Heavy ions

23rd FLUKA Beginner's Course
Lanzhou University
Lanzhou, China

June 2–7, 2024

Introduction-1

- Heavy Ions in FLUKA are all nuclei, from deuterons up
- They can be primary particles, for instance in hadron therapy or cosmic showers
- They can be secondary particles, generated in interactions through Coalescence / Evaporation /Break Up/ Radioactivity[1] etc.

To remember

Heavy Ion transport/interactions may be needed even if they are NOT the source.

Warning

Heavy Ion transport/interactions are NOT switched on by default (with exceptions, as always)

[1]yes: the (α,n) σ on some light elements exhibits resonances and is not negligible even at few MeV

ION CODES

Fluka does NOT pre-define all possible ions. Only a few ones, from now on called *light ions* are:

Ion symbol	Fluka name	Fluka particle index
^{2}H	DEUTERON	-3
^{3}H	TRITON	-4
^{3}He	3-HELIUM	-5
^{4}He	4-HELIUM	-6
All others	HEAVYION	-2

Note the negative numbering

What happens to ions?

Well, depends on the option you choose:

1. Nothing: they are stopped at the point where they are generated, their energy is deposited there
2. Approximate transport : trasported in the geometry, energy loss and multiple scattering according to what described in the *Ionization and transport* lecture. No nuclear interactions
3. Full transport : trasported in the geometry, energy loss and multiple scattering, plus nuclear interactions.

To enable transport and interactions of ions, use the IONTRANS card, i.e:

IONTRANS -2 : Full transport of all

WHAT(1) ≥ 1 : no transport of any ion
= 0 : ignored
= -1 : approximate transport (without interactions) of all light and heavy ions
= -2 : full transport and interactions of all light and heavy ions
≥ -6 and ≤ -3 : full transport of light ions with FLUKA id $\geq$ WHAT(1) and transport without interactions of all others

example :
IONTRANS -4 :
Only deuterons and tritons will interact
Default: +1 : no ion transport, unless a ion beam is requested by the BEAM card

BEAM

To request a beam of ions: the BEAM card:

BEAM -0.4 0.0 0.0 0.0 0.0 0.0 **HEAVYION**

WHAT(1) $\geq$ 0.0 : average beam momentum **per nuclear mass unit nucleon** (GeV/c/nmu)
WHAT(1) $\leq$ 0.0 : average beam kinetic energy **per nuclear mass unit nucleon** (GeV/nmu)

however:

BEAM -0.4 0.0 0.0 0.0 0.0 0.0 **4-HELIUM**

WHAT(1) $\geq$ 0.0 : average beam momentum **per nucleus** (GeV/c)
WHAT(1) $\leq$ 0.0 : average beam kinetic energy **per nucleus** (GeV)

All other WHAT's as for standard BEAM

Remember

Generic HeavyIon energy (or momentum) per nucleon
Specific predefined Light ion energy (or momentum) per nucleus

Which Ion?
HI-PROPE

For a HEAVYION beam, one has to define which ion:

HI-PROPE Z A Isomer

WHAT(1) $>$ 0.0 : Atomic number Z of the heavy ion Default: 6.0
WHAT(2) $>$ 0.0 : Mass number A of the heavy ion Default: 12.0
WHAT(3) $>$ 0 : isomeric state of the heavy ion
= 0 : heavy ion on the ground state (default)

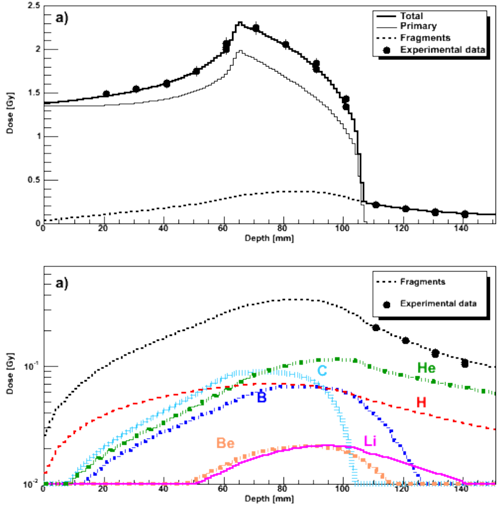
Example

to define an Oxygen beam , 400 MeV kinetic per mass unit (6.4 GeV total)

```
BEAM       -0.4   0.0   0.0   0.0   0.0   0.0   HEAVYION
HI-PROPE    8.0  16.0   0.0
```

If no HI-PROPE card is given: ^{12}C is the default

- In hadron – nucleus interactions, evaporation reaction products and residuals come mostly from the TARGET nucleus
- In nucleus-nucleus interactions, reaction products and residuals come from both TARGET and PROJECTILE nuclei.
- Indeed, except for complete fusion, one often refers to “projectile-like” and “target-like” fragments
- $\rightarrow$ projectile-like fragments travel with $\approx$ the projectile speed, thus they can be energetic, and travel longer /shorter than the average projectile range (range $\propto A/Z^2$ at given β)

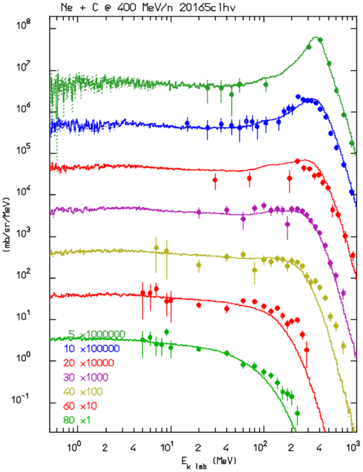


^{12}C spread-over Bragg peak in water. ^{12}C energies roughly between 170 and 230 MeV/nucleon.
Top: total dose, calculated and experimental. Note the tail due to projectile fragments
Bottom: Contributions from the various fragments.

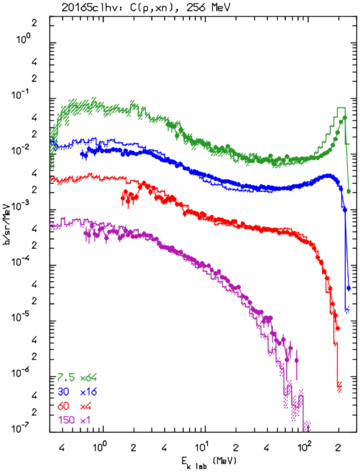
Dose to healthy tissue

A good simulation of fragments from ion nuclear interactions is extremely important in hadrontherapy

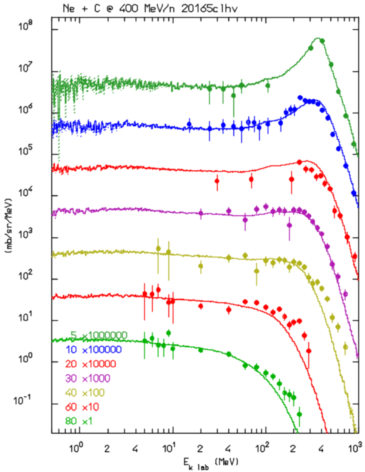
Interactions
Introduction-III



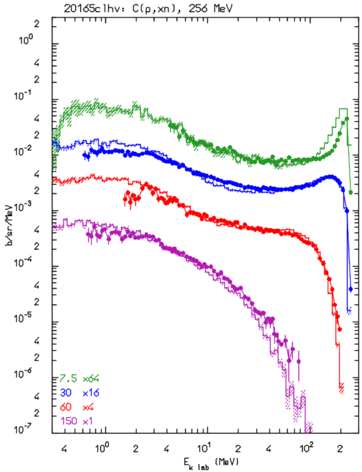
Left : Ne+C at 400 MeV/A
Right: p+C at 256 MeV
neutron energy spectra at different angles



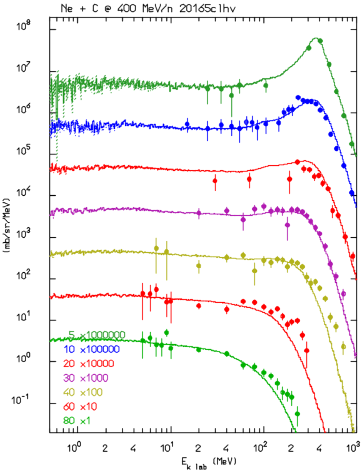
Note the high energy (>E/A) tails with ion projectiles



Left : Ne+C at 400 MeV/A
Right: p+C at 256 MeV
neutron energy spectra at different angles



Note the harder spectrum. In A-A, even evaporation products can be fast



Left : Ne+C at 400 MeV/A
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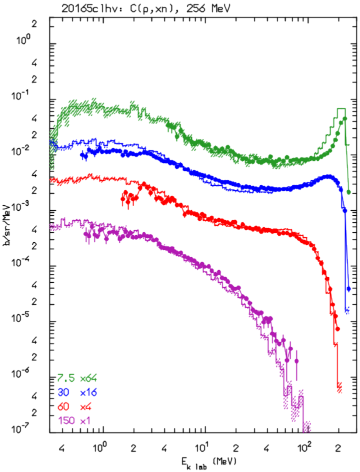
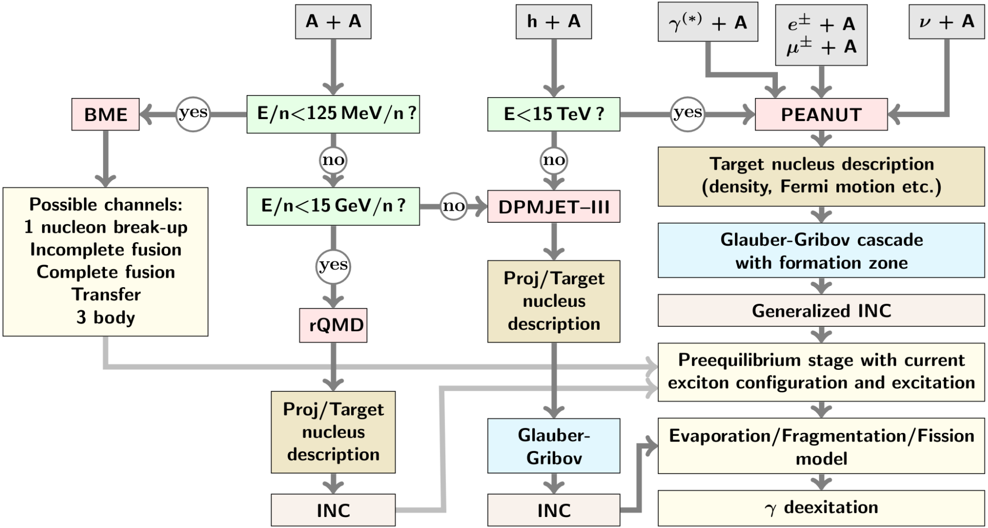


Heavy Ion interactions in FLUKA



Heavy Ion interactions in FLUKA

Interfaces to different generators depending on ion energy:

E > 12.5 GeV/n	Dual Parton Model (DPM) **DPMJET-III Version 3.19** A.Fedynitch and R. Engel, CERN Proceedings 01/2015, 291 (2015)), S.Roesler et al., Proc. MC2000, 1033 (2001), FLUKA implementation in V.Andersen et al., Advances in space research 34, 1302 (2004)
0.125 GeV/n < E < 15 GeV/n	Relativistic Quantum Molecular Dynamics Model (RQMD) **RQMD-2.4** (H.Sorge et al., Nucl. Phys. A498,567 (1989) ,Fluka implementation in V.Andersen et al., Advances in space research 34, 1302 (2004)
E < 0.125 GeV/n	Boltzmann Master Equation (BME) theory **BME** (E.Gadioli et al., Nucl. Phys. A643, 15 (1998) , Fluka implementation in F.Cerutti et al.,Proc. 11th International Conference on Nuclear Reaction Mechanisms (2006)
All Energies	Electro-Magnetic dissociation **EMD**, native FLUKA

Fragments from all generators are treated by the PEANUT deexcitation models

Not all interfaces are enabled by default (see later)

BME (E< 125 MeV/A)

The original BME code describes the evolution of a Compound Nucleus, formed by complete fusion of projectile and target, with a sophisticated pre-equilibrium model. Its implementation in FLUKA includes

- Multiplicities of the pre-equilibrium particles and their double differential spectra, parametrized from results of the BME theory. Valid for complete fusion and low-mass projectiles.
- FLUKA native preequilibrium for complete fusion systems not covered by the above parametrization
- Reaction processes different from complete fusion (see next slide)
- FLUKA native preequilibrium + evapoation etc for all fragments from the above processes

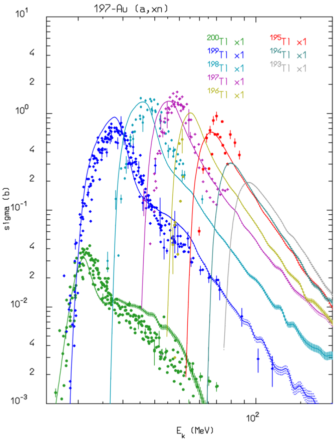
FLUKA BME processes

Higher impact parameter

- **Complete Fusion:** projectile and target nuclei interact and merge in a composite nucleus
- **Transfer:** pickup reaction where the smaller nucleus is fully overlapped by the density distribution of the bigger one and collects some of the partner nucleons
- **3body :** projectile and target nuclei interact with partial overlap of the density distributions, a hot region is produced (middle source X) and 3 outgoing fragments result
- **Incomplete FUSion:** as 3 body, with the middle source absorbed by one nucleus, resulting in two fragments
- **"Inelastic" collisions:** either the projectile or the target loses a single nucleon, possibly absorbed by the partner nucleus

Lines: FLUKA , dots:experimental data

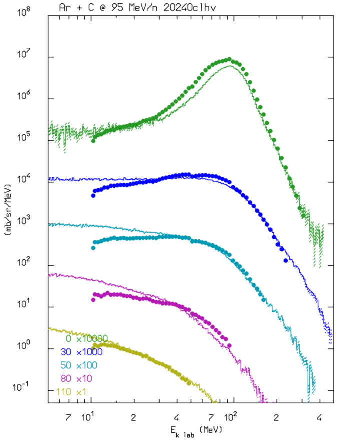
Data: EXFOR (https://www-nds.iaea.org/exfor)



Left: Production of different isotopes as a function of the projectile energy, for α particles incident on ^{197}Au

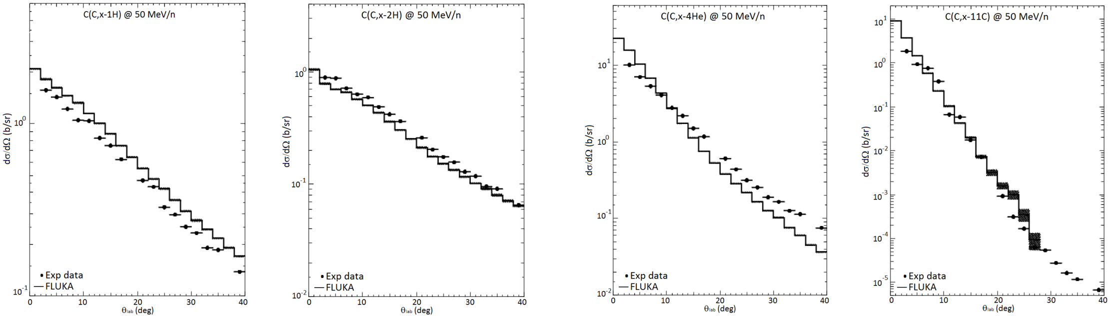
Right: Neutron spectra at different angles from Argon reations on Carbon at 95 MeV/n

Data: Sato et al., PRC 64, 034607



BME Benchmarks -II

Single differential fragment spectra from C+C at 50 MeV/n



Production of protons, deuterons, α, ^{11}C as a function of emission angle.
Experimental data (dots) from Divay et al (2017) Phys Rev C 95 044602.

BME Input

- BME is included in the standard FLUKA library and executable.
- It is called automatically if full ion transport is enabled.
- If the higher energy generators are linked (see later), FLUKA makes a smooth transition from BME to RQMD in between 100 and 150 MeV/c
- Advanced: the transition energy and the transition zone can be changed with the card PHYSICS. See manual.

Deuterons

BME cannot handle interactions of deuterons.
Thus, you need a new option: IONSPLIT

IONSPLIT

PHYSICS y/n Emin Emax Amin Amax flag **IONSPLIT**

With this option, ions having

- Energy between Emin and Emax (GeV/n)
- Mass number between Amin and Amax (included)

can be splitted into A nucleons, with a recipy according to WHAT(6).

Since the existence of heavy ion generators in FLUKA, IONSPLIT is useful and necessary only for deuterons:

Split deuterons

PHYSICS 1.0 0.005 0.15 2.0 2.0 2.0 **IONSPLIT**

Otherwise

If no IONSPLIT, deuterons below 125 MeV/n will not interact they will lose energy by ionization and eventually range out.

RQMD
0.125 GeV $<$ E/n $<$ 12.5 GeV

RQMD: a relativistic Quantum Molecular Dynamics (QMD) model, adapted to FLUKA: RQMD-2.4

- H. Sorge, Phys. Rev. C 52, 3291 (1995);
- H. Sorge, H. Stöcker, and W. Greiner, Ann. Phys. 192, 266 (1989), Nucl. Phys. A 498, 567c (1989)

QMD: Follows the Time evolution of the combined A+A system performing n-n interactions considering mean field effects and short range interactions Re-calculation of the nuclear potentials from sum of two-body fields

- fields due to the nucleons of the same nuclei
- fields due to the nucleons of the other particle

In FLUKA used in its faster cascade-like version

- Identification of residual fragments and their excitation was not provided by the original RQMD: added in the FLUKA implementation.
- Fragment de-excitation (pre-equilibrium (since fluka2020) , evaporation, fission, Fermi break-up, γ de-excitation) is performed in PEANUT
- Correct energy/momentum conservation:
  - Nuclear final state reworked out of the information on spectators
  - Excitation energy and exciton number deduced from the holes left
  - Use of experimental binding energies

V.Andersen et al., Advances in space research 34, 1302 (2004)

RQMD and DPMJET are external packages

They are distributed with FLUKA, but

- They are contained in libraries separated from the standard libflukahp.a
- They are NOT included in the standard flukahp executable and in executables built using the $FLUPRO/lfluka script

You need to do something:

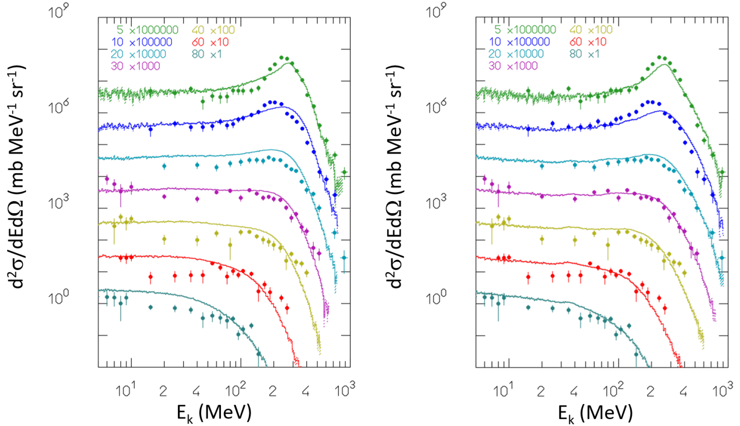
The **$FLUPRO/flutil/ldpmqmd** script produces a FLUKA executable that contains RQMD and DPMJET

The standard name of this executable is flukadpm3

Name can be changed: $FLUPRO/flutil/ldpmqmd -o myflukaexe

The same script can be used through FLAIR, in the Compile page

RQMD
Benchmarks



290 MeV/n C ions on C Neutron Energy spectra at 6 lab angles:

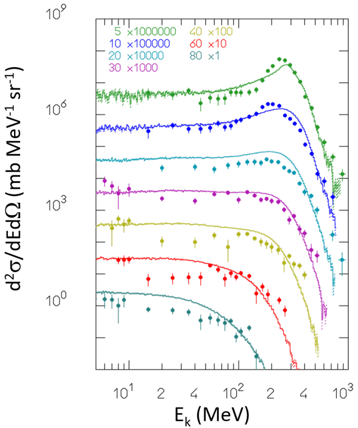
- 5° (green)
- 10° (blue)
- 20° (cyan)
- 30° (purple)
- 40° (gold)
- 60° (red)
- 80° (dark green).

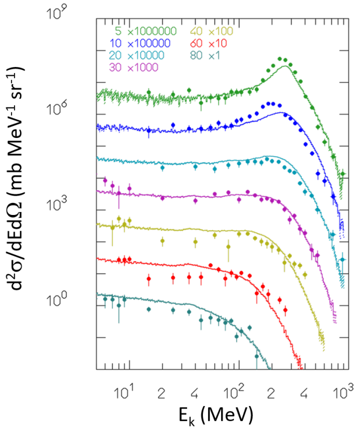
each scaled by a factor 10.

Right: with PEANUT pre-eq after RQMD. Left: without pre-eq.

Symbols: data (Iwata et al, PRC64, 10 (2001), revised in Satoh et al, NIMA583, 507 (2007))

RQMD
Benchmarks





290 MeV/n C ions on C Neutron Energy spectra at 6 lab angles:

- 5° (green)
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- 30° (purple)
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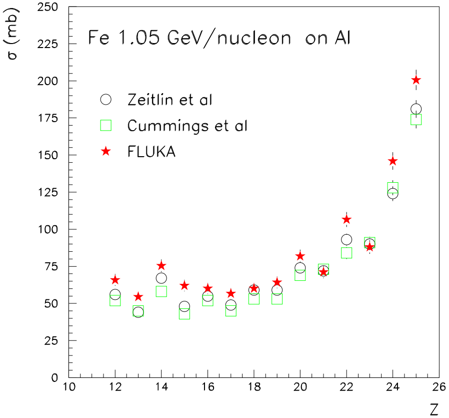
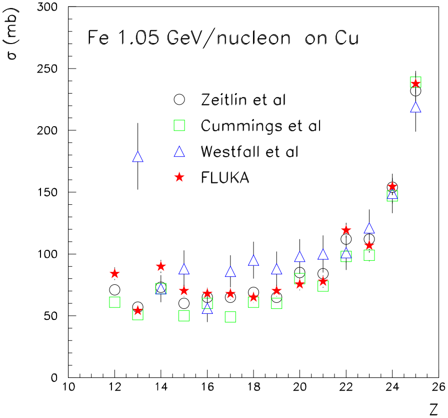
- 60° (red)
- 80° (dark green).

each scaled by a factor 10.

With pre-eq (right plot): higher yield at high energy (shielding!!) and intermediate angles, in better agreement with data

RQMD
Benchmarks -II





Fragment charge cross section for 1.05 GeV/n Fe ions on Al (left) and Cu (right).
Exp. data from PRC56, 338 (1996) , PRC42,5208 (1990) and PRC19, 1309 (1979)
Figures from Advances in space research 34, 1302 (2004)

DPMJET
E/n>12.5 GeV

DPMJET = Dual Parton Model and JETs

- A.Fedynitch and R. Engel, CERN Proceedings 01/2015, 291 (2015), S.Roesler et al., Proc. MC2000, 1033 (2001)

DPMJET - Version III.19

- hadron-nucleus collisions
- nucleus-nucleus collisions
- photon-nucleus collisions

Energy range: 5 GeV/nucleon – 10^{11} GeV/nucleon

In FLUKA:

- nucleus-nucleus collisions above 12.5 GeV/nucleon
- hadron-nucleus collisions above 15 TeV

DPMJET is an external package: remember to link it with ldpmqmd

DPMJET: (as well as the FLUKA high energy h–A generator) is based on the Dual Parton Model in connection with the Gribov-Glauber formalism.

Parton model: to analyze high-energy hadron collisions. Hadrons are considered made of "partons".

Glauber-Gribov formalism: elastic, quasi-elastic and absorption hadron-nucleus (h-A) cross sections are derived from the hadron-nucleon (h-N) cross sections. Inelastic interactions are equivalent to multiple interactions of the projectile with thetarget nucleons.

Hadron-nucleon: DPM

- Gribov's reggeon field theory for soft and perturbative interactions
- QCD improved parton model for hard interactions

Hadron-nucleon: JET

- Hadronization of the strings produced in DPM
- Performed with the PHYTIA[2] package, based on the Lund[3] model

Nuclear environment: Intranuclear cascade

- Fundamental ideas as in FLUKA, simplified implementation
- Includes the formation time concept

Excited fragments: PEANUT

- Evaporation, Break-up, γ de-excitation

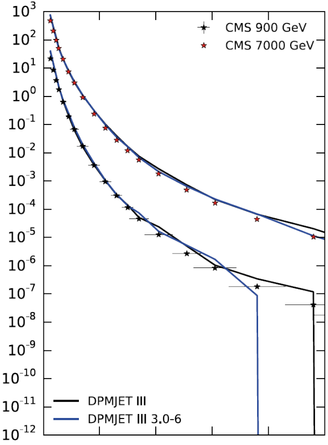
[2] T.Sjostrand et al.„ JHEP 0605:026,2006
[3] Phys. Rep. 97 (1983) 31, Nucl. Phys. B248 (1984) 469

- Internally, DPMJET uses Glauber impact parameter distributions depending on energy, project and target.
- The computations are CPU intensive for colliding systems with heavier nuclei and it would not be practical to produce the required distributions repeatedly while processing full showers in
- For FLUKA: procedure to provide pre-computed impact parameter distributions for a complete matrix of projectile-target combinations up to a mass number of A=246 over the entire available energy range[4]

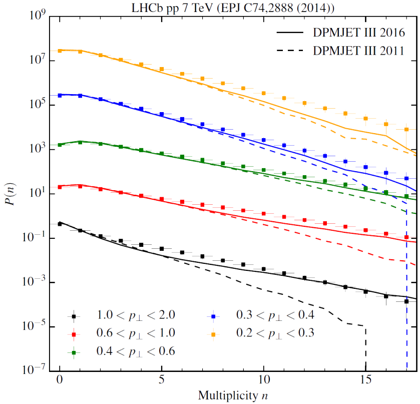
[4] Empl et. al, proc. 12th ANS RPSD topical meeting, SantaFè 2002

DPMJET Benchmarks

proton-proton at LHC



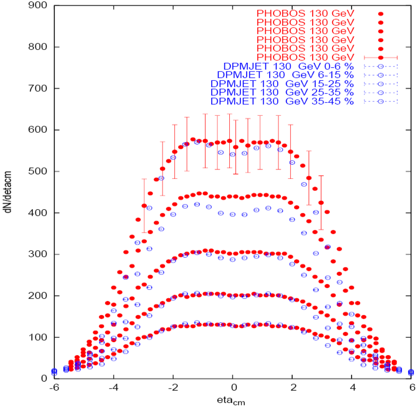
Invariant σ for charged particles production vs of transverse momentum for p-p at various energies

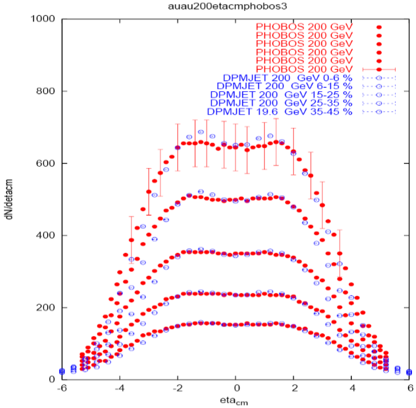


Charged particle multiplicity distribution for different p_T ranges in the forward region as measured by LHCb at $\sqrt{s}$=7 TeV

DPMJET Benchmarks

Nucleus-nucleus





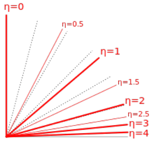
pseudorapidity: η

$\eta = -ln\left(tan\frac{\theta}{2}\right)$

where

$tan\theta = p_T/p_L$

$\eta = \frac{1}{2}ln\left(\frac{p+p_{||}}{p-p_{||}}\right)$



Wikipedia, Mets501

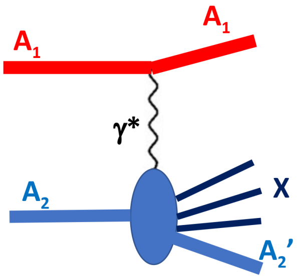
Pseudorapidity distribution of charged hadrons produced in Au-Au collisions at a c.m. energy of 130GeV/A (left) and 200GeV/A (right) for different ranges of centralities. Exp. data: PHOBOS-Collaboration. (from J. Ranft, AIP Conf. Proc. 896, 102 (2007))

Electro-Magnetic dissociation

Remember from Hadronic lecture:

- Break-up of one of the colliding nuclei in the electromagnetic field of the other nucleus
- Through the exchange of a virtual photon
- Multiplicity of emitted particles peaked at few nucleons, tails extend to many.
- Its importance grows with ion energy and ion Z

See PhysRevSTAB 17 021006 (2014)



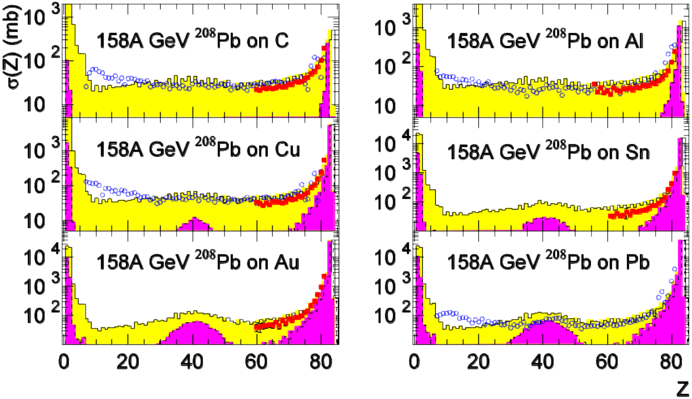
Electro-Magnetic dissociation
when and how

E-M Dissociation is in the standard library, but it is NOT active by default.
For light systems, such as Carbon on water, it is important only at ultra-relativistic energies
For heavy sytems it is already important at energies $<$ 1GeV/n
As usual, the counterindication is CPU time and initialization time
In doubt, a test run w/wo can drive the decision

To activate EM-Dissociation if needed

PHYSICS flag 0.0 0.0 0.0 0.0 **EM-DISSO**
recommended (if EMD needed): flag=2.0 (both target and projectile dissociation)

DPMJET and EMD benchmark



Fragment charge cross sections for 158GeV/n Pb ions on various targets.

FLUKA: solid histogram. Purple contribution from electromagnetic dissociation

Exp. data: NPA662, 207 (2000), NPA707, 513 (2002) (blue circles), PRC70, 014902 (2004), (red squares)

Summary

Ion interactions and transport are not on by default

IONTRANS -2 : Full transport of all

To request a beam of ions: the BEAM card:

```
BEAM      -E/n  0.0  0.0  0.0  0.0  0.0  HEAVYION
HI-PROPE   Z   A   Isomer
```

BME does not perform deuteron interactions

To approximate them:

```
PHYSICS  1.0  0.005  0.15  2.0  2.0  2.0  IONSPLIT
```

To activate EM-Dissociation if needed

```
PHYSICS  2.0  0.0  0.0  0.0  0.0       EM-DISSO
```

Summary -II

RQMD, DPMJET

For ion energy >125 MeV/n, external generators are needed: Use the $FLUPRO/flutil/ldpmqmd script to build the fluka executable

Fragments from all three ion interaction models are handled by PEANUT. If residual nuclei are of interest (and not only) , do not forget to switch on the precise PEANUT low energy processes:

PEANUT setup

```
PHYSICS    1.0   0.0   0.0   0.0   0.0   0.0   COALESCE
PHYSICS    3.0   0.0   0.0   0.0   0.0   0.0   EVAPORAT
```

Note: FLUKA perform consistency checks when it reads the input file: For instance, it stops if RQMD/DPMJET are not included in an high energy problem where full IONTRANS is on. A message is written at the end of .out and .err files