MCNPX Models and Applications
Hadronic Shower Simulation Workshop

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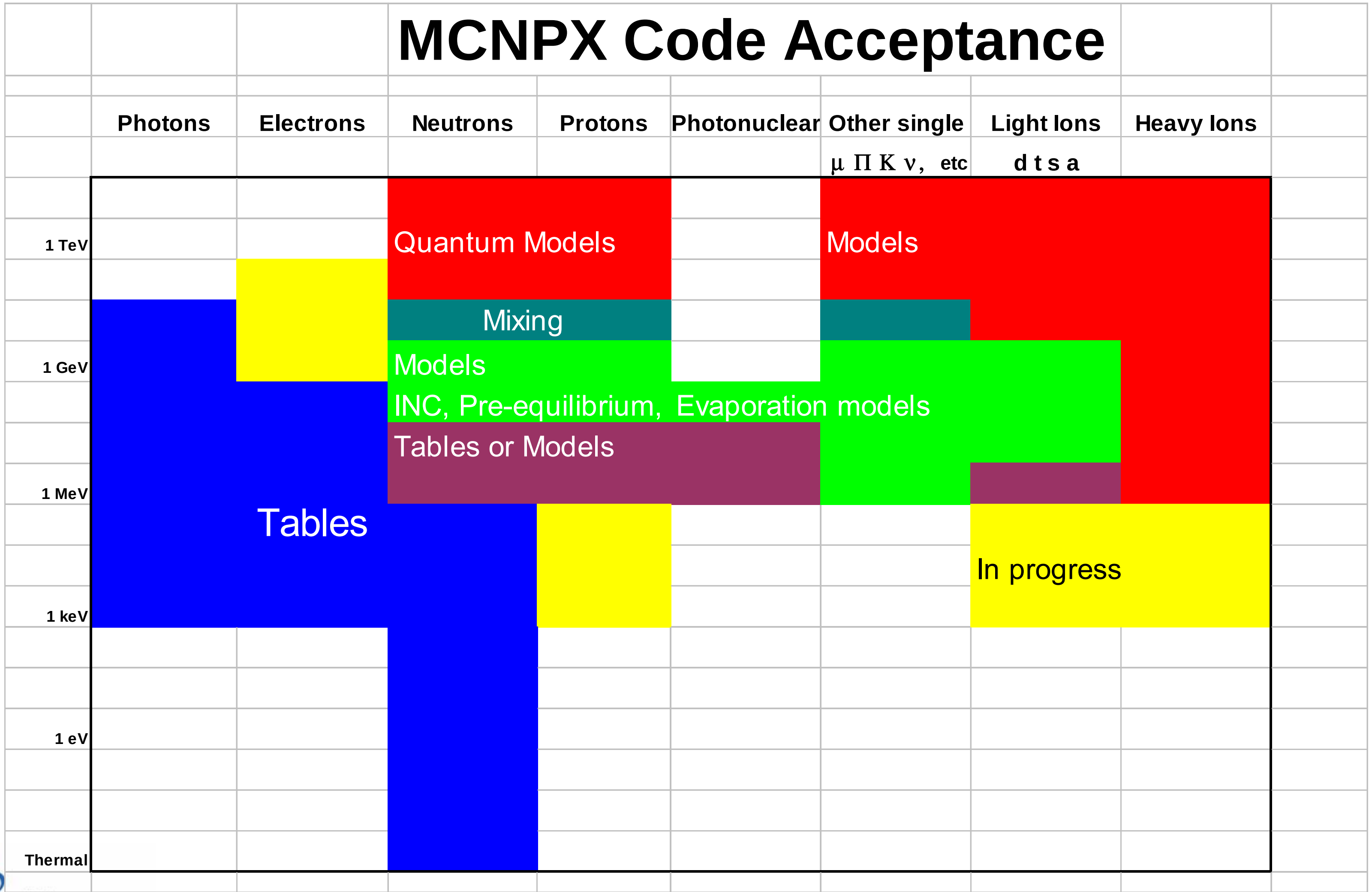
Where MCNPX is very strong

- Neutronics (table-based)
  - Inherent difficulty with correlations (ORNL Polimi patch – need analog processes)
  - Few exceptions hardwired in.
- Criticality
- Transmutation
  - Burnup
  - Enables delayed particle production
- Variance Reduction
  - Next-event-estimators
- Statistical Convergence Checks (Figure of Merit = $1/(T\sigma^2)$)
  - 10 separate checks (not just the standard deviation)
- Ease of Use
  - Don't have to code anything
  - All standard shapes + torus, lattices, repeated structures, basically no limit on geometry. (no formally released magnetic fields)
  - 2 Commercial GUIs
- Quality Assurance, Security, Support
- Extension outside of traditional neutronics arena
  - 30 particles, 4 light ions, all heavy ions
  - Models in addition to libraries (solves the correlation problem)

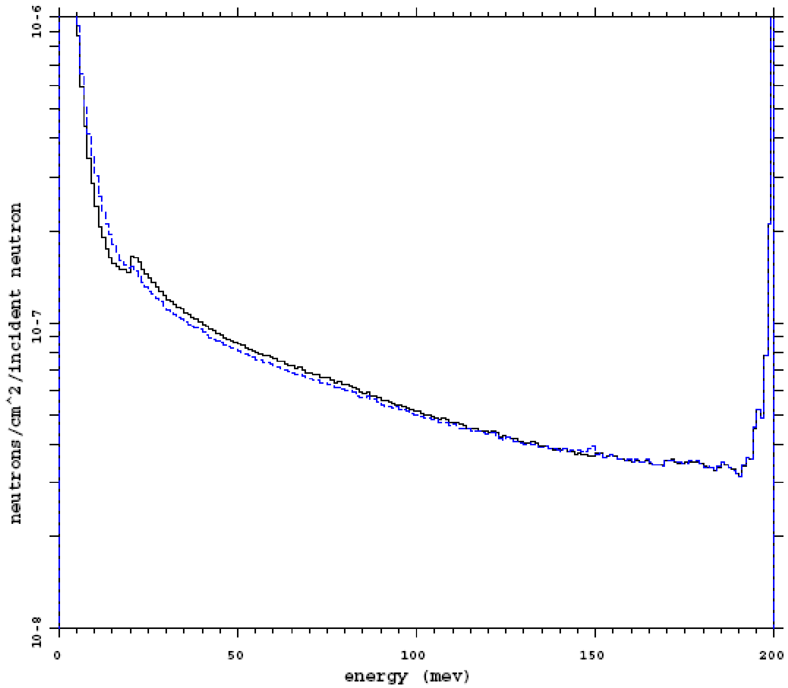
MCNPX Particle and Energy Acceptance



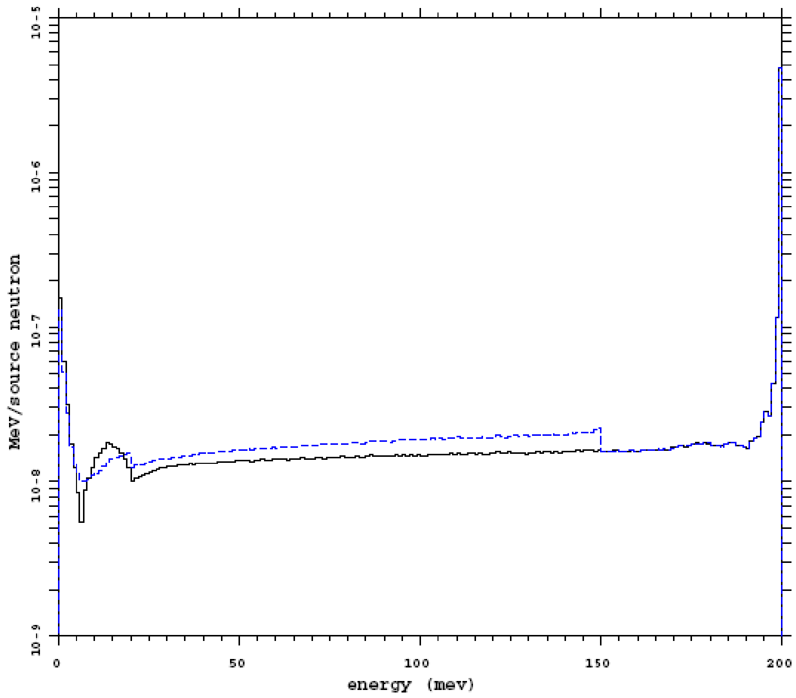
Selecting Tables or Models in MCNPX

```
mode n h p
m1      1001 1 1002 1 1003.6 1 6012 1 20040 1 nlib .24c
mx1:n   j     model   j       6000   20000
mx1:h   j     model   1001    j      j
Mx1:p   0     6012    0       j      j
```

Matching Tables and Models



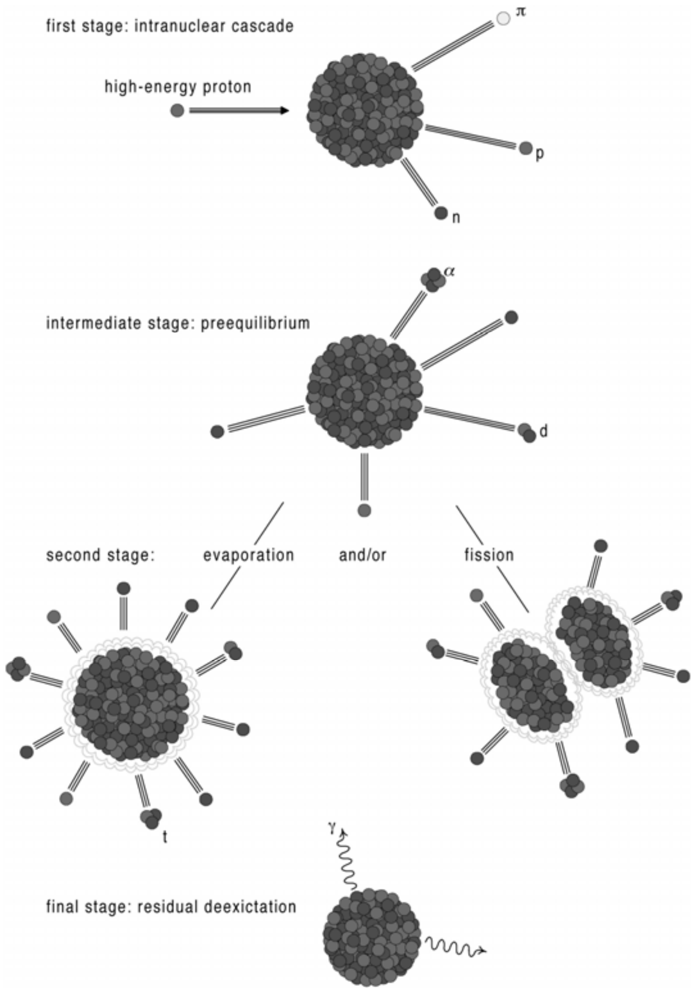
Neutrons in aluminum, flux



Neutrons in aluminum, energy deposition

Black- 20 MeV library, Blue, 150 MeV library

Model Choices in MCNPX



Model Choices in MCNPX

Physics Process	Bertini	ISABEL	CEM
Method	INC + EQ or INC + PE + EQ	INC + EQ or INC + PE + EQ	INC + PE + EQ
Intranuclear Cascade Model	Bertini INC	ISABEL INC	improved Dubna INC
Monte Carlo Technique	"spacelike"	"timelike"	"spacelike"
Nuclear Density Distribution	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r) = \alpha_i\rho(0)$; i - 1,...,3 $\alpha_1=0.9$, $\alpha_2=0.2$ $\alpha_3=0.01$	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho(r) = \alpha_i\rho(0)$; i - 1,...,16	$\rho(r)=\rho_0\{\exp[(r-c)/a]+1\}$ $c=1.07A^{1/3}$ fm a=0.545 fm $\rho_n(r)/\rho_p(r) = N/Z$ $\rho(r)=\alpha_i\rho(0)$; i=1,...,7 $\alpha_1=0.95$, $\alpha_2=0.8$ $\alpha_3=0.5$ $\alpha_4=0.2$ $\alpha_5=0.1$ $\alpha_6=0.05$ $\alpha_7=0.01$
Nucleon Potential	$V_N = T_F + B_N$	Nucleon kinetic energy (T_N) dependent potential $V_N=V_i(1-T_n/T_{max})$	$V_N = T_F + B_N$
Pion Potential	$V\pi = V_N$	$V\pi = 0$	$V\pi$ = 25 MeV
Mean Nucleon Binding Energy	B_N ~ 7 MeV	initial B_N from mass table; the same value is used throughout the calculation	B_N ~ 7 MeV
Elementary Cross Sections	standard BERTINI INC (old)	standard ISABEL (old)	new CEM97, last update March 1999

Model Choices in MCNPX

Physics Process	Bertini	ISABEL	CEM
A + A interactions	not considered	allowed	not considered
γA interactions	not considered	not considered	may be considered
Condition for passing from the INC stage	cutoff energy ~ 7 MeV	different cutoff energies for p and n, as in VEGAS code	$P = \| (W_{mod} - W_{exp}) / W_{exp} \|$ P = 0.3
Nuclear density depletion	not considered	considered	not considered
Pre-equilibrium stage	MPM (LAHET) model	MPM (LAHET) model	Improved MEM (CEM97)
Equilibrium stage	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	CEM97 model for n, p, d, t, ^{3}He ^{4}He emission (+ fission) (+γ)
Level density	3 LAHET models for a = a(Z, N, E*)	3 LAHET models for a = a(Z, N, E*)	CEM97 models for a = a(Z, N, E*)
Multifragmentation of light nuclei	Fermi breakup as in LAHET	Fermi breakup as in LAHET	Fermi breakup as in LAHET
Fission models	ORNL or RAL models	ORNL or RAL models	CEM model for σ_f, RAL fission fragmentation

New INCL model, improved H and He emission

Model Energy Limits

Variable	Bertini	Isabel	CEM
Lower energy[a]	20 - 150 MeV	20-150 MeV	~100 MeV
Upper Energy	3.5 GeV (nucleon-nucleon 2.5 GeV (pion-nucleon)	1 GeV	5GeV
Nuclei	all	all	carbon and heavier
Incident particles	p, n, pions	A<=4 and antiprotons	p, n, pions

FLUKA’89

LAQGSM

Charged Particle Transport (not electrons)

- Energy Loss
  - Bethe -Bloch
  - The ionization potentials have been enhanced to the values and interpolation procedures recommended in ICRU Report 37 (ICR84), bringing the model into closer ICRU compliance.
  - The density effect correction now uses the parameterization of Sternheimer and Peierls (STE71).
  - For high-energy protons and other light charged projectiles, the approximate SPAR model (ARM73) has been replaced with a full implementation of the maximum kinetic energy transfer.
  - For intermediate energies, the shell corrections to the stopping power have been adapted from Janni (JAN82).
    - A continuous transition in the stopping power between the ranges 1.31 MeV/AMU (Atomic Mass Unit) for the high-energy model, and 5.24 MeV/AMU (the low energy SPAR model) is achieved with a linear interpolation between the two models.
  - No very very low (less than 1 MeV for protons) model is present.
- Small angle Coulomb Scattering
  - Rossi-Greisen scattering algorithm (Rossi, B. & Griesen, K., “Cosmic-Ray Theory”, Rev. Mod Phys 13, Oct 1941 pp 262-268)
  - Overpredicts large angle, high-Z Coulomb scattering
  - MCNPX does not yet accommodate transverse displacements in charged-particle substeps

Charged Particle Transport (not electrons)

- Energy Straggling
  - At low energies and large step sizes, the Vavilov distribution approaches a Gaussian.
  - At very high energies, or small step sizes (and for electrons in almost all circumstances), the Vavilov distribution approaches a Landau distribution.
    - The module implemented in MCNPX to represent the Vavilov model does not currently account for the Gaussian and Landau limits
  - Updated logic applies the Vavilov algorithm to each substep and to each partial substep, and makes a better estimate of the continuous-slowing-down energy loss (mean energy loss) across energy-group boundaries.

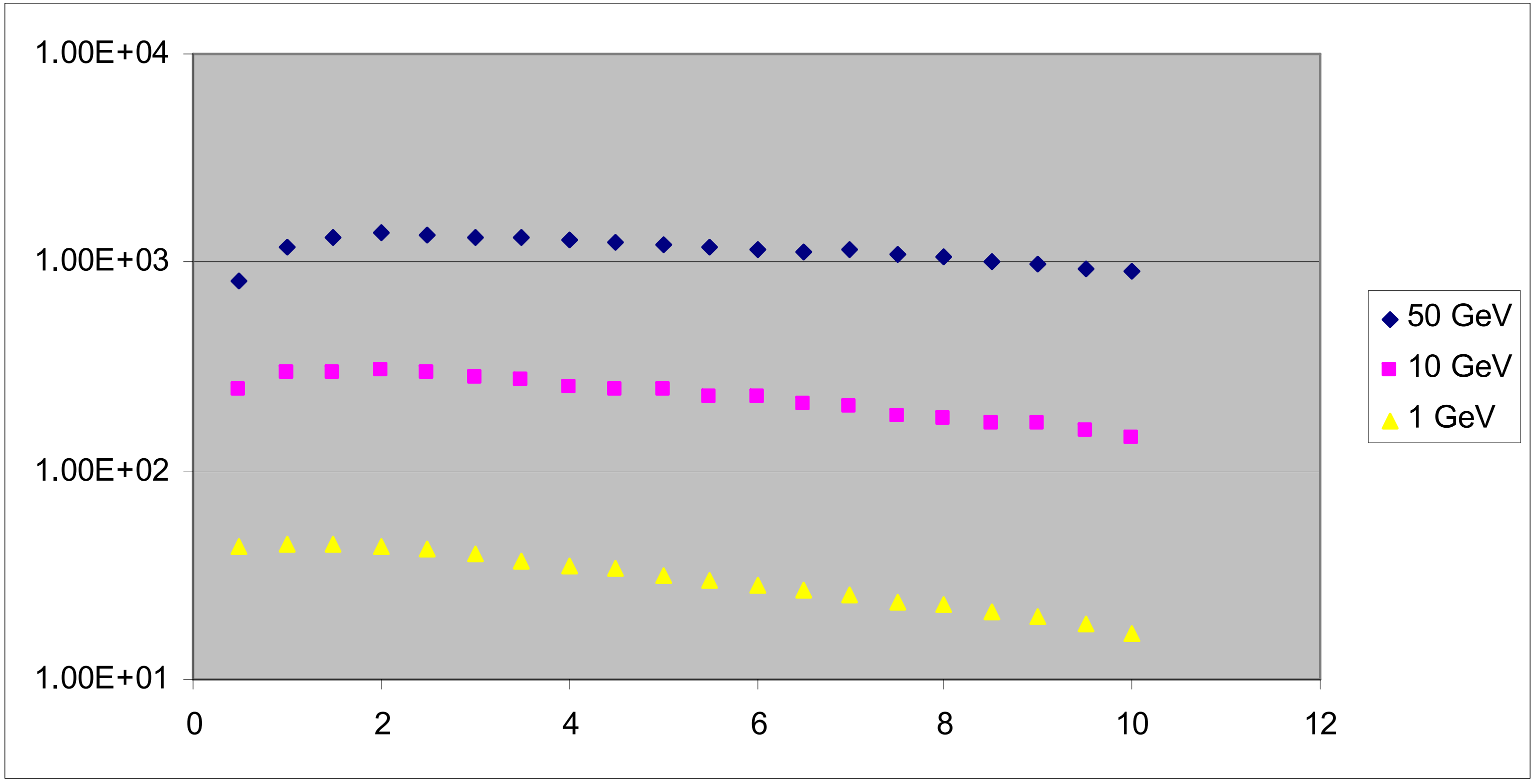
Other

- Evaporation
  - Dresner
  - ABLA (goes with INCL)
- Fission
  - Rutherford Appleton (does sub-actinide fission)
  - ORNL
  - Fission multiplicity (in tabular region)
- Light ion recoil (in tabular region)

Tallies

- F1 - Current $= W_i$
- F2 - Surface Flux $= W/(|\mu|*A)$
- F4 - Flux = $W*\lambda/V$
- F5 – Detector Fluence = $W*p(\mu)\&exp(-s)/2\pi R^2$
- F6 – Energy Deposition – $W* \lambda*\sigma_T(E)*H(E)*\rho_a/m$
  - +F6, mean to be used in model region, adds dE/dx + recoil + cufoff energies
- F7 – Fission Energy Deposition – $W*\lambda*\sigma_F(E)*Q*\rho_a/m$
- F8 – Pulse Height – W_s in bin E_d $*W/W_s$
  - Pulse height light coincidence tally

Benchmark Task 7



Input file for Task 7

```
task 7  energy dep profile in a thick target for proton beam
1 1 -19.3 -1    u=1
2 0          1    u=1
3 0         -2    lat=1 fill=1 u=2
4 0         -3    fill=2
5 0          3 -4
6 0          4

1 rcc 0 0 0  0 0 .5  1
2 rpp -2 2 -2 2 0 .5
3 rcc 0 0 0 0 0 10 2
4 so 100.0

mode n p h d t s a | / z k l + -
Imp:n 1 1 1 1 1 0
phys:n 1000.0
phys:p 1000.0 j j 5
phys:h 1000.0
lca 8j 1
sdef x=0 y=0 z=-10 vec 0 0 1 dir 1 par=h erg=1000.
m1 74180 .12 74182 26.3 74183 14.28 74184 30.7 74186 28.6
+f6      (1<3[0 0 0]<4) (1<3[0 0 1]<4) (1<3[0 0 2]<4) (1<3[0 0 3]<4)
         (1<3[0 0 4]<4) (1<3[0 0 5]<4) (1<3[0 0 6]<4) (1<3[0 0 7]<4)
         (1<3[0 0 8]<4) (1<3[0 0 9]<4) (1<3[0 0 10]<4) (1<3[0 0 11]<4)
         (1<3[0 0 12]<4) (1<3[0 0 13]<4) (1<3[0 0 14]<4) (1<3[0 0 15]<4)
         (1<3[0 0 16]<4) (1<3[0 0 17]<4) (1<3[0 0 18]<4) (1<3[0 0 19]<4) T
```

MCNPX Applications

- Medical
  - Design of proton therapy facilities
  - Heavy ions
- Space
  - Space power reactors
  - Cosmic ray shielding
  - Comic ray backgrounds, SEE
  - Cosmochemistry
- Threat Reduction
  - Active Interrogation
  - Detector design and performance, espec. neutrons
  - Signal backgrounds
  - Nonproliferation
  - Wide variety of applications

MCNPX Applications

- Reactors
  - Materials damage
  - Criticality and burnup
  - ASCI, GNEP
- Intermediate Energy Accelerators
  - APT, SNS