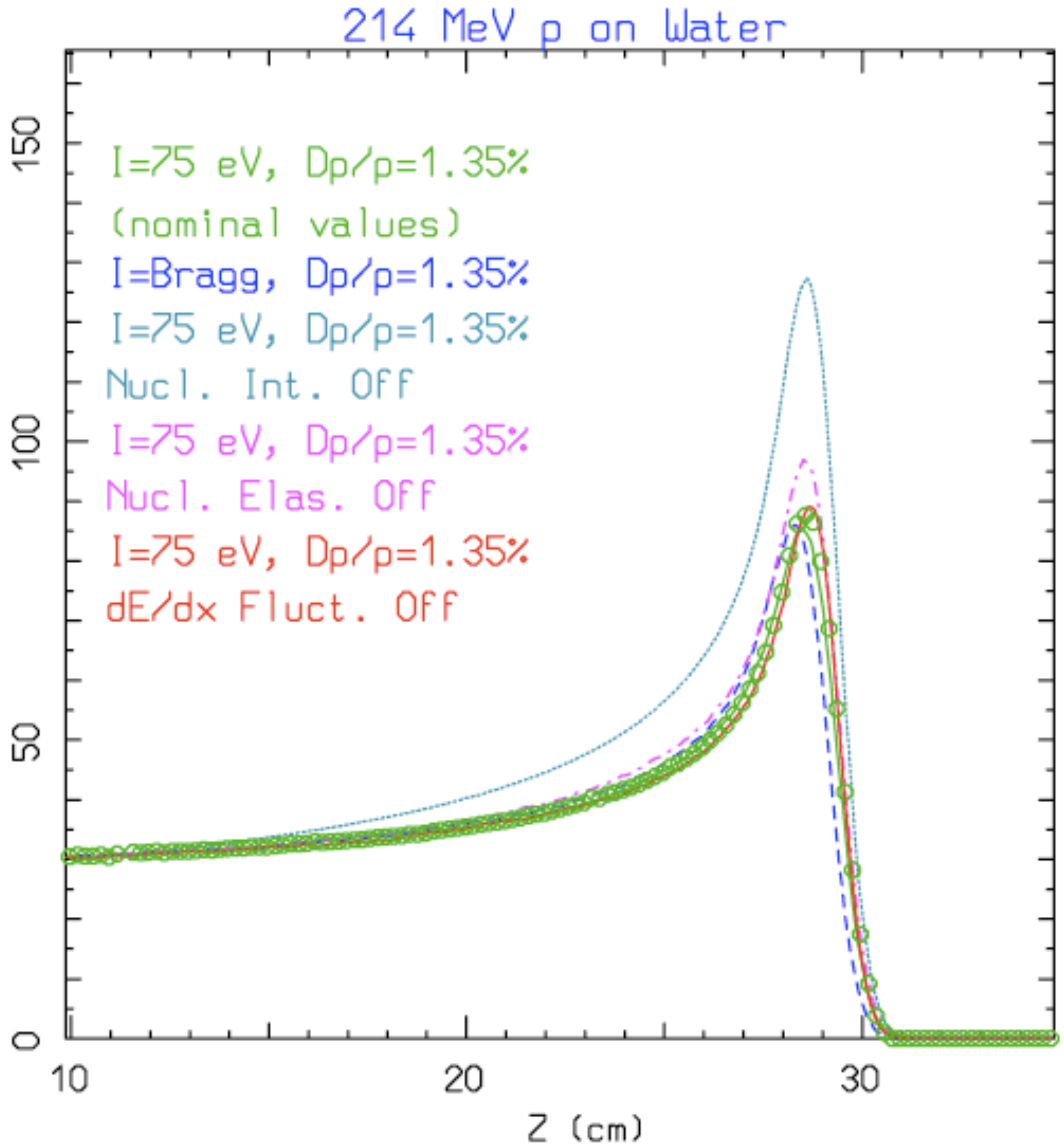
$\boldsymbol{\alpha}$ *particles :*

$$\frac{dE}{dx} \leq \frac{7 \cdot 10^{3}\ pairs}{mm}$$

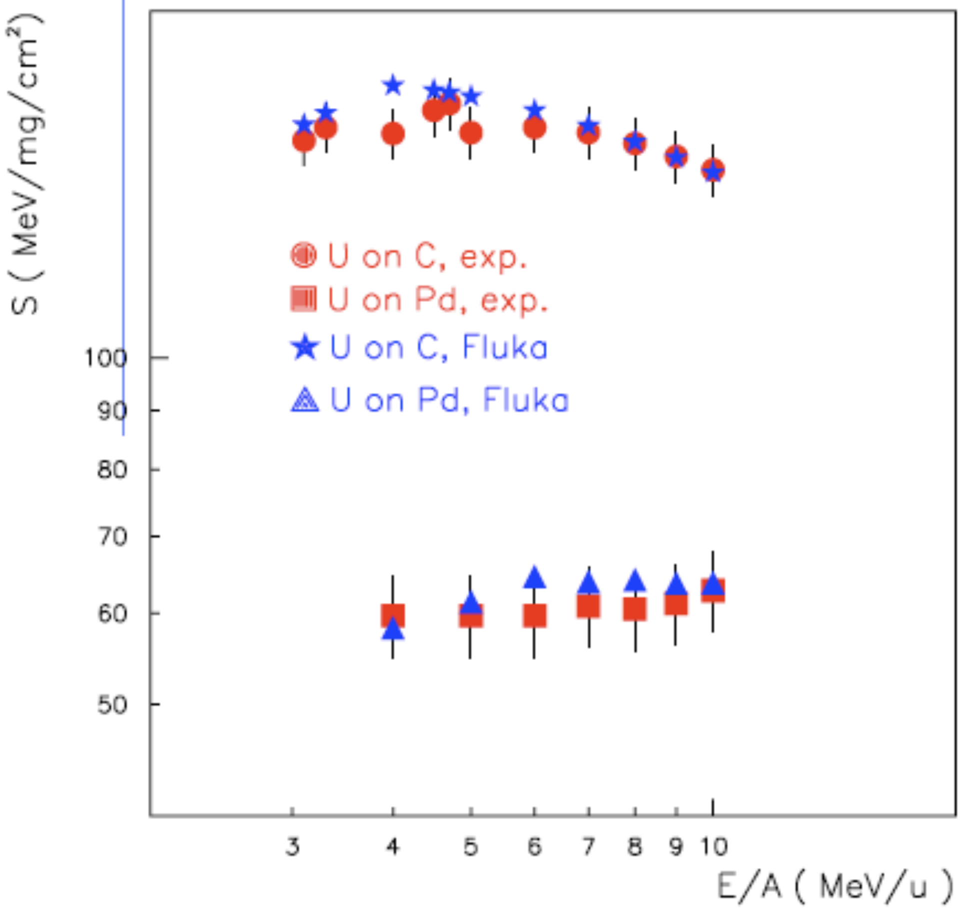
Playing with a proton beam II part

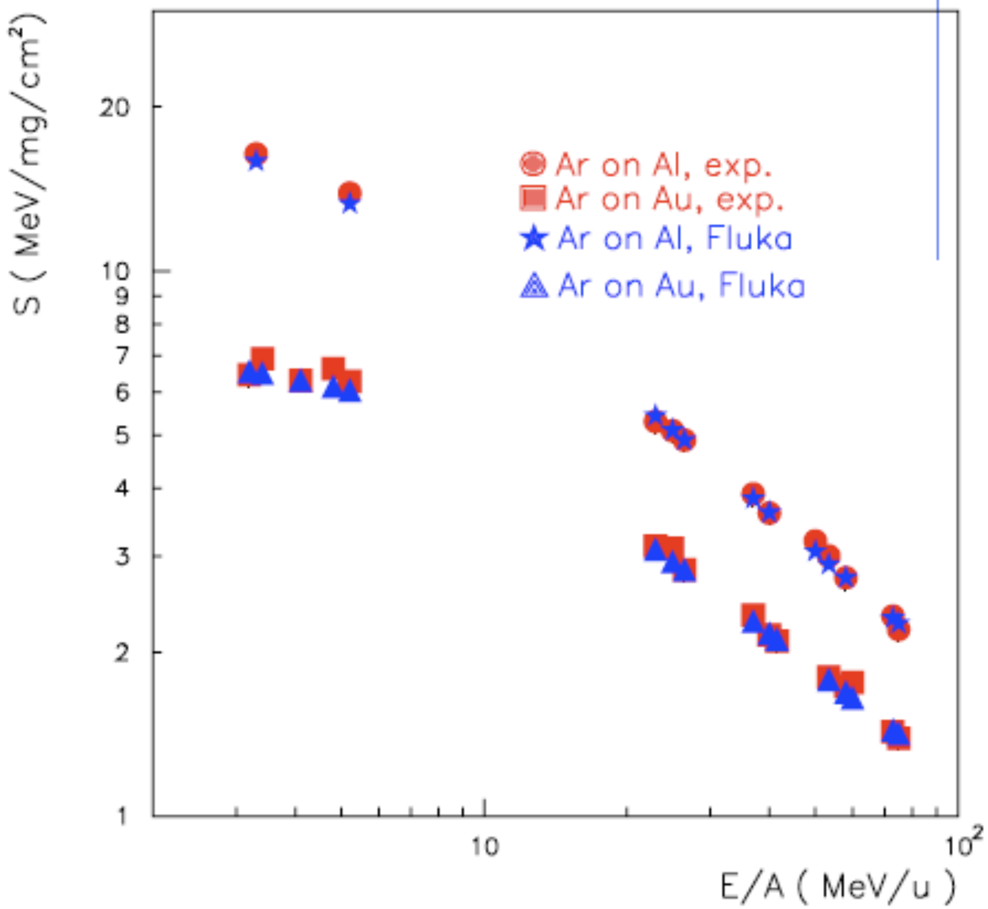
Dose vs depth energy deposition in water for a 214 MeV real p beam under various conditions.

Exp. Data from PSI



Heavy ions dE/dx

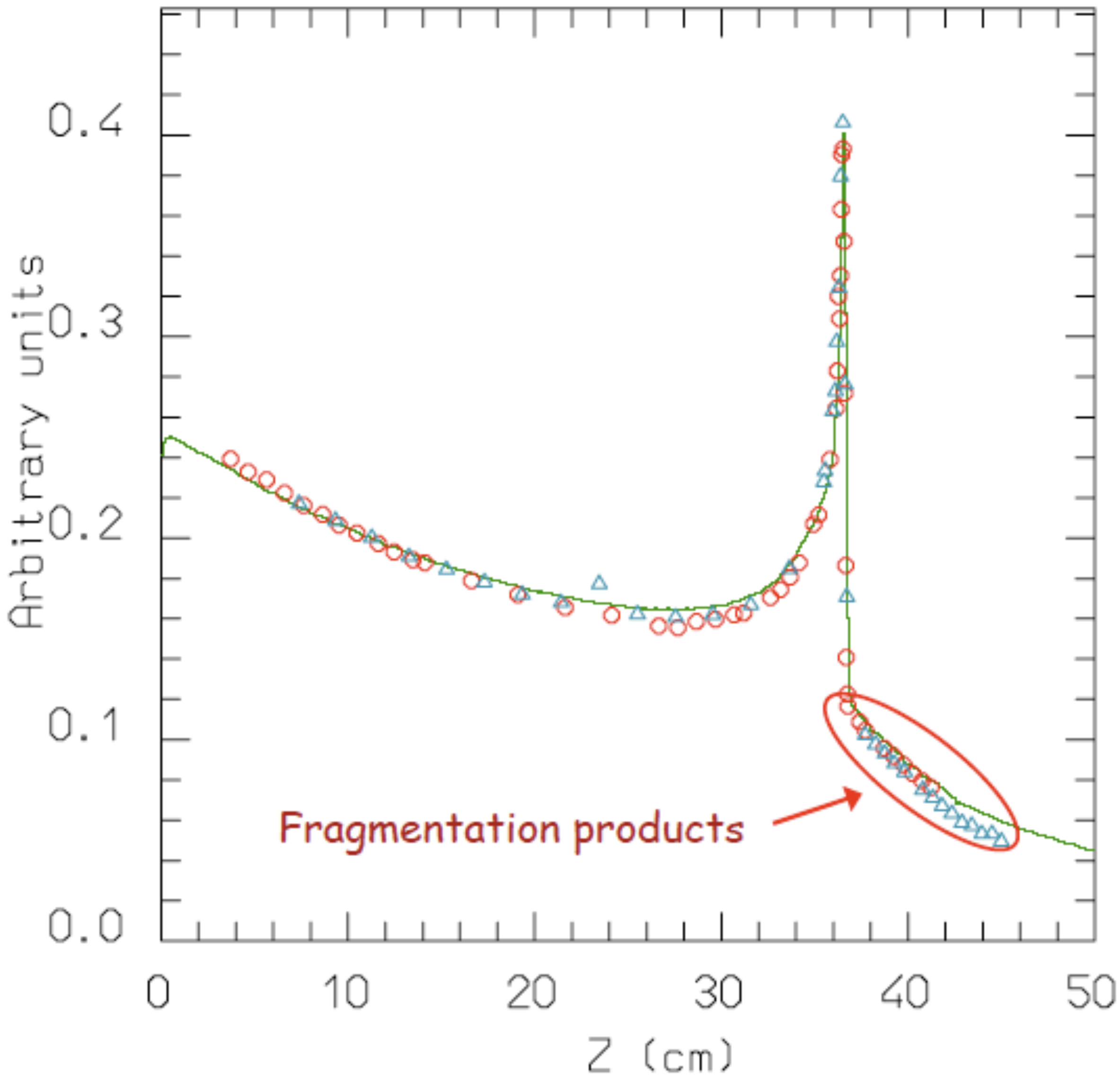




Comparison of experimental (R.Bimbot, NIMB69 (1992) 1) (red) and FLUKA (blue) stopping powers of Argon and Uranium ions in different materials and at different energies.

Bragg peaks vs exp. data: ^{20}Ne @ 670 MeV/n

Dose vs depth distribution for 670 MeV/n ^{20}Ne ions on a water phantom.
The green line is the FLUKA prediction
The symbols are exp data from LBL and GSI



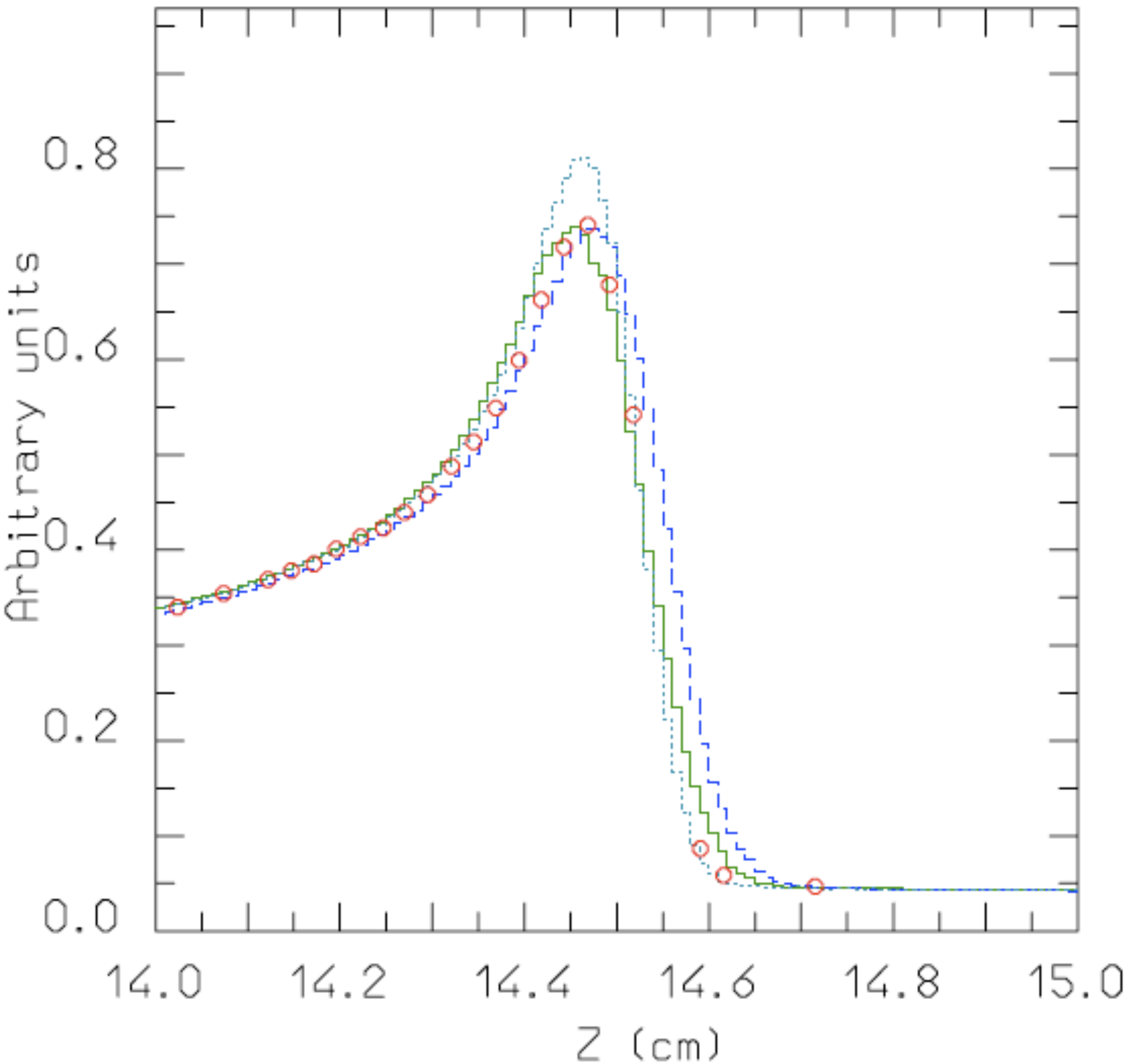
Exp. Data
Jpn.J.Med.Phys. 18, 1,1998

Bragg peaks vs exp. data: ^{12}C @ 270 MeV/n

Close-up of the dose vs depth distribution for 270 MeV/n ^{12}C ions on a water phantom.

The green line is the FLUKA prediction with the nominal 0.15% energy spread

The dotted light blue line is the prediction for no spread, and the dashed blue one the prediction for *I* increased by 1 eV

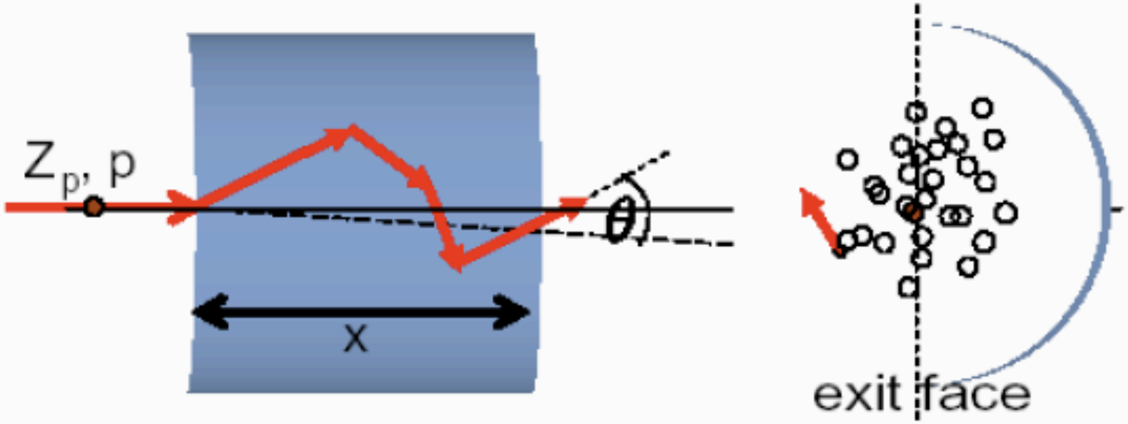


Exp. Data Jpn.J.Med.Phys. 18, 1,1998

Angular Straggling

Theory by Moliere, see W.T. Scott, Rev. Mod. Phys. 35, 231 (1963)

HI : M. Wong et al., Med. Phys. 17, 163 (1990)



Non-trivial geometry !

$$\frac{d\sigma_{MS}(\theta)}{d\Omega} = \frac{1}{2\pi\theta_0^2} \exp\left\{-\frac{\theta^2}{2\theta_0^2}\right\}$$ *cross section*

Assume multiple Coulomb scattering

$$\theta_0 \approx \frac{13.6\,MeV}{\beta pc} Z_p \sqrt{\frac{x}{L}} \left[1 + 0.038 \ln\left(\frac{x}{L}\right)\right]$$

Gaussian angular distribution

$$L \approx \frac{716.4\, A_T}{Z_T (Z_T + 1) \ln\left(287/\sqrt{Z_T}\right)} \frac{g}{cm^2}$$ *radiation length*

- *mean distance over which a high-energy e⁻ reduces to 1/e of its energy by bremsstrahlung*
- *7/9 of the mean free path for pair production by a high-energy photon*
- *appropriate scale length for high-energy electromagnetic cascades*

Charged particle transport

Besides energy losses, charged particles undergo scattering by atomic nuclei. The Molière multiple scattering (MCS) theory is commonly used to describe the cumulative effect of all scatterings along a charged particle step. However

- Final deflection wrt initial direction
- Lateral displacement during the step
- Shortening of the straight step with respect to the total trajectory due to "wiggliness" of the path (often referred to as PLC, path length correction)
- Truncation of the step on boundaries
- Interplay with magnetic field

MUST all be accounted for accurately, to avoid artifacts like unphysical distributions on boundary and step length dependence of the results

The FLUKA MCS

- Accurate PLC (not the average value but sampled from a distribution), giving a complete independence from step size
- Correct lateral displacement even near a boundary
- Correlations:

  PLC ⇔ lateral deflection

  lateral displacement ⇔ longitudinal displacement

  scattering angle ⇔ longitudinal displacement
- Variation with energy of the Moliere screening correction
- Optionally, spin-relativistic corrections (1st or 2nd Born approximation) and effect of nucleus finite size (form factors)
- Special geometry tracking near boundaries, with automatic control of the step size
- On user request, single scattering automatically replaces multiple scattering for steps close to a boundary or too short to satisfy Moliere theory. A full Single Scattering option is also available.
- Moliere theory used strictly within its limits of validity
- combined effect of MCS and magnetic fields

The FLUKA MCS - II

- As a result, FLUKA can correctly simulate electron backscattering even at very low energies and in most cases without switching off the condensed history transport (a real challenge for an algorithm based on Moliere theory!)
- The sophisticated treatment of boundaries allows also to deal successfully with gases, very thin regions and interfaces
- The same algorithm is used for charged hadrons and muons

Single Scattering

- In very thin layers, wires, or gases, Molière theory does not apply.
- In FLUKA, it is possible to replace the standard multiple scattering algorithm by single scattering in defined materials (option MULSOPT).
- Cross section as given by Molière (for consistency)
- Integrated analytically without approximations
- Nuclear and spin-relativistic corrections are applied in a straightforward way by a rejection technique

Electron Backscattering

Energy (keV)	Material	Experim. (Drescher et al 1970)	FLUKA Single scattering	FLUKA Multiple scattering	CPU time single/mult ratio
9.3	Be	0.050	0.044	0.40	2.73
	Cu	0.313	0.328	0.292	1.12
	Au	0.478	0.517		1.00
102.2	Cu	0.291	0.307	0.288	3.00
	Au	0.513	0.502	0.469	1.59

Fraction of normally incident electrons backscattered out of a surface.
All statistical errors are less than 1%.

NUCLEAR INTERACTIONS

The FLUKA hadronic Models

Hadron-nucleus: PEANUT

Elastic,exchange
Phase shifts
data, eikonal

P<3-5GeV/c
Resonance prod
and decay

low E
π,K
Special

High Energy
DPM
hadronization

Sophisticated
G-Intranuclear Cascade

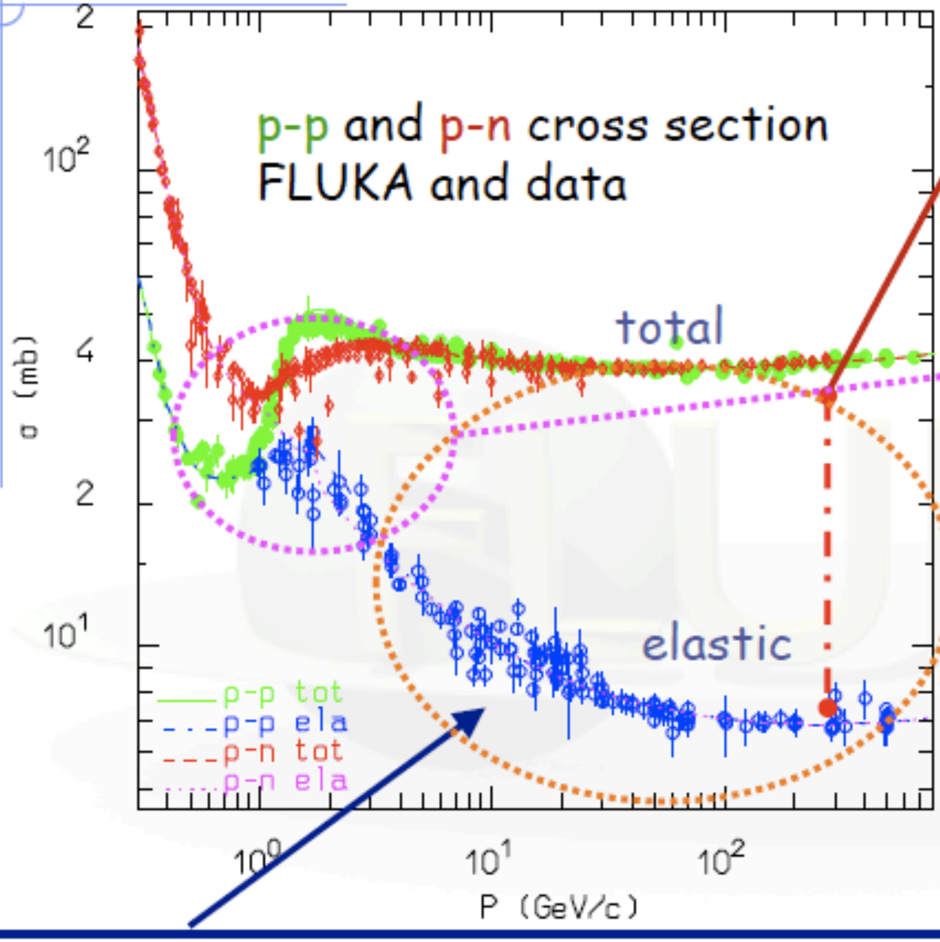
Gradual onset of
Glauber-Gribov multiple
interactions

Preequilibrium

Coalescence

Evaporation/Fission/Fermi break-up
γ deexcitation

Hadron-nucleon interaction models



Particle production interactions: two kinds of models

Those based on "resonance" production and decays, cover the energy range up to 3-5 GeV

Those based on quark/parton string models, which provide reliable results up to several tens of TeV

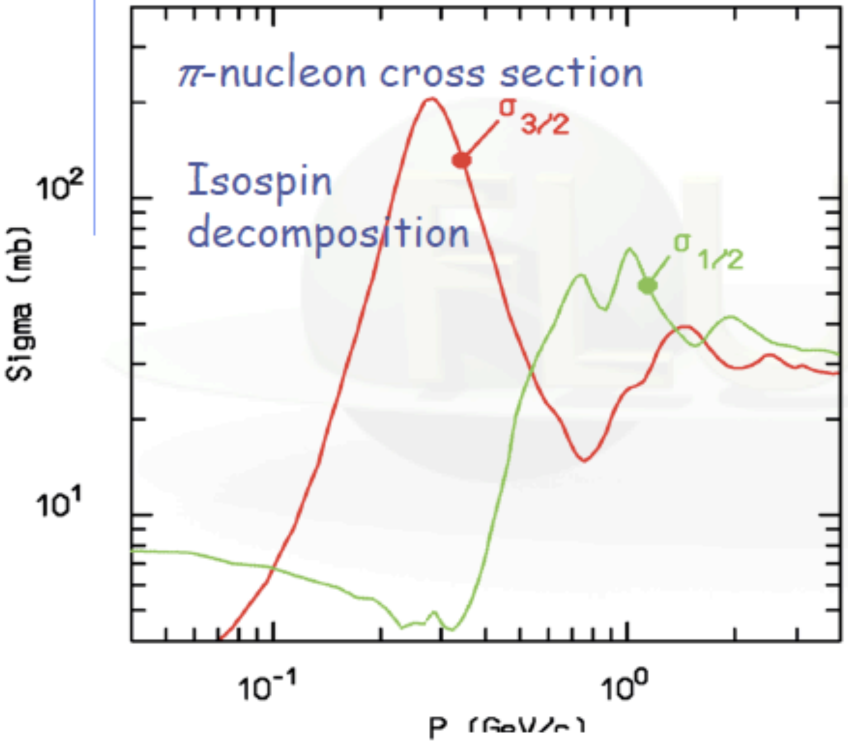
Elastic, charge exchange and strangeness exchange reactions:

- Available phase-shift analysis and/or fits of experimental differential data
- At high energies, standard eikonal approximations are used

Nonelastic hN interactions at intermediate energies

- $N_1 + N_2 \rightarrow N'_1 + N'_2 + \pi$ threshold at 290 MeV, important above 700 MeV,
- $\pi + N \rightarrow \pi' + \pi'' + N'$ opens at 170 MeV.

Anti-nucleon -nucleon open at rest !



Dominance of the Δ resonance and of the N* resonances

→ isobar model

→ all reactions proceed through an intermediate state containing at least one resonance.

Resonance energies, widths, cross sections, branching ratios from data and conservation laws, whenever possible. Inferred from inclusive cross sections when needed

$$N_1 + N_2 \rightarrow N''_1 + \Delta(1232) \rightarrow N'_1 + N'_2 + \pi$$
$$\pi + N \rightarrow \Delta(1600) \rightarrow \pi' + \Delta(1232) \rightarrow \pi' + \pi'' + N'$$
$$N_1 + N_2 \rightarrow \Delta_1(1232) + \Delta_2(1232) \rightarrow N'_1 + \pi_1 + N'_2 + \pi_2$$

Nuclear interactions in PEANUT:

Target nucleus description (density, Fermi motion, etc)

⇩

Glauber-Gribov cascade with formation zone

⇩

Generalized IntraNuclear cascade

⇩

Preequilibrium stage with current exciton configuration and excitation energy
(all non-nucleons emitted/decayed + all nucleons below 30-100 MeV)

⇩

Evaporation/Fragmentation/Fission model

⇩

γ deexcitation

t (s)

10^{-23}

10^{-22}

10^{-20}

10^{-16}

Preequilibrium emission

For E > π production threshold → only (G)INC models
At lower energies a variety of preequilibrium models

Two leading approaches

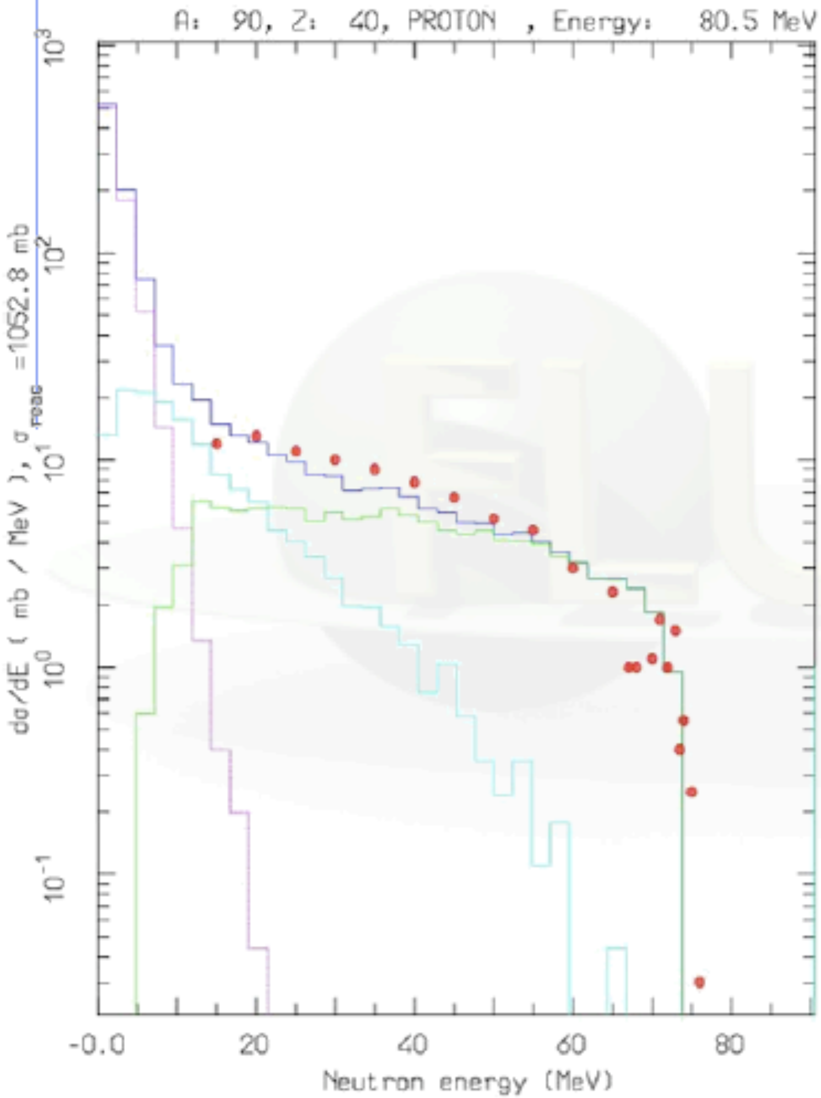
The quantum-mechanical multistep model:
Very good theoretical background
Complex, difficulties for multiple emissions

The semiclassical exciton model
Statistical assumptions
Simple and fast
Suitable for MC

Statistical assumption:
any partition of the excitation energy E^* among N, $N = N_h + N_p$, excitons has the same probability to occur
Step: nucleon-nucleon collision with $N_{n+1}=N_n+2$ ("never come back approximation)
Chain end = equilibrium = N_n sufficiently high or excitation energy below threshold

N_1 depends on the reaction type and cascade history

Thin target example



Angle-integrated $^{90}Zr(p,xn)$ at 80.5 MeV

The various lines show the total, INC, preequilibrium and evaporation contributions

Experimental data from M. Trabandt et al., Phys. Rev. C39, 452 (1989)

Equilibrium particle emission (evaporation, fission and nuclear break-up)

From statistical considerations and the detailed balance principle, the probabilities for emitting a particle of mass m_j, spin $S_j\hbar$ and energy E, or of fissioning are given by:
(i, f for initial/final state, Fiss for fission saddle point)

Probability per unit time of emitting a particle j with energy E

$$P_J = \frac{(2S_j+1)m_j c}{\pi^2\hbar^3}\int_{V_j}^{U_i-Q_j-\Delta_f}\frac{\rho_f(U_f)}{\rho_i(U_i)}\sigma_{inv}(E)\,E\,dE$$

Probability per unit time of fissioning

$$P_{Fiss} = \frac{1}{2\,\pi\,\hbar}\int_0^{U_i-B_{Fiss}}\frac{\rho_{Fiss}(U_i-B_{Fiss}-E)}{\rho_i(U_i)}\,dE$$

- ρ's: nuclear level densities
- U's: excitation energies
- V_j's: possible Coulomb barrier for emitting a particle type j
- B_{Fiss}: fission barrier

- Q_j's: reaction Q for emitting a particle type j
- σ_{inv}: cross section for the inverse process
- Δ's: pairing energies

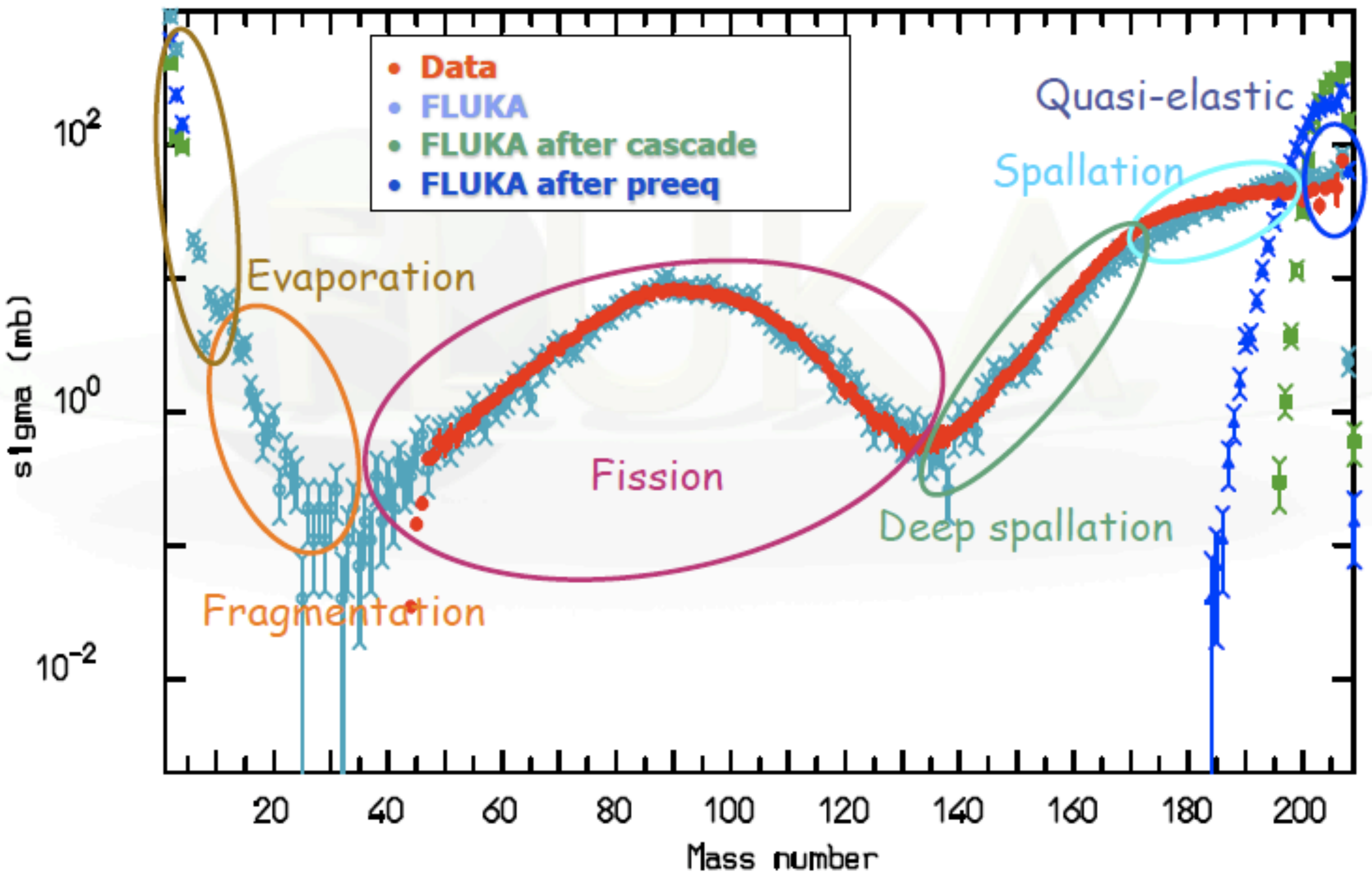
Neutron emission is strongly favoured because of the lack of any barrier
Heavy nuclei generally reach higher excitations because of more intense cascading

Equilibrium particle emission

- Evaporation: Weisskopf-Ewing approach
  - ~600 possible emitted particles/states (A<25) with an extended evaporation/fragmentation formalism
  - Full level density formula with level density parameter A,Z and excitation dependent
  - Inverse cross section with proper sub-barrier
  - Analytic solution for the emission widths (neglecting the level density dependence on U, taken into account by rejection
  - Emission energies from the width expression with no. approx.
- Fission: past, improved version of the Atchison algorithm, now
  - Γ_{fis} based of first principles, full competition with evaporation
  - Improved mass and charge widths
  - Myers and Swiatecki fission barriers, with exc. en. Dependent level density enhancement at saddle point
- Fermi Break-up for A<18 nuclei
  - ~ 50000 combinations included with up to 6 ejectiles
- γ de-excitation: statistical + rotational + tabulated levels

Example of fission/evaporation

1 A GeV ^{208}Pb + p reactions Nucl. Phys. A 686 (2001) 481-524



Heavy ion interaction models in FLUKA - 1

E > 5 GeV/n

Dual Parton Model (DPM)
DPMJET-III (original code by R.Engel, J.Ranft and S.Roesler,
FLUKA-implemenation by T.Empl *et al.*)

0.1 GeV/n < E < 5 GeV/n

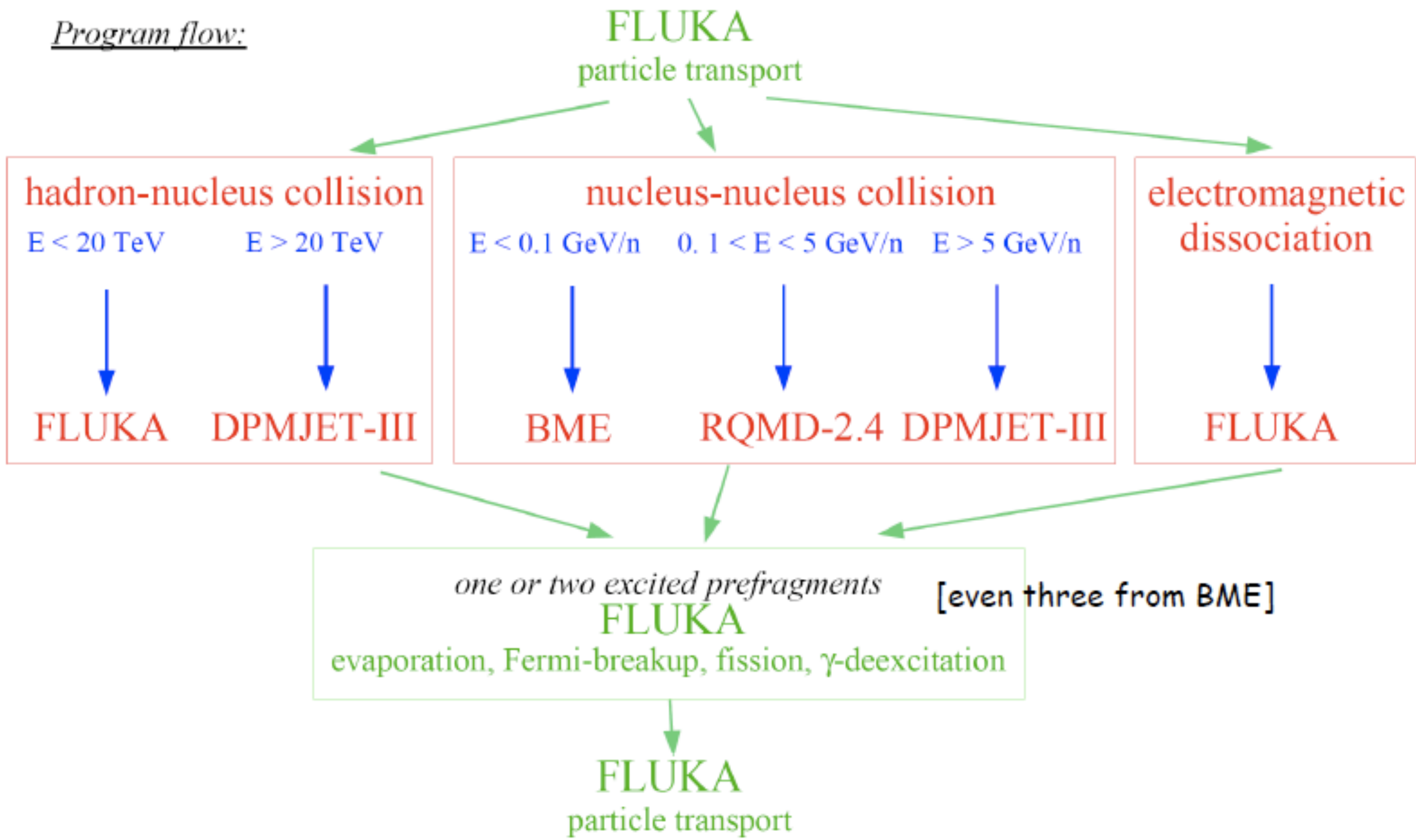
Relativistic Quantum Molecular Dynamics Model (RQMD)
RQMD-2.4 (original code by H.Sorge *et al.*,
FLUKA-implementation by A.Ferrari *et al.*)

E < 0.1 GeV/n

Boltzmann Master Equation (BME) theory
BME (original code by E.Gadioli *et al.*,
FLUKA-implementation by F.Cerutti *et al.*)

Heavy ion interaction models in FLUKA - 2

Program flow:



RQMD

E > 5 GeV/n

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E < 0.1 GeV/n

Boltzmann Master Equation (BME) theory
BME (original code by E.Gadioli et al.,
FLUKA-implementation by F.Cerutti et al.)

RQMD - *References*

interface to a suitably modified **RQMD model**

RQMD-2.4 (H. Sorge, 1998) was successfully applied

to relativistic A-A particle production over a wide energy range

[H. Sorge, Phys. Rev. **C 52**, 3291 (1995);

H. Sorge, H. Stöcker, and W. Greiner, Ann. Phys. **192**, 266 (1989)

and Nucl. Phys. **A 498**, 567c (1989)]

RQMD - *The original code*

The RQMD-2.4 code

INITIAL CONDITION two Fermi gases (projectile and target)

Fermi momentum $p_{F0} = \hbar \left(3\pi^2 \frac{A}{2V}\right)^{1/3}$ $V = (4/3)\,\pi\,\left(r_0 A^{1/3}\right)^3$ $r_0 = 1.12\,fm \Rightarrow \rho = 0.17\,\frac{nucl.}{fm^3}$

nucleon momentum $\boxed{p = p_{F0}\left(\frac{\rho(r)}{\rho_0}\right)^{\frac{1}{3}} \epsilon^{1/3}}$ $\epsilon \in [0,1]$ random

$\phi = 2\pi\epsilon$ $\cos\theta = 1 - 2\epsilon$

$$
\begin{aligned}
p_x &= p \sin\theta\cos\phi & -\left(\sum p_x\right)/A \\
p_y &= p \sin\theta\sin\phi & -\left(\sum p_y\right)/A \\
p_z &= p \cos\theta & -\left(\sum p_z\right)/A
\end{aligned}
$$

so $\sum p_x = \sum p_y = \sum p_z = 0$

FINAL STATE

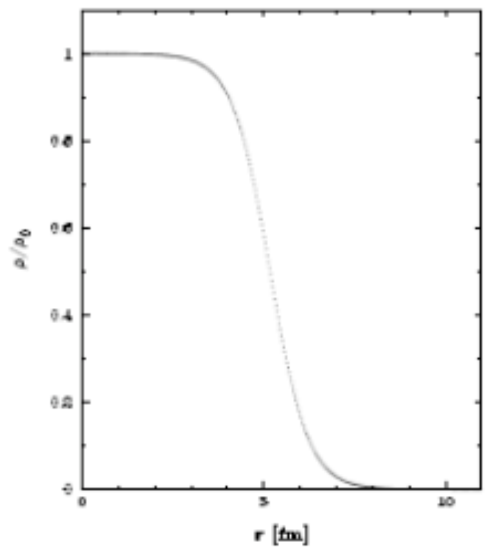
- $\left(p^0, p_x, p_y, p_z\right)$ for nucleons (and produced particles) in the LAB frame
- the spectators are marked
- no residue and fragment identification
- energy non-conservation issues, particularly when run in full QMD mode

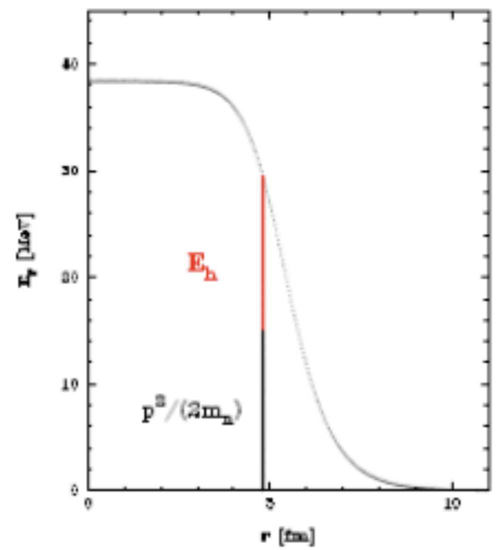
RQMD - *The interfaced code*

Implemented developments

- construct the **projectile- and target-like** nuclei by gathering *spectator* nucleons,

$$\text{assuming } E^*_{PL} = \sum_{pa.,\ P} E_h \qquad (TL)$$





$$\rho(r) \propto \left(1 + \exp\left(\frac{r-R}{a}\right)\right)^{-1}$$

$$R = 1.19\,A^{1/3} - 1.61\,A^{-1/3}\ fm \qquad a = 0.52\ fm$$

$$E_h = \frac{1}{2m_n}\left\{\left[p_{F0}\left(\rho(r)/\rho_0\right)^{1/3}\right]^2 - p^2\right\}$$

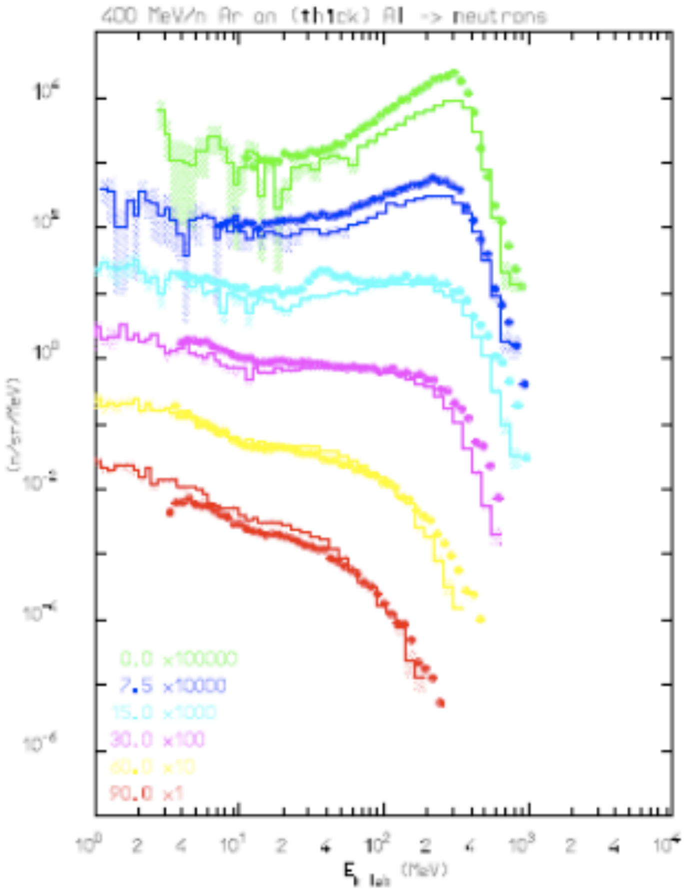
$$r, p\,(t=0)$$

- fix the remaining energy-momentum conservation issues taking into account **experimental binding energies**
- use the FLUKA evaporation/fission/fragmentation module

RQMD - *FLUKA benchmarks*

Double differential neutron yield

Ar ions

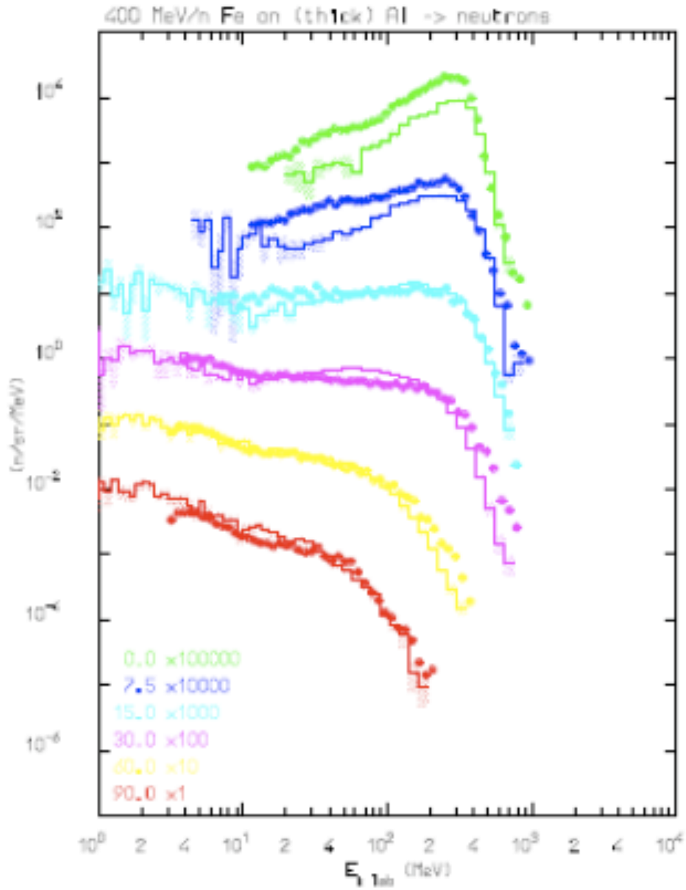


400 MeV/n

on *thick*

Al targets

Fe ions



exp. data from T. Kurosawa *et al.*, Phys. Rev. **C 62**, 044615 (2000)

BME

E > 5 GeV/n

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E < 0.1 GeV/n

Boltzmann Master Equation (BME) theory
BME (original code by E.Gadioli *et al.*,
FLUKA-implementation by F.Cerutti *et al.*)

BME - *The interfaced code*

two different reaction paths have been adopted:

1. COMPLETE FUSION

$P_{CF}=\sigma_{CF}/\sigma_R$

pre-equilibrium
according to the BME theory

2. PERIPHERAL COLLISION

$P = 1 - P_{CF}$

work in progress

three body mechanism
pickup/stripping (for asymmetric systems at low *b*)
inelastic scattering (at high *b*)

FLUKA evaporation

1. In order to get the multiplicities of the pre-equilibrium particles and their double differential spectra, the BME theory is applied to a few representative systems at different bombarding energies and the results are parameterized.

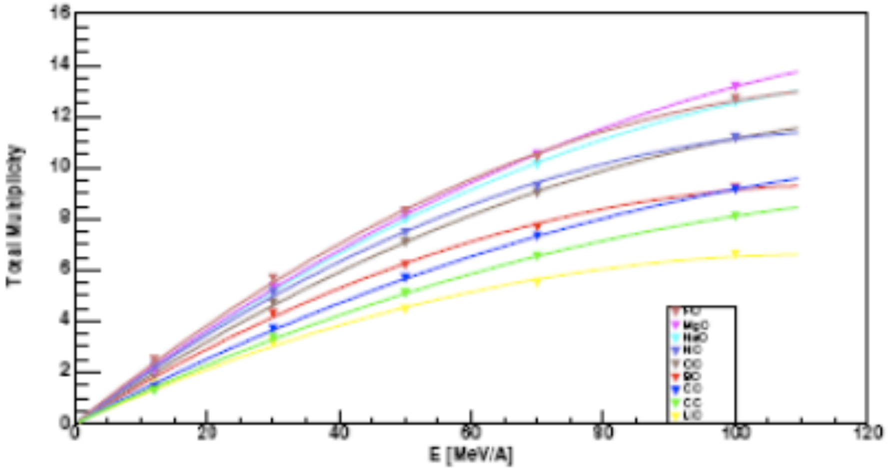
2. The complete fusion cross section decreases with increasing bombarding energy. We integrate the nuclear densities of the projectile and the target over their overlapping region, as a function of the impact parameter, and obtain a preferentially excited "middle source" and two fragments (projectile- and target-like). The kinematics is suggested by break-up studies.

BME - *The database for the pre-equilibrium emissions*

^{16}O + ^{6}Li, ^{8}Li, ^{8}B, ^{10}B, ^{12}C, ^{14}N, ^{16}O, ^{19}F, ^{20}Ne, ^{24}Mg, ^{27}Al, ^{56}Fe, ^{197}Au

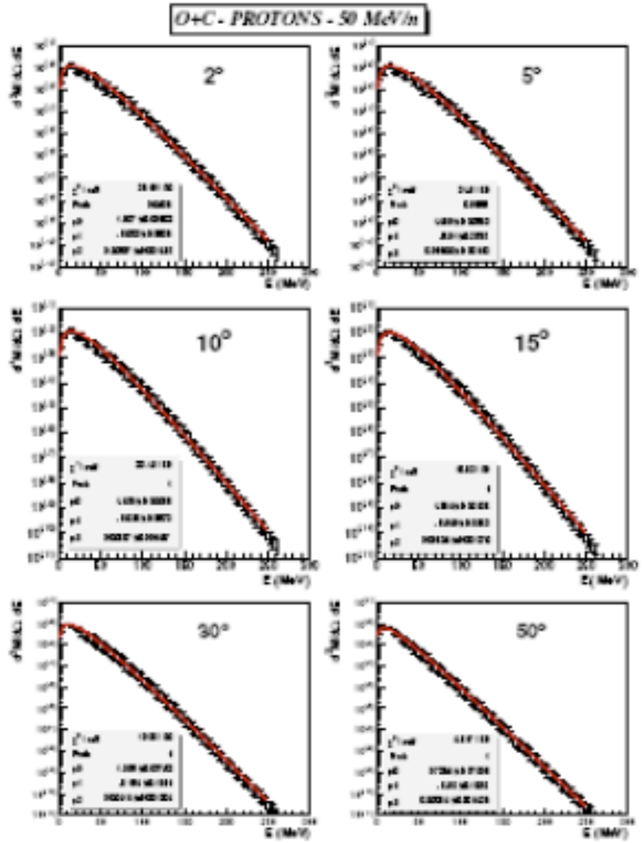
^{12}C + ^{8}Li, ^{8}B, ^{12}C, ^{27}Al, ^{40}Ca

@ 12, 30, 50, 70, 100 MeV/n



total multiplicity

$$M = P_1 E_{nucl} - P_2 E_{nucl}^2$$



energy spectra

$$d^2M/(dEd\Omega) = E^{P_0(\theta)} \exp(-P_1(\theta) - P_2(\theta)E)$$

BME - *Theoretical framework*

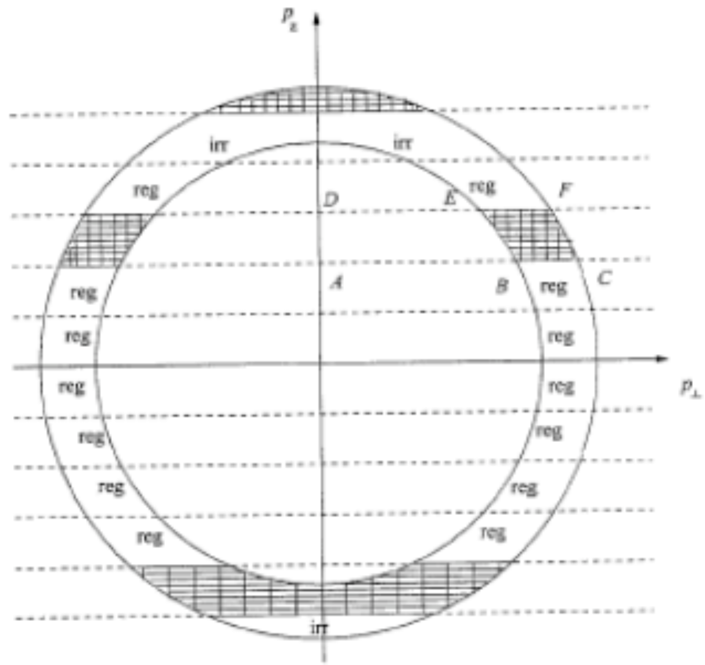
Calculation of preequilibrium for the composite nucleus

proton and neutron momentum spaces divided into bins

$$\left\{(p_x, p_y, p_z) : p_z \in [p_{zi}, p_{zi} + \Delta p_z),\ \varepsilon = (2m)^{-1}\left(p_x^2 + p_y^2 + p_z^2\right) \in [\varepsilon_i, \varepsilon_i + \Delta\varepsilon)\right\}$$

(**Z** is the beam direction)

of volume $2\pi m\,\Delta\varepsilon\,\Delta p_z$



The BME system

$$N_i = n_i \, g_i$$

- N_i: nucleon number
- n_i: occupation probability
- g_i: number of states in bin i

$$\begin{aligned}
\frac{d(n_i^\pi g_i^\pi)}{dt} = & \sum_{jlm} [\omega_{lm\to ij}^{\pi\pi} \, g_l^\pi \, n_l^\pi \, g_m^\pi \, n_m^\pi \, (1-n_i^\pi)(1-n_j^\pi) \\
& - \omega_{ij\to lm}^{\pi\pi} \, g_i^\pi \, n_i^\pi \, g_j^\pi \, n_j^\pi \, (1-n_l^\pi)(1-n_m^\pi)] \\
& + \sum_{jlm} [\omega_{lm\to ij}^{\pi\nu} \, g_l^\pi \, n_l^\pi \, g_m^\nu \, n_m^\nu \, (1-n_i^\pi)(1-n_j^\nu) \\
& - \omega_{ij\to lm}^{\pi\nu} \, g_i^\pi \, n_i^\pi \, g_j^\nu \, n_j^\nu \, (1-n_l^\pi)(1-n_m^\nu)] \\
& - n_i^\pi g_i^\pi \omega_{i\to i'}^\pi \, g_{i'}^\pi \, \delta(\varepsilon_i^\pi - \varepsilon_{i'}^\pi - \varepsilon_F^\pi - B^\pi) - \frac{dD_i^\pi}{dt}
\end{aligned}$$

BME - *Theoretical framework*

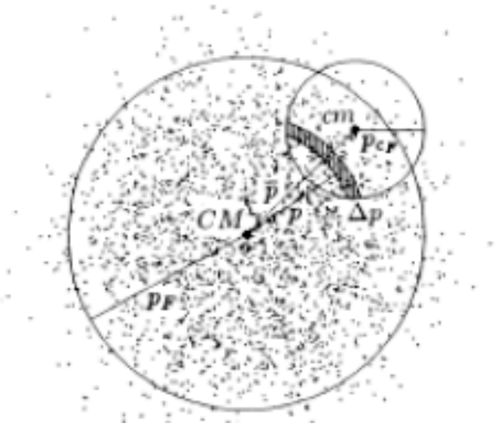
Multiplicity spectra

of emitted nucleons
$$\frac{d^2M(\varepsilon',\theta)}{d\varepsilon'\,d\Omega} = \frac{1}{2\pi\sin\theta}\int_0^{t_{eq}} n(\varepsilon,\theta,t)\,\frac{\sigma_{inv}\,V}{V}\,\rho(\varepsilon',\theta)\,dt$$

of a cluster c
$$\frac{d^2M_c\,(E_c',\theta_c)}{dE_c'\,d\Omega} = \frac{R_c}{2\pi\sin\theta}\int_0^{t_{eq}} N_c\,(E_c,\theta_c,t)\,\frac{\sigma_{inv,c}\,V_c}{V}\,\rho_c\,(E_c',\theta_c)\;dt$$

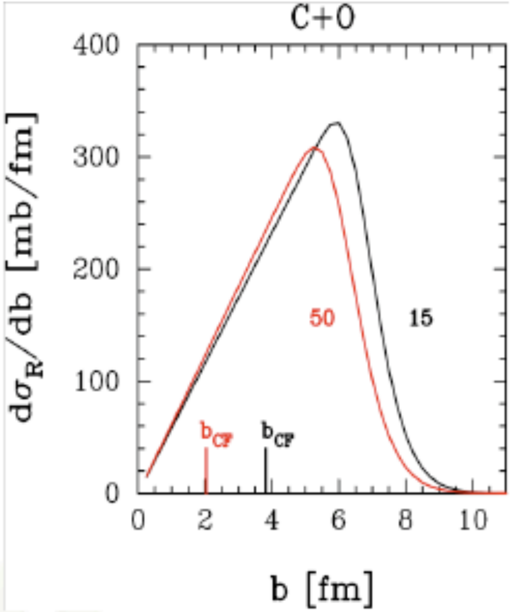
$$N_c\,(E_c\,,\theta_c\,,t) = \prod_i\,(n_i^{\pi}(\varepsilon,\theta,t))^{P_i(E_c\,,\theta_c)Z_c}\cdot\prod_i\,(n_i^{\nu}(\varepsilon,\theta,t))^{P_i(E_c\,,\theta_c)N_c}$$

joint probability



BME - *Peripheral collisions*

i. selection of the *impact parameter b*



ii. kinematics determination

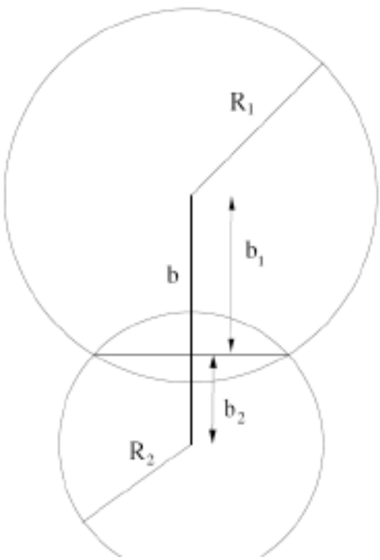
θ_{PL}, θ_{TL} chosen according to $[d\sigma/d\Omega]_{cm} \sim \exp(-k\theta_{cm})$
θ_{MS} momentum conservation
p_{PL}, p_{TL} chosen according to a given energy loss distribution
p_{MS} momentum conservation
ϕ_{PL} free
ϕ_{TL}, ϕ_{MS} same reaction plane

work in progress

PL

MS

TL



iii. excitation energy sharing

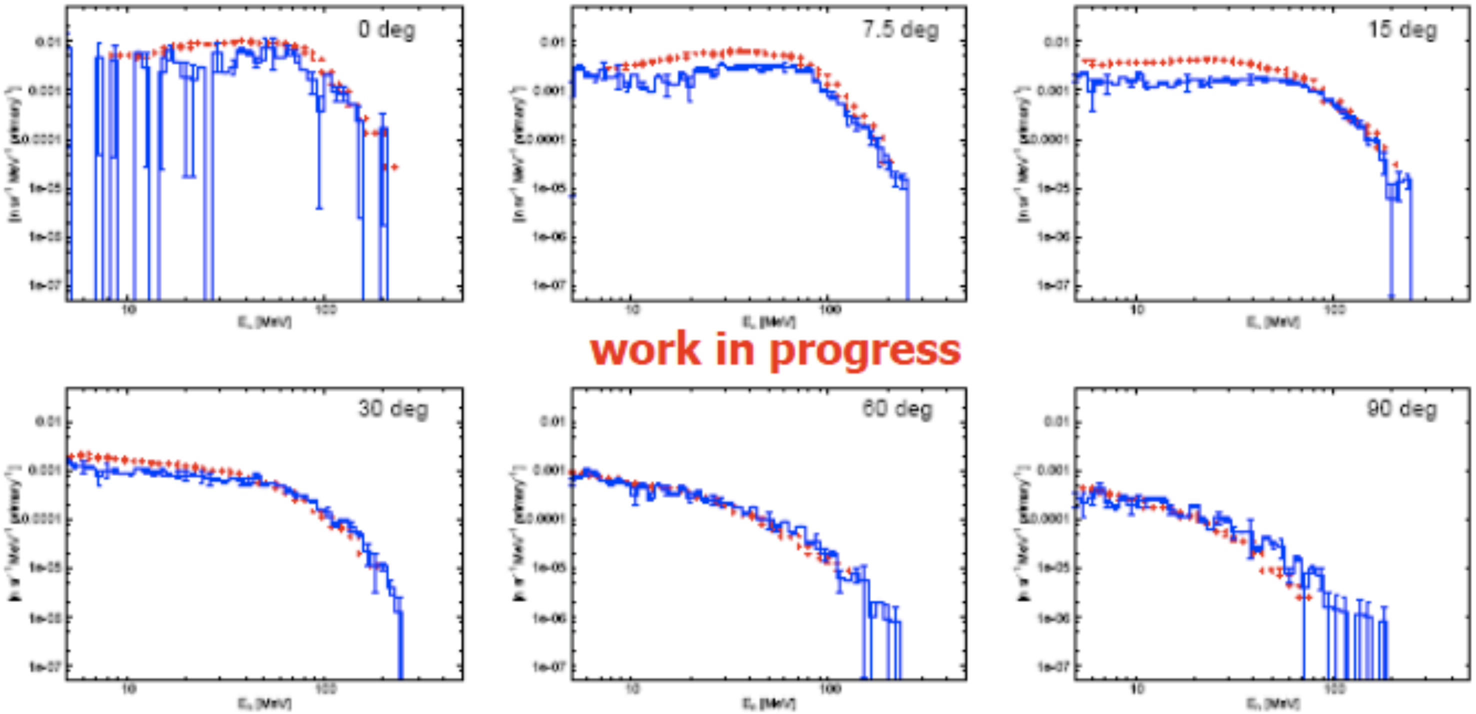
$$E^*_{MS} = (A_{MS}/A_{tot})E^*_{tot} \sum_{n=0}^{k} (1 - A_{MS}/A_{tot})^n$$

$$E^*_{PL} = f(A_{PL}, A_{TL})\,(E^*_{tot} - E^*_{MS})$$

$$E^*_{TL} = (E^*_{tot} - E^*_{MS} - E^*_{PL})$$

Double differential neutron yields from thick targets

exp. data from T. Kurosawa, N. Nakao, T. Nakamura *et al.*, Nucl. Sci. Eng. **132**, 30-57 (1999)



100 MeV/n ^{12}C ions on C target

Material sources:

- "Advanced dosimetric concepts for radiation therapy"
  Dr K Parodi, Heidelberg, Germany

- FLUKA Course Material (www.fluka.org)